Abstract book

Contents

Oral

AMO

When: 2026-06-26, 11:40 - 12:05, Where: Heinz-Otto Kreis

O1 - Attohallen - A High-Resolution Attosecond Facility for XUV Spectroscopy

AMO

Raimund Feifel[1]
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Abstract text: Attohallen, a new attosecond science facility at the University of Gothenburg, combines high temporal and high spectral resolution for ultrafast photoionization studies. The facility is based on a CEP-stabilized OPCPA-HE laser system delivering sub-10 fs pulses with pulse energies up to 50 mJ at 100 Hz repetition rate, enabling the generation of extreme-ultraviolet (XUV) radiation in rare gases via loose-focusing high-order harmonic generation. The setup incorporates a Mach–Zehnder-type interferometer for attosecond pump–probe experiments together with a 5.6 m magnetic bottle electron time-of-flight spectrometer providing exceptionally high spectral resolving power.

To demonstrate the capabilities of the facility, I will present measurements of spin–orbit-resolved Wigner electron emission time delays in rare-gas atoms using the RABBIT (reconstruction of attosecond beating by interference of two-photon transitions) technique. While previous studies have reported spin–orbit resolved delays in Kr and Xe, analogous measurements in Ar have remained experimentally challenging due to the small 0.18 eV splitting of the 3p ionic states. The combined temporal and spectral performance of Attohallen enables resolving these closely spaced channels.

I will also discuss ongoing developments of a second high-harmonic generation beamline, together with the scientific motivation driving its design and the new experimental opportunities it will enable for attosecond science.

When: 2026-06-22, 14:00 - 14:25, Where: Heinz-Otto Kreis

O2 - Deeper insights into molecular photodynamics by deep core ionization

AMO

Edwin Kukk[1]
[1] University of Turku

Abstract text: Organic molecules containing heavy elements are rewarding targets for experimental and theoretical investigations of the complex series of processes, triggered by the absorption of an X-ray photon. The ensuing dynamics is primarily determined by the nature of the initial electron vacancy. Ionization of deep core atomic orbitals adds a new dimension of lengthy Auger cascades with charge multiplication, running concurrently with the nuclear dynamics. The latter, owing to the relatively high charge reached after the Auger cascades, even when absorbing a single photon, can approach the conditions of a full Coulomb explosion (CE) that leads to complete atomization. However, for the medium-sized (few tens of atoms) organic molecules with heavy-atom substitution, the natural photodynamics regime is the *incomplete Coulomb explosion* (ICE) with surviving molecular fragments.

We present the latest experimental results on the ICE by core ionization of a specific class of molecules, halogenated (I, Br) cyclic compounds, using energy-and-momentum-resolved multicoincidence set-up MUSTACHE, installed at the GALAXIES beamline of SOLEIL synchrotron. We combine our experimental findings with an empirical molecular mechanics model designed to be directly comparable with the ion-ion coincidence experimental data. Such combined approach allows to draw conclusions on the timescales and spatial distribution of the positive charge accumulation process and provides comparison with theoretical works. Developing computationally inexpensive models for predicting the outcome of molecular core ionization – fragment abundances and energy distributions – has also an applied aspect. The released fragments and electrons can play an important role in radiotherapy of cancers, using halogenated radiosensitizer drugs.

When: 2026-06-23, 11:15 - 11:40, Where: Sonja Lyttkens

O3 - Development and Commissioning of TRÉSOR, a High-Resolution Time-Resolved Electron Spectrometer at the SQS Instrument of European XFEL

AMO

John BOZEK[1]
Alberto DE FANIS[2], Sylvain BETOULE[3], Iyas ISMAIL[3], Renaud GUILLEMIN[3], Thomas M. BAUMANN[2], Olle BJÖRNEHOLM[4], Rebecca BOLL[2], Klemen BUCAR[5], Luis CARDENAS[6, 7], Simon DOLD[2], Gilles DOUMY[8], Benjamin ERK[9], Rebecca INGLE[10], Edwin KUKK[11], Alexander MAGUNIA[12], Tommaso MAZZA[2], Tatiana MARCHENKO[3], Saikat NANDI[13], Yevheniy OVCHARENKO[2], Ralph PÜTTNER[14], Hamid RASHTABADI[2], Matthew ROBINSON[2], Daniel ROLLES[15], Sayantan SARKAR[3], Philip SCHMIDT[2], Florian TRINTER[16], Oksana TRAVNIKOVA[3], Sergey USENKO[2], Matjaz ZITNIK[5], Michael MEYER[2], **Marc SIMON**[3, 6]
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Abstract text: Time-resolved high-resolution electron spectroscopy in the X-ray domain is a long-sought goal, as it enables the detailed study of ultrafast dynamics and non-linear processes on femtosecond timescales. To address this challenge, we have developed an experimental endstation featuring a hemispherical electron analyzer equipped with a Delay-Line anode, capable of performing time-resolved high-resolution electron spectroscopy in the gas phase.

The spectrometer was commissioned at the PLÉIADES beamline of SOLEIL Synchrotron and at the SQS instrument of European XFEL. By leveraging the high repetition rate of European XFEL and the high-resolution capability of our analyzer, we achieved unprecedented resolution for high kinetic energy electrons using an XFEL. We also investigated the effects of the high intensity of XFEL X-ray pulses, which produce a large number of electrons and ions that interact with the detected electrons via Coulomb interactions, leading to spectral shifts and distortions.

During the talk, the performance of the electron analyzer, the first experimental results, and original scientific findings obtained during the commissioning phase will be presented.

When: 2026-06-23, 15:20 - 15:45, Where: Eva von Bahr

O4 - Double-Blind Holography and Spectral Interferometry for Attosecond Characterization of Free-Electron Laser Pulses and Electron Dynamics

Oliviero Cannelli[1, 2], Agata Azzolin[1, 2, 3], Sabine Rockenstein[1, 3], Kai-Fu Wong[1, 2, 3], Lina Hedewig[4], Venkata J.Yallapragada[5], Erik P. Månsson[1], Christina Papadopoulou[6], Elisa Appi[7], Ulrike Frühling[6], Alexander Magunia[4], Marc Seitz[1, 3], Josina Hahne[1, 2, 3], Ammar Bin Wahid[1, 3], Ana Oliveira Silva[1, 3], Peer Biesterfeld[8], Philip Mosel[8], Sven Fröhlich[8, 9], Markus Braune[6], Sebastian Schulz[6], Stefan Düsterer[6], Milutin Kovacev[8, 9], Uwe Morgner[8, 9], Robert Moshammer[4], Tino Lang[6], Christoph M. Heyl[6, 10, 11], Thomas M. Baumann[12], Terry Mullins[1, 2], Vincent Wanie[1, 2], Oren Raz[13], Fatemeh S. Ghaffari[1], Felix Ritzkowsky[1], Pranav Sreekumar[8], Huseyin Cankaya[6], Bianca Iwan[8], Giovanni Cirmi[6], Oender Akcaalan[6], Sangkil Son[1, 2], Robin Santra[1, 2], Christian Ott[4], Thomas Pfeifer[4], Evgeny Schneidmiller[6], Nirit Dudovich[13], Dan Oron[13], Andrea Trabattoni[1, 8, 9], Francesca Calegari[1, 2, 3]

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Abstract text: Attosecond light pulses provide the time resolution necessary for real-time tracking of electron dynamics in matter. Recently, several works have demonstrated the generation of few-femtosecond or sub-femtosecond pulses at free-electron laser (FEL) facilities, opening a new horizon for attosecond science. Crucial requirements are the accuracy of the pulse characterization methods in terms of spectral content, coherence, and temporal duration, as well as a precise delay tagging ideally with attosecond resolution. Overcoming these limitations is key to fully exploiting FEL sources for this purpose. Here, we show two complementary approaches to achieve attosecond capabilities at FEL facilities.

First, we demonstrate double-blind holography (DBH) as an all-optical scheme for the retrieval of amplitude and phase of FEL pulses on a single-shot basis. We report the full characterization of ultrashort 10-fs self-amplified spontaneous emission (SASE) FEL pulses in the extreme ultraviolet (XUV) through interference with a synchronized HHG source at FL26 beamline of FLASH, paving the way for extending single-shot DBH characterization in the soft X-ray domain. Second, we present spectral-interferometry experiments in noble gases. A split-and-delay unit generates two replicas of the FEL pulses, one propagating through the gas target, the other bypassing the sample. The two beams are spatially overlapped producing spectral fringes, from which the amplitude and phase of the atomic resonances are extracted. By varying the FEL intensity, we directly track intensity-dependent Stark shifts of the Fano resonances and their effect on the attosecond electron-wavepacket dynamics, retrieved via Fourier analysis of the complex spectral response of the excitation process.

When: 2026-06-26, 12:05 - 12:25, Where: Heinz-Otto Kreis

O5 - Emission and absorption spectroscopy of xenon-noble gas mixtures for Bose-Einstein condensation of VUV-photons

AMO

Eric Boltersdorf[1]
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Abstract text: Photons confined in a dye-filled microcavity can exhibit Bose-Einstein condensation upon thermalization through repeated absorption and (re-)emission processes on the dye molecules. This has been experimentally demonstrated for photons in the visible spectral regime in 2010 [1]. The most important prerequisite for the dye molecules to be a suitable thermalization mediator is the fulfillment of the so-called Kennard-Stepanov relation, a thermodynamic, Boltzmann-like scaling law connecting the absorption and emission lineshapes.

In the present work, we show an experimental approach to realize Bose-Einstein condensation of photons in the vacuum-ultraviolet spectral regime via repeated absorption and (re-)emission cycles between the $5p^6$ ground state and the $5p^5 6s$ (J = 1) excited state ($\lambda_{res} = 146.96$nm [2]) of xenon-noble gas excimer molecules in dense gaseous ensembles with pressures of up to 100bar. We present absorption and emission data on this transition giving strong evidence for a Kennard-Stepanov scaling of photons in these dense xenon-noble gas ensembles [3]. We observe a spectral temperature of 140-160K, which is well below the temperature of the room temperature gas cell, but nevertheless expected to allow for thermalization of a VUV photon gas at the measured spectral temperature.

[1] J. Klärs et al., Nature **468**, 545-548 (2010)
[2] Brandi et. al., Phys. Rev. A **64**, 032505 (2001)
[3] E. Boltersdorf et al., Phys. Rev. A **112**, 012811 (2025)

When: 2026-06-22, 16:10 - 16:35, Where: Heinz-Otto Kreis

O6 - Femtosecond non-adiabatic dynamics induced by ultrafast molecular photoionization

AMO

Saikat Nandi[1]
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Abstract text: The rapid development of high-order harmonic generation based tabletop sources providing attosecond (1 as = 10^{-18} s) extreme ultraviolet (XUV) pulses has opened up novel avenues to explore ultrafast molecule dynamics. As the photon energies of these pulses are relatively high (between 10 to 100 eV), they can easily remove an electron from the valence or, inner-valence molecular orbital, leading to simultaneous ionization and excitation of the target. The molecular cation is usually promoted to a highly excited state from where the relaxation to the cationic ground state is accompanied by non-adiabatic dynamics due to strong coupling between the electronic and nuclear degrees of freedom.

Here, using an attosecond XUV pulse train as pump and an intense, femtosecond near-infrared pulse as probe, we investigated the ultrafast photoionization dynamics in ethylene molecules. In particular, we studied how isotope-induced explicit symmetry breaking can speed up the ethylene to ethylidene photo-isomerization process in the molecular cation [1]. Furthermore, we observed that the yield of the ethylene dication can be confined to a narrow temporal window of a few femtoseconds, which originates from the competition between pump-induced non-adiabatic processes and probe-induced resonance enhanced multi-photon processes [2].

The results obtained for such model systems, can further be used to understand better similar photoionization dynamics in complex photo-switches, such as spiropyran, interacting with femtosecond X-ray pulses from a free-electron laser.

References:

1. A. N. Nardi *et al.*, *Commun. Chem.* **8**, 222 (2025).
2. C. Marante *et al. J. Phys. Chem. Lett.* **17**, 797–803 (2026).

When: 2026-06-22, 15:45 - 16:10, Where: Heinz-Otto Kreis

O7 - From atoms to aerosols: research on low density matter at the FinEstBeAMS beamline of MAX IV

AMO

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Calle Preger[1], Kirill Chernenko[1], Gunnar Öhrwall[1], Maxim Tchaplyguine[1], Noelle Walsh[1]
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Abstract text: FinEstBeAMS [1] is a multi-purpose undulator beamline at the MAX IV Laboratory (Lund, Sweden). It covers a wide photon energy range of 4.5-1300 eV, allowing studies at both valence and core level thresholds. Studies on dilute gas-phase samples typically utilize photon energies up to ~750 eV due to a significant decrease in flux at higher photon energies. The elliptically polarizing undulator of the beamline can deliver linearly and circularly polarized radiation.

FinEstBeAMS has three dedicated end stations that are or can be installed at two branch lines: a gas-phase end station (GPES) [2], a photoluminescence end station, and a solid-state end station. The GPES was designed for coincidence measurements between energy-resolved electrons and ions, but it can, of course, be used for stand-alone electron spectroscopy and ion time-of-flight spectroscopy. Different sources such as a liquid jet, a cluster source, and an aerosol sample delivery system [3] have been coupled to the GPES.

Temporary installation of other experimental setups is also possible at FinEstBeAMS, when the GPES is removed from the beamline. For instance, a reaction microscope/COLTRIMS apparatus and a magnetic bottle electron spectrometer have been used at the beamline with single-bunch operation, which is typically available for 6-8 days in a semester.

[1] K. Chernenko *et al.*, *J. Synchrotron Rad.* **28** (2021) 1620.
[2] K. Kooser *et al.*, *J. Synchrotron Rad.* **27** (2020) 1080.
[3] C. Preger *et al.*, *J. Synchrotron Rad.* **31** (2024) 1382.

When: 2026-06-25, 10:20 - 10:40, Where: Sonja Lyttkens

O8 - Identification of Roaming Mechanism and the Formation of H3+ in Core Ionised Cyclopropane

AMO

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Smita Ganguly[2], Noelle Walsh[3], Mathieu Gisselbrecht[1], Stacey Sorensen[1]
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[3] MAX IV Laboratory, Lund University, Lund, Sweden

Abstract text: Three-dimensional electron and ion imaging spectrometry is used to study the dynamics of gas-phase cyclopropane, C_3H_6, after inner-shell electron excitation. In this study, one particular dynamic is studied, the formation of the H_3^+ ion through the roaming dissociation mechanism from the cyclopropane dication $C_3H_6^{2+}$. The roaming pathway in cyclopropane revolves around the neutral H_2 roaming around the dication $C_3H_4^{2+}$ and eventually abstraction of a H^+ forming the H_3^+ ion [1,2]. This study utilises momentum imaging to study primarily the incomplete fragmentation $H_2/H^+/C_3H_3^+$ where a CH bond has broken before the abstraction occurs, interrupting the roaming process. Fig. 1 shows the momentum correlation and the kinetic energy release during the roaming process. Two channels emerge, the X and Y channel, these are identified as roaming and asynchronous concerted dissociation, respectively. Branching ratios of the X, Y and H_3^+ channels at different total kinetic energy release values reveal that the interrupted roaming (X channel) is converted into the successful roaming (H_3^+ channel) when the internal energy is sufficiently high. In conclusion, this study shows with momentum imaging that the formation pathway of the H_3^+ ion in the fragmentation of cyclopropane occurs via the roaming mechanism. This experiment was carried out at the MAX IV Laboratory in Lund, Sweden, at the FlexPES beamline.

[1] D. Townsend *et al.*, (2004), Science 306, 1158-1161. DOI: 10.1126/science.1104386.
[2] Sung Kwon *et al.*, J. Phys. Chem. A 2023, 127, 41, 8633–8638.

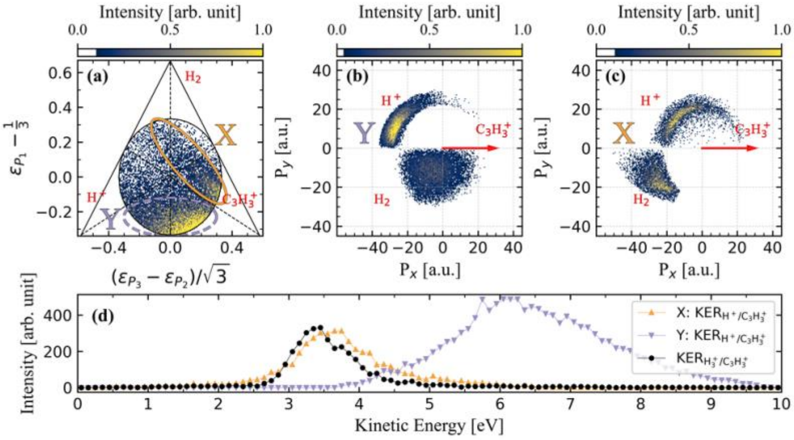

Figure 1: (a) Dalitz plot for the fragmentation $H_2/H^+/C_3H_3^+$. Newton diagrams for respective pathway Y (b) and X (c) show the distribution of momentum vectors. (d) The kinetic energy release for the X and Y channels compared with $H_3^+/C_3H_3^+$.

When: 2026-06-25, 11:15 - 11:40, Where: Sonja Lyttkens

O9 - Inner-shell photoionization of free atomic and molecular ions

AMO

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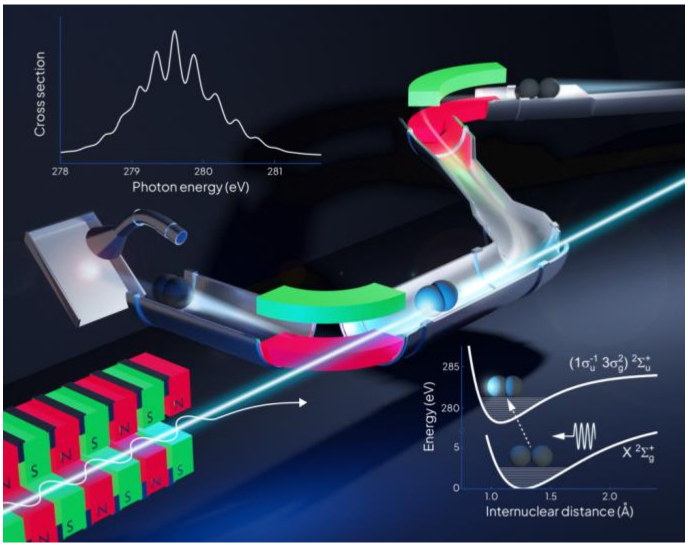
Abstract text: The photon-ion merged-beams technique is a powerful approach for studying the interaction of energetic radiation of atomic and molecular ions and of other charged small quantum systems. A salient feature of the technique is its capability of providing reaction cross sections on an absolute scale. I will review results from the Photon-Ion end station at PETRA III (PIPE), where photon energies are available in the range 260-2700 eV and, consequently, inner-shell phenomena can be addressed. The record high photon flux at the PETRA III beamline P04 permits high-resolution studies with thin targets, which provide a wealth of information on the ionic structure and on the dynamics, which sets in after the creation of an inner-shell hole by an energetic photon. The results are of fundamental interest and have prompted corresponding quantum-theoretical research [1]. Moreover, they are relevant for a number of fields such as fusion plasmas and astrophysics [2,3]. In my talk I will focus on negatively charged atomic and molecular ions, where the extra electron is bound by strong correlation effects. Our studies, e.g. [4,5], provide a unique access to core-valence correlation effects in such highly correlated systems.

[1] A. Müller et al, Phys. Rev. A **110**, 062802 (2024), doi: 10.1103/PhysRevA.110.062802.
[2] L. Corrales et al., Astrophys. J. **965**, 172 (2024), doi: 10.3847/1538-4357/ad2939.
[3] M. Looshorn et al., Astrophys. J. **997**, 199 (2026), doi: 10.3847/1538-4357/ae3089.
[4] A. Perry-Sassmannshausen et al., Phys. Rev. Lett. **124**, 083203 (2020), doi: 10.1103/PhysRevLett.124.083203.
[5] S. Schippers et al., ChemPhysChem **24**, e202300061 (2023), doi: 10.1002/cphc.202300061.



When: 2026-06-25, 12:05 - 12:25, Where: Sonja Lyttkens

O10 - Investigating Photoelectron Circular Dichroism as a Function of Distance from the Stereocenter

AMO

Emilia Heikura[1]
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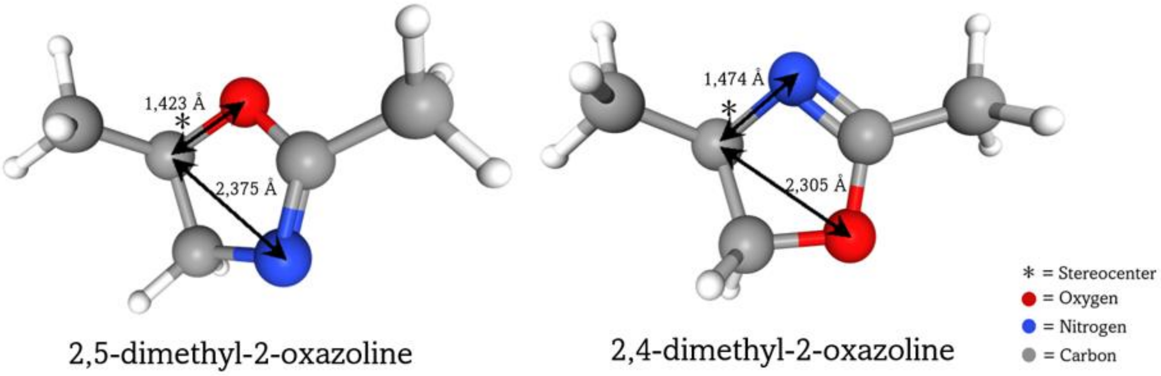
Abstract text: Photoelectron circular dichroism (PECD) is one of the most powerful methods for investigating the physical properties of molecular chirality in the gas phase. PECD arises from a forward-backward asymmetry of emitted photoelectrons in chiral molecules after interaction with circularly polarized light. This forward-backward asymmetry can be observed even in randomly oriented chiral molecules. It is still unknown how the magnitude of PECD is affected as a function of the distance between the emission site and the stereocenter. The site-selectivity of inner-shell photoelectrons enables the investigation of this aspect of molecular chirality. For this experimental work, the synthesis of specifically tailored molecules was necessary to achieve the required experimental properties, such as high volatility and a rigid molecular structure. Most importantly, these experiments require two distinct molecules in which the distances between the stereocenter and a marker atom are different, while the changes to the main structure of the molecule are minimal. These properties were fulfilled by the molecules 2,5-dimethyl-2-oxazoline and 2,4-dimethyl-2-oxazoline shown in the figure. In these oxazoline derivatives, the distance dependency of PECD can be investigated by ionization of not only one but two different marker atoms, nitrogen and oxygen, with respect to the stereocenter. The existence of these two marker atoms enables investigation of distance dependency for the two different elements but also a comparable study of element-specific PECD.



2,5-dimethyl-2-oxazoline

2,4-dimethyl-2-oxazoline

When: 2026-06-24, 14:55 - 15:20, Where: Eva von Bahr

O11 - Investigation of non-linear processes and photoinduced dynamics using soft X-ray Free-Electron Lasers

AMO
Michael Meyer[1]
[1] European XFEL

Abstract text: Soft X-ray pulses of high intensities (more than 10^{18} W/cm^2) and ultrashort pulse durations (less than 1 fs) are available for experiments at the Small Quantum Systems (SQS) scientific instrument of the European X-ray Free-Electron Laser [1]. Many novel investigations of non-linear processes as well as time-resolved dynamical studies have been performed taking advantage of these unique properties. Beside introducing these general research topics, the talk will focus on some recent experiments. As typical example for multi-photon processes, the formation and relaxation of double-core holes (DCH) resonances in atoms (Ne, Ar) and molecules (N_2) will be discussed, which were explored using high-resolution photon or electron spectroscopy. Insight into molecular fragmentation dynamics was obtained using time-resolved experiments, combining either two soft X-ray FEL pulses (X-ray/X-ray) or a soft X-ray FEL with an optical laser pulse (X-ray/OL) in a pump-probe arrangement [2]. Special attention will be given here to the availability of soft X-ray FEL pulses, characterized by attosecond (>300 as) durations and intensities of up to 1 mJ, and their first applications [3]. Some of the results have been made possible only by the recently installed diagnostic section at the SQS instrument enabling pulse-resolved, on-line characterization of the spectral and temporal profile of the strongly varying FEL pulses as well as the precise optimization of the focus size using a Shack-Hartmann-type wavefront sensor.

References

[1] W. Decking et al., Nature Photon. **14**, 391 (2020).
[2] D. E. Rivas et al., Phys.Rev. X **16**, 011051 (2026).
[3] L. Funke et al., https://doi.org/10.48550/arXiv.2408.03858

When: 2026-06-22, 14:25 - 14:50, Where: Heinz-Otto Kreis

O12 - Nitrogen K-edge Time-Resolved XAS for Probing Photoinduced Dynamics in Azobenzene

AMO

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Abstract text: Azobenzene is often considered the classic example of a photoswitch, undergoing photoisomerization resulting in a significant photochromic shift. Good photoswitching fatigue resistance and selective wavelength control over the forward and backswitching processes have made azobenzene-based motifs ubiquitous in molecular switching applications. However, there have been a relatively limited number of experimental ultrafast spectroscopies studies on isolated azobenzene. Using time-resolved X-ray absorption spectroscopy (TR-XAS) at the nitrogen K-edge, we demonstrate how the excellent sensitivity of TR-XAS to states of different electronic character and site-specific probing capabilities can be used to map the photoinduced dynamics across multiple electronic states as well as changes in the nuclear configuration.

When: 2026-06-24, 11:15 - 11:40, Where: Sonja Lyttkens

O13 - Non-local X-ray intermolecular radiative decay probes solvation shell of ions in water

AMO

Johan Söderström[1], **Lucas Cornetta**[2], Victor Ekholm[3], Vincenzo Carravetta[4], Arnaldo de Brito[5], Ricardo Marinho[6, 7], Marcus Agåker[1, 3], Takashi Tokushima[3], Conny Såthe[3], Anirudha Ghosh[3], Dana Bloß[8], Andreas Hans[8], Florian Trinter[9], Iyas Ismail[10], Debora Vasconcelos[1], Joel Pinheiro[1], Yi-Ping Chang[11], Manuel Harder[11], Zhong Yin[12], Joseph Nordgren[1], Gunnar Öhrwall[3], Hans Ågren[1], Jan-Erik Rubensson[1], Olle Björneholm[1]

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[9] Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
[10] Sorbonne Université, CNRS, Laboratoire de Chimie Physique - Matière et Rayonnement, LCPMR, Paris, France
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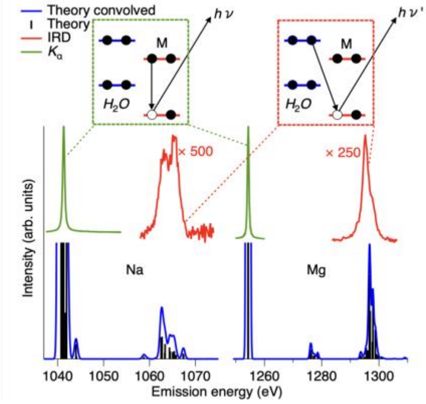
[12] International Center for Synchrotron Radiation Innovation Smart, Tohoku University, Sendai, Japan

Abstract text: Aqueous solutions are crucial in chemistry, biology, environmental science, and technology. The chemistry of solutes is influenced by the surrounding solvation shell of water molecules, which have different chemical properties than bulk water due to their different electronic and geometric structure. It is experimentally challenging to selectively investigate this property-determining electronic and geometric structure. Here, we report experimental results on the non-local X-ray emission process Intermolecular Radiative Decay, for the prototypical ions Na$^+$ and Mg^{2+} in water. We show that, in Intermolecular Radiative Decay, an electron from the solvation shell fills a core hole in the solute, and the released energy is emitted as an X-ray photon. We interpret the underlying mechanism using theoretical calculations, and show how Intermolecular Radiative Decay will allow us to meet the challenge of selectively probing the solvation shell from within.



When: 2026-06-24, 15:20 - 15:40, Where: Eva von Bahr

O14 - Nonlinear atomic tunnelling boosted by bright squeezed vacuum

AMO

Shengzhe Pan[1]
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Abstract text: Nonlinear optical processes, mediated by multiphoton interactions rather than single-photon response, are routinely exploited to enable a range of light-based functionalities in devices and applications. Nonlinear effects are enhanced by higher-intensity fields, which is a limiting strategy owing to potential radiation damage. An alternative strategy relies on the fluctuation redistribution typical of quantum light, but experimental demonstrations at the most fundamental level have been limited. Here we report experimental nonlinear tunnelling ionization of isolated atoms, a pivotal nonlinear process that drives high-harmonic generation and forms the basis of attosecond science, boosted by quantum light—bright squeezed vacuum (BSV). A BSV light with an average pulse energy of 300 nJ achieves an effective intensity equivalent to that of a coherent light with 7.1 μJ, demonstrating a more than 20-fold quantum boost in the nonlinear effect from BSV light. This boost is revealed by matching the peaks of the photoelectron momentum spectra produced by the BSV and coherent light as measured by angular streaking. Furthermore, we demonstrate control of the effective intensity of the BSV by tuning the correlation function at fixed average pulse energy, establishing a robust method to tailor nonlinear processes by quantum statistics rather than classical intensity scaling. These findings may facilitate the development of quantum-controlled strong-field dynamics using tailored quantum light sources.

When: 2026-06-22, 14:50 - 15:10, Where: Heinz-Otto Kreis

O15 - Photoelectron tomography for high-order partial waves in multiphoton ionization

AMO

Lulu Han[1], Wenyu Jiang[1], Luke Roantree[2], Boren Shen[3], Kiyoshi Ueda[1, 4], Andrew Brown[2], Yang Li[3], Shengzhe Pan[1], Feng He[3], Jian Wu[1]

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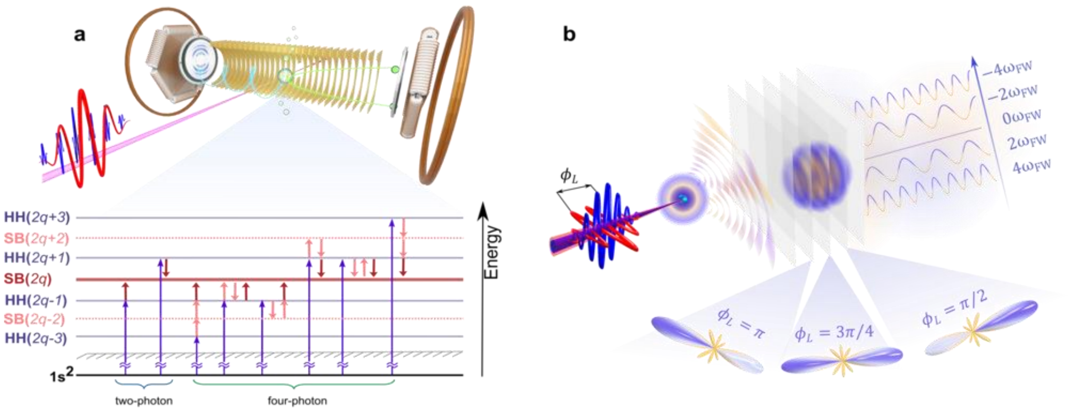
Abstract text: The characterization of photoionization dynamics on the attosecond timescale requires detailed knowledge of both the partial-wave composition of the continuum electron wave packet and the quantum pathways involved in multiphoton ionization. Here, we report recent progress in photoelectron tomography methods designed to reconstruct high-order partial waves and to disentangle photon interaction pathways in few-photon and strong-field ionization regimes. We first present a heterodyne analysis approach based on delay-resolved anisotropy parameters, which extends the Reconstruction of Attosecond Beating By Interference of Two-photon Transitions (RABBITT) technique beyond the perturbative regime. This method enables the identification of weak high-angular-momentum partial-wave contributions in near-infrared-assisted photoionization via Rydberg states. We show that even small contributions from high-order partial waves can significantly influence photoelectron angular distributions through interference with dominant channels and can lead to observable deviations in reconstructed spectral phases.In addition, we introduce a photoelectron quantum-path tomography method for multiphoton ionization, in which phase-resolved photoelectron angular distributions obtained from orthogonally polarized two-color laser fields are used to extract complex partial-wave amplitudes. Fourier analysis of these amplitudes yields a quantum-path spectrum that identifies the contributing ionization pathways according to the number of absorbed and emitted photons. Supported by time-dependent Schrodinger equation simulations, this approach reveals selection rules, propensity effects, and interference mechanisms governing the formation of continuum electron wave packets.These results establish a general tomographic framework for resolving partial waves and reconstructing quantum paths, providing new insight into non-perturbative photoionization dynamics and attosecond strong-field physics.



a.Schematic of attosecond coincidence interferometer and transition map of photoionization in helium atoms.
b.Schematic illustration of the photoelectron quantum-path tomography.

When: 2026-06-23, 12:05 - 12:30, Where: Sonja Lyttkens

O16 - Probing transient nanoplasma dynamics using high-harmonic beamline at ELI Beamlines facility

AMO

Eva Klimešová[1]
Keshav Sishodia[1], Martin Albrecht[1], Andreas Hult Roos[1, 2], Matyáš Staněk[1, 3], Lucie Jurkovičová[1, 3], Ondřej Hort[1], Jaroslav Nejdl[1, 3], Martin Matys[1], Dmitrij Ševaev[3], Andrei Nomerotski[3, 4, 5], Peter Švihra[3, 4], Jakob Andreasson[1], Maria Krikunova[1, 6]
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Abstract text: ELI Beamlines facility, operated within the Extreme Light Infrastructure ERIC, operates ultrafast high-power lasers and laser-driven sources of radiation and accelerated particles for user applications. The high-harmonic (HHG) beamline and the MAC end-station at ELI Beamlines provide a combination of a laser-driven VUV beam and an auxiliary beam for femtosecond time-resolved investigations primarily in the field of AMO sciences. Typical experiments at MAC are focused on photoelectron spectroscopy of atoms, molecules, gas-phase clusters and nanoparticles [1,2].

After presenting an overview of the HHG beamline and the MAC end-station at ELI, we will address user experiments studying anisotropic nanoplasma dynamics in nanoscale clusters using velocity map imaging spectrometer equipped with time-stamping Timepix3 optical camera [3]. These investigations aim to explore the non-homogeneous charging and disintegration of large atomic clusters ionized by VUV pulse from the HHG beamline, and the subsequent dynamics of the localized nanoplasma created by a near-infrared (NIR) pulse. We will present different cases of non-uniform field distribution in clusters: (i) shadowing in clusters in VUV fields and (ii) nanofocusing in clusters in NIR fields. We will address microscopic mechanisms of ion acceleration and other distinct phenomena in confined nanoplasmas.

The presented results, relevant for electron and ion manipulation on the nanoscale, showcase the reliable performance HHG-MAC instrument at ELI Beamlines.

[1] E. Klimešová et al., Eur. Phys. J. Spec. Top. **230**, 4183 (2021) https://doi.org/10.1140/epjs/s11734-021-00192-z
[2] O. Hort *et al.,* Opt. Express **27**, 8871 (2019) https://doi.org/10.1364/OE.27.008871
[3] D. Ševaev *et al.*, J. Instrum. **21**, C03022 (2026) https://doi.org/10.1088/1748-0221/21/03/C03022

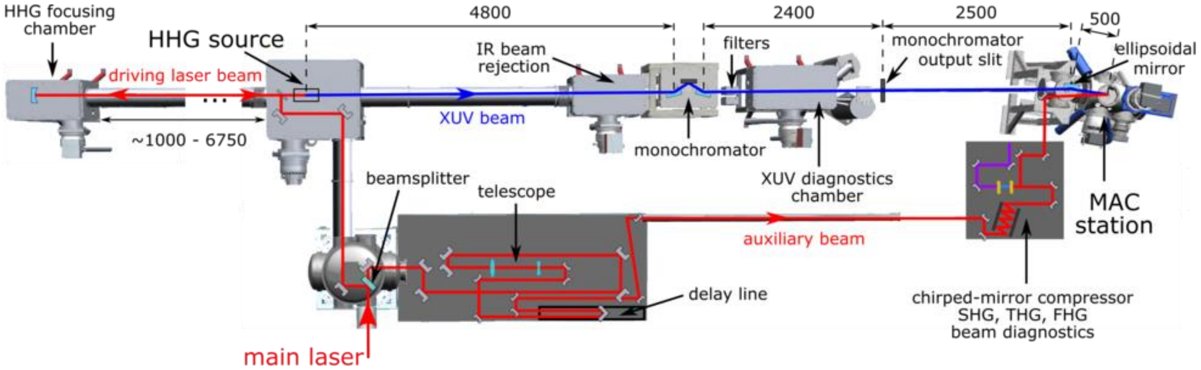

Figure 1: HHG-MAC beamline at the ELI Beamlines facility. The main laser beam is split into a main part, driving the high-harmonic source, and auxiliary beam for time-resolved experiments at MAC end-station. Adapted from Ref. [1].

When: 2026-06-26, 12:05 - 12:25, Where: Eva von Bahr

O17 - Experimental opportunities with 1D imaging spectrometer at the SQS instrument at the European XFEL

AMO

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Abstract text: Capabilities of the novel 1D imaging soft X-ray spectrometer [1] installed at the SQS instrument at the European XFEL are presented and discussed. The instrument aims at monitoring non-linear X-ray phenomena as high-intensity short-duration X-ray pulses propagate through dense gaseous media [2] and time-evolution via spatially resolved X-ray emission spectroscopy. Examples of measurements from of three beamtimes granted for community proposals will be discussed. These measurements involve a large number of researchers, their contributions are gratefully acknowledged.

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[2] Svyatoslav Blinov, Pavel Krasnov, Faris Gel'mukhanov, Jan-Erik Rubensson, Sergey Polyutov, and Victor Kimberg, Phys. Rev. Research **8**, 013110 (2026)

When: 2026-06-22, 11:55 - 12:15, Where: Eva von Bahr

O18 - RIXS on Neon: Fano-Like Interference and Coster-Kronig-Like Autoionization

AMO

Jan-Erik Rubensson[1]
Marcus Agåker[1, 2], Ji-Cai Liu[3, 4], Takashi Tokushima[2], Anirudha Ghosh[2], Conny Såthe[2], Jian Wang[3, 4], Moritz Grunwald-Delitz[5], Thomas Baumann[5], Michael Meyer[5], Manuel Harder[5], Zhong Yin[6], Olle Björneholm[1], Joseph Nordgren[1], Stephan Fritzsche[7, 8, 9], Victor Kimberg[10], Johan Söderström[1], Faris Gel'mukhanov[10, 11]
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Abstract text: We present resonant inelastic X-ray scattering spectra excited at single- and double-excitation resonances of neon. For the single $1s^{-1}n'p$ excitations we observe interference between scattering channel leading to final states $2p^{-1}np$ as main configuration, where large-amplitude one-electron ($n'=n$) channels interfere with small-amplitude two-electron ($n'\neq n$) channels. The interference is manifested in an asymmetric line profile where the two-electron resonance occurs in the tail region of the one-electron resonance. This slowly varying tail plays the role of the continuum for the Fano effect, and the asymmetric profile is well modelled by means of a single asymmetry parameter [1]. At resonances due to $1s^{-1}2p^{-1}3pnl$ double excitations we observe transitions to several doubly excited final states of the $2p^{-2}3pnl$ type which have not been resolved before. We discuss the behavior at the $1s^{-1}2p^{-1}3p$ ionization thresholds and find an unusual Coster-Kronig-like autoionization transition from core-excited to core-ionized states, mediated by spin-recoupling of the inner electrons.

References

[1] Johan Söderström, Marcus Agåker, Ji-Cai Liu, Takashi Tokushima, Anirudha Ghosh, Conny Såthe, Jian Wang, Andreas Pantelis Frey Koudouridis, Moritz Grunwald-Delitz, Thomas M. Baumann, Michael Meyer, Manuel Harder, Zhong Yin, Olle Björneholm, Joseph Nordgren, Stephan Fritzsche, Victor Kimberg, Jan-Erik Rubensson, and Faris Gel'mukhanov, Phys. Rev. Lett. 135, 233001 (2025), https://doi.org/10.1103/c5mk-trlz

When: 2026-06-23, 14:55 - 15:20, Where: Eva von Bahr

O19 - Shake-down spectroscopy as state- and site-specific probe of ultrafast chemical dynamics

AMO

Henry J. Thompson[1], Matteo Bonanomi[2, 3], Jacob Pedersen[4, 5], Felix Allum[6], Michael Ashfold[7], Alexander D. Brynes[8], Marcello Coreno[9], Miltcho B. Danailov[8], Piero Decleva[10], Alexander Demidovich[8], Michele Devetta[3], Avijit Duley[11], Davide Faccialà[3], Raimund Feifel[12], Ruaridh Forbes[6, 13], Cesare Grazioli[14], David M. P Holland[15], Rebecca Ingle[16], Nitish Pal[8], Paolo Piseri[17], Oksana Plekan[8], Stephen Pratt[18], Kevin C. Prince[8, 19], Weronika Razmus[1], Daniel Rolles[11], Michael S. Schuurman[20, 21], Alberto Simoncig[8], Richard J. Squibb[12], Bruno N. C. Tenorio[4], Caterina Vozzi[3], Marco Zangrando[8, 14], **Carlo Callegari**[8], Sonia Coriani[4], Russell S. Minns[1], Michele Di Fraia[8, 14]

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[11] Department of Physics, Kansas State University, Manhattan, United States of America
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Abstract text: Tracking electronic and structural changes occurring in a molecule during a photochemical transformation benefits from recent experimental and computational progress in time-resolved valence- and core-shell photoelectron spectroscopy (hereafter tr-PES and tr-XPS, respectively). The former provides a global picture of the bonding structure of the molecule, the latter of the local environment.

Weak tr-XPS satellites resulting from shake-down processes provide a unique fingerprint that is

sensitive to both valence-state electronic evolution and nuclear motion. The seeded free-electron laser FERMI delivers pulses at the S2p edge with a duration of few tens of femtoseconds, narrow bandwidth, and negligible timing jitter, producing high-dynamic-range spectra and enabling the observation of shake-down processes.

We performed high-resolution tr-XPS on CS_2 and 2-iodothiophene. In CS_2, where the role of internal conversion and intersystem crossing in determining the pre-dissociation dynamics is controversial, we derive a propensity rule that demonstrates the spin selectivity of the shake-down signals. This selectivity allows us single-out contributions from the bright and dark singlet excited states along the dissociation pathway. In 2-iodothiophene the direct XPS signal shows very limited changes during the dissociation reaction, whereas the shake-down signal spans approximately 5 eV as the C–I bond stretches; mapping this shift onto classical trajectory simulations yields precise bond-length evolution. Together these results demonstrate that shake-down satellites provide an element-specific, simultaneous window on electronic state evolution and bond-length changes, offering a powerful tool for real-time structural mapping in complex photochemical reactions. This approach opens a new avenue for ultrafast light-matter interaction studies at advanced light sources.

When: 2026-06-24, 15:40 - 16:00, Where: Eva von Bahr

O20 - Single-shot single-particle electron and ion spectroscopy of large XUV-excited neon clusters

AMO

Frederic Ussling[1]
Yves Marc Acremann[1], David Carey[1], Alessandro Colombo[1], Indrani Dey[1], Linos Hecht[1], Moritz Heinemann[1], Katharina Kolatzki[1], Jannis Lehmann[1], Changji Pan[1], Mario Sauppe[1], José Gómez Torres[1], Angela Vidoni[1], Michael Wenger[1], Daniela Rupp[1]
[1] Physics Department, ETH Zurich, Zurich, Switzerland.

Abstract text: We report on the development and implementation of a high-intensity high-harmonic generation (HHG) beamline designed for single-shot coherent diffractive imaging (CDI) of isolated, free-flying nanotargets, such as atomic and molecular clusters. The recording of a single diffraction pattern provides detailed information about the sample's size, geometry, and irradiation intensity [1, 2]. In a complementary approach, single-particle imaging is combined with coincidence electron and ion time-of-flight (TOF) spectroscopy, offering a quasi-complete measurement of the XUV-cluster interaction. In this study, we investigate cluster size- and XUV intensity-dependent energy transfer dynamics upon XUV irradiation in large neon clusters. Using CDI as a tool allows us to sort the single-shot electron and ion spectra, thus circumventing previously unavoidable ensemble averaging over cluster size and focal intensity distributions. The analysis of the size- and intensity-sorted charged residuals reveals complex recombination and relaxation dynamics in the dense and cold nanoplasma created upon the interaction. We identify signatures of recombination-induced intra-Rydberg interatomic Coulombic decay (ICD) [3, 4] between neutral excited atoms which form via electron-ion recombination during the expansion of the cluster. By identifying these intra-Rydberg ICD processes and tracing their evolution as a function of cluster size and XUV exposure intensity, this work offers new insights into energy transfer processes on the nanoscale.

[1] D. Rupp et al., Phys. Rev. Lett. 117, 153401 (2016)
[2] T. Gorkhover et al., Phys. Rev. Lett. 108, 245005 (2012)
[3] K. Nagaya et al., Nat. commun 7, 13477 (2016)
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When: 2026-06-23, 11:40 - 12:05, Where: Sonja Lyttkens

O21 - Spatial and temporal evolution of ionic fragments produced by deep core-level ionization

AMO

Oksana TRAVNIKOVA[1]
[1] Laboratoire de Chimie Physique-Matière et Rayonnement (LCPMR), CNRS, Sorbonne Université

Abstract text: Deep-inner-shell ionisation triggers Auger cascades, providing a natural framework to probe coupled electron-nuclear dynamics under conditions of high and evolving transient charge, central to XFEL science, pump-probe experiments, and radiation-damage processes. In the tender and hard X-ray regime, relaxation of a deep-core vacancy proceeds via sequential decay, in contrast to the single-step processes extensively studied using soft X-rays. This multi-step character defines a qualitatively distinct regime: intermediate states are populated progressively, and their effective lifetimes are governed not only by intrinsic decay rates but also by population flow during the cascade. Consequently, intermediates bearing inner-shell vacancies can persist for hundreds of femtoseconds, orders of magnitude longer than typical single-core-hole lifetimes, enabling nuclear dynamics to develop over large internuclear distances.

As a case study [1], we examine the Coulomb-fragmentation regime, where charge build-up and nuclear dynamics evolve concurrently under long-range Coulomb interactions. Using HCl as a prototypical system, we probe Cl K-shell ionisation and identify long-lived intermediate states surviving to internuclear separations exceeding 100 a.u. These results align with our soft X-ray L-emission studies of SF_6 [2], where S K-shell ionisation drives complete dissociation via intermediates with a S 2p core vacancy, producing neutral atomic sulfur, with all six fluorines detached before the final decay step. These results show that deep-inner-shell ionisation defines a regime where molecular dynamics unfolds alongside charge build-up, revealing charge redistribution and fragmentation pathways beyond single-step decays.

[1] Travnikova et al. PRA 113, 012823 (2026)
[2] Travnikova et al. PRL 134, 063003 (2025)

When: 2026-06-25, 09:55 - 10:20, Where: Sonja Lyttkens

O22 - Studying metal-molecule interface on isolated plasmonic nanoparticles by on-the-fly soft X-ray spectroscopies

AMO

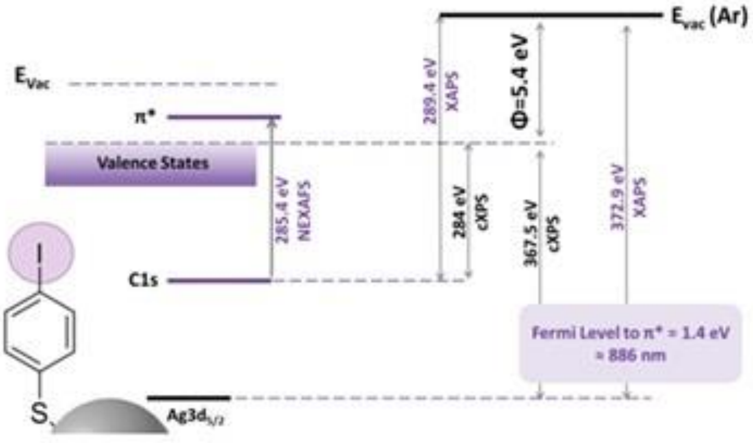
Namitha Deepak[1], **Aleksandar Milosavljevic**[2], Anahita Heraji Esfahani[1], John Bozek[2], Christophe Nicolas[2], Sergio Kogikoski Junior[1], Ilko Bald[1]
[1] University of Potsdam, Institute of Chemistry, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany
[2] Synchrotron SOLEIL, L’Orme des Merisiers Départementale 128, 91190 Saint-Aubin, France

Abstract text: Light-induced chemistry on functionalized metallic plasmonic nanomaterials attracts significant attention due to a wide range of potential applications [1]. In these systems, visible light induces localized surface plasmon resonance in e.g. gold or silver nanoparticles, triggering chemical reactions in adsorbed molecules. These processes are governed by diverse mechanisms, including enhanced electromagnetic fields, charge transfer, and heat. Gaining a fundamental understanding of these reaction pathways requires profound knowledge of the electronic structure at the metal-molecule interface.

In this contribution, we describe a state-of-the-art experimental setup at the PLEIADES beamline (SOLEIL Synchrotron, France) for X-ray Aerosol Photoelectron Spectroscopy (XAPS) of nanoparticles isolated in vacuum. The nanoparticle beam is generated from a colloidal solution, focused by an aerodynamic lens, and crossed with the photon beam in front of a hemispherical analyzer. This arrangement offers several advantages over table-top techniques: it completely avoids substrate influence and radiation damage, allows direct alignment to the vacuum level, and enables depth profiling via tunable photon energy. Moreover, using soft X-rays provides exceptional sensitivity to the nanoparticle surface.

We will present recent results for silver nanoparticles modified with 4-iodothiophenol. Combining XPS and NEXAFS provides an unprecedented energy diagram for such system, including the relative position of ligand unoccupied states with respect to the Fermi level (Figure). We briefly discuss perspectives on combining XAPS with liquid jet spectroscopy, utilizing mass/charge-selected X-ray spectroscopy to investigate ligands alone, and probing light-activated nanoparticles *in situ*.

[1] Ilko Bald, Adv. At. Mol. Phys. Interfaces Nat. Sci., pp. 165-190 (2026)



When: 2026-06-24, 16:00 - 16:20, Where: Eva von Bahr

O23 - The end-stations for atomic, molecular and optical physics at the Shanghai X-ray Free Electron Laser facilities

AMO

Xincheng Wang[1]
Mingjie Zhang[1], Jianfei Tao[1], Zhenjie Shen[1], Jianfeng Liao[1], Jinze Feng[1], Yikang Zhang[1], Wentao Zhu[1], Hailong Guo[1], Huanyu Ma[1], Yunfei Feng[1], Ruichao Dong[1], Yuhai Jiang[1], Kiyoshi Ueda[1, 2], Xiaojing Liu[1]
[1] Center for Transformative Science, Shanghaitech University, Shanghai, China
[2] Tohoku University, Sendai, Japan

Abstract text: Free-electron lasers (FELs) are characterized by their high pulse energy, ultrashort pulse width, and exceptional properties such as high coherence and continuously tunable wavelengths. These unique features have established FELs as a novel and powerful platform for exploring light-matter interactions, offering unprecedented capabilities in nonlinear physics and ultrafast processes research with high spatial and temporal resolution. The development of the Shanghai Free-Electron Laser (SXFEL) facility has significantly advanced these applications, particularly in studies of X-ray induced ultrafast dynamics.

Up to now, Shanghai Soft X-ray Free-Electron Laser (SXFEL) has achieved first lasering in 2021 and the Shanghai High repetition rate XFEL and Extreme light facility (SHINE) has entered its final phase. The AMO end-station at the Shanghai Soft X-ray Free-Electron Laser (SXFEL) has successfully completed commissioning and is now officially available for user experiments. This provides valuable experience and a solid foundation for the development, commissioning, and future operation of the SHINE-AMO end-station, which is dedicated to exploring ultrafast dynamics at the atomic and molecular level.

These developments present significant opportunities for researchers to investigate complex systems with unprecedented precision, paving the way for groundbreaking discoveries in atomic and molecular physics. The successful commissioning of the SXFEL's AMO end-station and the imminent completion of the SHINE facility underscore our development in advancing FEL-based research infrastructure for global scientific collaboration and innovation.

When: 2026-06-23, 14:00 - 14:45, Where: Eva von Bahr

O24 - The world of atoms at the attosecond time scale

AMO

Anne L'Huillier[1]
[1] Lund University

Abstract text: Attosecond pulses have enabled the study of photoionization of atoms and molecules in a completely new way. Using a synchronized probe field and interferometric measurements, it is possible to measure small time delays in photoionization and the phase change of an electron wavepacket across a Fano resonance. Recently, the use of multicolor probe fields has allowed us to perform the quantum state tomography of a photoelectron. This presentation will review advances in atomic physics enabled by attosecond techniques.

When: 2026-06-23, 10:15 - 10:35, Where: Sonja Lyttkens

O25 - Thermal Stability of DTDCTB Systems for Reliable Organic Solar Cells

AMO
Ambra Guarnaccio[1]
Cesare Grazioli[2], Teng Zhang[3], Fredrik Johansson[4], Iulia Brumboiu[5], Monica de Simone[2], Carla Puglia[4]
[1] CNR-ISM Italy
[2] CNR-IOM Italy
[3] Beijing Institute of Technology, China
[4] Uppsala University, Sweden
[5] Nicolaus Copernicus University in Toruń, Poland

Abstract text: Organic solar cells (OSCs) are promising alternatives to silicon-based photovoltaic cells due to their lower production costs, simpler fabrication processes, and compatibility with large-area and flexible substrates. However, their power conversion efficiency remains lower than that of conventional silicon technologies. In OSCs, solar energy conversion occurs within photoactive donor–acceptor (D–A) systems, typically composed of electron-rich (donor) and electron-deficient (acceptor) molecular units.

Efficient D–A systems can be designed by covalently linking triphenylamine (TPA)-based donor units with suitable acceptor counterparts. Such molecular engineering has significantly advanced photovoltaic performance and remains essential for further progress in the field.

In this study, the commercially available molecule 2-{[7-(5-N,N-ditolylaminothiophen-2-yl)-2,1,3-benzothiadiazol-4-yl]methylene}malononitrile (DTDCTB) and its constituent building blocks are investigated. DTDCTB features a donor–acceptor–acceptor (D–A–A) architecture, combining a TPA-based donor moiety, a benzothiadiazole acceptor, and a dicyanovinylene electron-withdrawing group. Particular attention is given to N,N-diphenylthiophen-2-amine (DPTA), where a thiophene ring enhances the electron-donating properties compared to conventional TPA systems.

The study aims to comprehensively characterize DTDCTB and its building blocks under different evaporation conditions using gas-phase synchrotron-based photoemission spectroscopy (PES), X-ray absorption spectroscopy (XAS), TGA/DTA under inert gas conditions, and FT-ATR analysis.

By integrating experimental results with theoretical simulations, this work provides detailed insight into the electronic structure and stability of the molecule, offering valuable knowledge for the development and implementation of advanced OSC materials.

When: 2026-06-24, 14:00 - 14:45, Where: Eva von Bahr

O26 - Title to be announced

AMO

Reinhard Dörner[1]
[1] Goethe University

Abstract text: To be added.

When: 2026-06-23, 09:55 - 10:15, Where: Sonja Lyttkens

O27 - Tuning interfacial charge transfer at PDI/Ag(111) interface through molecular functionalization

AMO

Giacomo Agnesod[1, 2], Simone Pistillo[3], Davide Piva[1, 2], Luca Schio[2], Luca Floreano[2], Daniele Toffoli[3], Alberto Morgante[1, 2], Albano Cossaro[2, 3], Giovanna Fronzoni[3], Martina Dell'Angela[2], Roberto Costantini[1, 2]
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Abstract text: Controlling electronic properties at organic/metal interfaces is fundamental to enhancing the efficiency of organic optoelectronic devices. In this work, we investigate the interfacial interactions of a π-conjugated monolayer of iPr-PDI on Ag(111), comparing it to its non-functionalized perylene diimide (PDI) derivative. Using a multi-technique approach, combining scanning tunneling microscopy (STM), X-ray photoemission and absorption (XPS, NEXAFS) and time-resolved two-photon photoemission (tr-2PPE), performed at the Elettra Synchrotron, and the support of Density Functional Theory (DFT) calculations, we characterize the impact of bulky 2,6-diisopropylphenyl (iPr) substituents on charge transfer and energy level alignment. Our results reveal that the iPr-functionalization at the imide sites induces an ordered herringbone arrangement featuring two distinct molecular configurations. Core-level spectra and DFT calculations identify two chemically inequivalent oxygen species, originating from a coexistence of different adsorption heights driven by steric interactions between the isopropyl groups. This structural divergence creates a heterogeneous electronic landscape: the LUMO of molecules closer to the Ag(111) surface is partially filled via substrate-to-molecule electron transfer, while the vertically displaced molecules remain electronically decoupled. In contrast to pristine PDI, this steric-driven decoupling significantly alters the energy level alignment and exciton dynamics at the heterointerface. Our findings demonstrate that while imide substitution is a powerful tool for engineering functional PDI self-assembly, it simultaneously induces local variations in interfacial charge transfer. Accounting for these substrate-mediated effects is critical for optimizing charge carrier dynamics in application-specific organic sensitized heterostructures.

A. Franco-Cañellas, *Phys. Rev. Materials*, 2017, **1**, 013001
Q. Yang, *Phys. Rev. B*, 2009, **80**, 115214

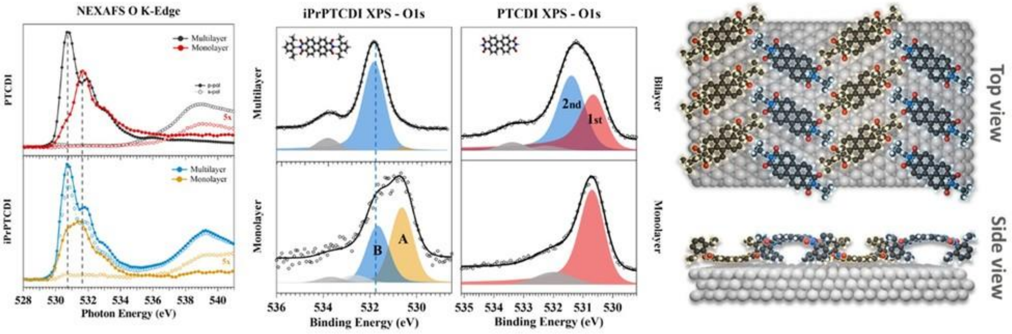


Figure: a) NEXAFS spectra of the organic overlayer (PDI on top and iPr-PDI at bottom) adsorbed on Ag(111) surface in both multilayer and monolayer configurations. b) O 1s XPS spectra of the molecular overlayers (PDI and iPr-PDI) at different thin film thicknesses. c) Atomistic model of the iPr-PDI monolayer on Ag(111) obtained with a DFT relaxation calculation.

When: 2026-06-23, 15:45 - 16:10, Where: Eva von Bahr

O28 - Ultrafast electron correlation dynamics in atomic krypton driven by HHG radiation

AMO

Andreas H. Roos[1], Eva Klimešová[2], Ltaief Ben Ltaief[3], Marcel Mudrich[4], Lucie Jurkovičová[2, 5], Ondrej Hort[2], Martin Albrecht[2], Matyáš Staněk[2, 5], Jaroslav Nejdl[2, 5], Jakob Andreasson[2], Maria Krikunova[2, 6]
[1] Department of Physics, University of Gothenburg, Origovägen 6B, 412 58, Gothenburg, Sweden
[2] ELI Beamlines facility, The Extreme Light Infrastructure ERIC, Za Radnicí 835, 252 41 Dolní Břežany, Czech Republic
[3] Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark
[4] Institute of Physics, University of Kassel, Kassel, 34132, Germany
[5] Czech Technical University in Prague, FNSPE, Břehová 7, 115 19 Prague 1, Czechia
[6] Technical University of Applied Sciences, Hochschulring 1, 15745 Wildau, Germany

Abstract text: The ELI Beamlines facility, part of the Extreme Light Infrastructure ERIC, provides high-power laser sources and laser-driven radiation for ultrafast science. At the high-harmonic generation (HHG) beamline, the MAC end-station serves as a versatile user platform for time-resolved studies of atomic and molecular dynamics. Combining monochromatized extreme ultraviolet (EUV) radiation with synchronized femtosecond near-infrared (NIR) pulses and advanced electron and ion spectroscopy, including coincidence detection, the station enables detailed investigations of ultrafast light-matter interactions.

We report time-resolved measurements of satellite-state dynamics in atomic krypton following excitation with single harmonics in the 29.6–35.9 eV range[1]. The EUV excitation populates Kr^{+*} satellite states, which are probed via NIR-induced ionization to Kr^{2+}. The transient Kr^{2+} yield exhibits a strong dependence on NIR intensity, enabling clear separation of sequential and non-sequential two-color double ionization pathways. By tuning the probe intensity, we demonstrate control over the relative contributions of these channels (see Figure 1). At low intensities, oscillatory features attributed to quantum beating between coherently excited satellite states are observed, while at higher intensities these oscillations are suppressed. The measurements also provide access to relaxation dynamics associated with doubly excited decay channels.

Recent developments extend the experimental capabilities using electron-ion coincidence detection. Measuring electrons and ions simultaneous, energy-resolved information on emitted electrons and final ionic states can be obtained, enabling direct mapping of the ionization pathways. This approach provides a detailed energy-resolved insight of the ultrafast dynamics and the competing processes in multi-electron systems.

[1] A. Roos et al., New J. Phys. **25**, 013038 (2023).

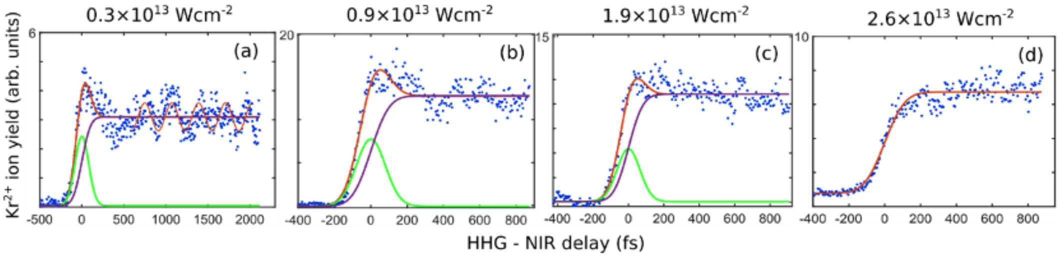


Figure 1: Transient Kr^{2+} ion yield as a function of XUV–NIR delay at a photon energy of 32.8 eV for different NIR intensities: (a)-(d). Blue dots represent the experimental data. Green lines show the fitted non-sequential ionization contribution, while purple lines correspond to the fitted sequential ionization. Red lines indicate the total fit to the transient signal, and the orange line in (a) highlights oscillations in the transient signal attributed to quantum beating, obtained from Fourier analysis.

Coincidences

When: 2026-06-25, 15:20 - 15:45, Where: Heinz-Otto Kreis

O29 - Tracking Ultrafast Charge-Transfer and Electron-Transfer-Mediated Decay Dynamics in Weakly Bound Systems

Coincidences

Florian Trinter[1]
[1] Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Abstract text: When electronically excited atoms or molecules are embedded in a chemical environment, they can relax via nonlocal decay pathways where neighboring species donate or accept energy or electrons. Processes such as electron-transfer-mediated decay (ETMD) and sequential charge-transfer (CT) events are governed by coupled electronic and nuclear dynamics that control efficiency and outcomes [1].

Here, we combine multi-particle coincidence detection [2] following site-selective synchrotron photoionization with ab initio calculations [3] to investigate ultrafast charge redistribution and decay in weakly bound systems. Tracking electron and nuclear motion in real space and time, we resolve coupled dynamics.

For a loosely bound triatomic system, we show that ETMD is strongly coupled to nuclear motion, with transient geometries favored at different decay times. The dynamics reveal roaming-like behavior prior to decay, offering an intuitive picture of nonlocal electronic relaxation [4].

For a heteronuclear dimer with covalent and van der Waals interactions, we resolve sequential CT events during fragmentation. Structural evolution triggers electron transfer, including back-and-forth charge flow mediated by nonadiabatic transitions via conical intersections [5].

Together, these results demonstrate how controlled model systems enable direct observation of coupled electronic and nuclear dynamics, providing insight into nonadiabatic reaction pathways and charge-transfer processes in complex environments.

[1] T. Jahnke et al., Chem. Rev. 120, 11295-11369 (2020).
[2] R. Dörner et al., Phys. Rep. 330, 95-192 (2000).
[3] J. Hofierka et al., J. Chem. Theory Comput. 21, 12026-12033 (2025).
[4] F. Trinter et al., J. Am. Chem. Soc. 148, 4126-4135 (2026).
[5] R. Dong et al., arXiv:2511:14201 (2026).

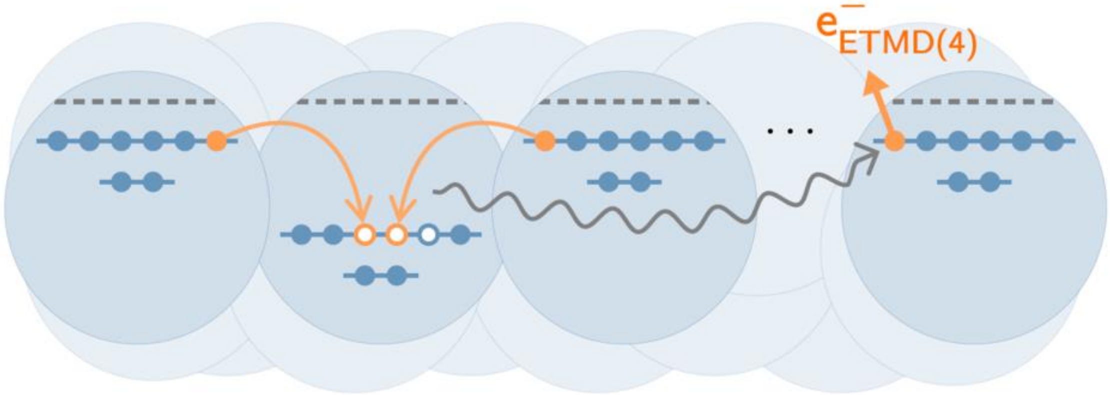
When: 2026-06-25, 14:55 - 15:20, Where: Heinz-Otto Kreis

O30 - X-ray-induced charge and energy transfer processes in atomic clusters studied by electron-photon coincidence spectroscopy

Coincidences

Andreas Hans[1]
[1] Universität Kassel

Abstract text: Over the last decades it has been discovered and intensively investigated that atoms and molecules, which have been excited and/or ionized by X-rays, can relax by interacting with their environment. Interatomic processes like Interatomic Coulombic Decay (ICD) and Electron-Transfer-Mediated Decay (ETMD) are autoionization mechanisms of extended systems, which crucially influence the final distribution of charge and energy in a quantum system upon photon absorption. They were found to proceed on ultrafast time scales and may be dominant decay channels if certain conditions are met. Also slower, radiative non-local channels like Radiative Charge Transfer (RCT) can play an important role. For the experimental investigation of such mechanisms in atomic clusters with a particular focus on the competition between photon and electron emission, we developed a scheme for the routine measurement of electrons and visible and ultraviolet photons in coincidence. It enables the observation of decay cascades including both non-radiative and radiative transitions with unprecedented sensitivity. Here, we will give an overview of recent results including examples like long-range ICD or collective ETMD(4) (cf. figure).



Correlated Materials

When: 2026-06-25, 11:40 - 12:05, Where: Heinz-Otto Kreis

O31 - Charge density waves in quantum materials

Correlated Materials

Yeongkwan Kim[1]
[1] Korea Advanced Institute of Science and Technology

Abstract text: The charge density wave (CDW), the ununiform distribution of itinerant charge density, has been found and studied in various low-dimensional systems for decades. Despite extensive investigations, the many characteristics of CDW remain unknown; a microscopic mechanism other than the Pierls instability is required, and how CDW intertwines with other competing phases, particularly with the superconductivity, should be investigated. Furthermore, the recent compelling evidence has cast light on the unexpected aspect of CDW, additional symmetry breakings that accompany or occur concurrently with the CDW transition. In this talk, I will discuss various aspects of CDWs in different quantum materials, i) the additional symmetry breaking in CDW phase of 1T-$TiSe_2$ and CsV_3Sb_5 systems, which are footprinted in the intensity of angle-resolved photoemission spectroscopy, ii) the possible role of CDW fluctuation on Cooper pairing, which is accomplished by analyzing the low-energy electronic structure of 2H-$TaSe_2$.

When: 2026-06-23, 14:55 - 15:20, Where: Heinz-Otto Kreis

O32 - Nodal metal and interlayer coupling in multilayer cuprate superconductors

Correlated Materials

Shin-ichiro Ideta[1]
[1] Research Institute for Synchrotron Radiation Science, Hiroshima University, Higashi-Hiroshima, Japan

Abstract text: In multilayer cuprates, the maximum T_c occurs at the numebr of CuO_2 plane (n) of $n = 3$ (triple-layer) in all cuprate families. In $n \geq 5$ systems, antiferromagnetic (AFM) order has been confirmed bu NMR, and ARPES studies have shown small hole Fermi pockets in the inner CuO_2 planes as a result of AFM band folding. Here, we report ARPES data of the triple-layer cuprates Bi2223 over a wide doping range covering from underdoped to overdoped samples, all of which are superconducting (SC) although the doping level of the inner CuO_2 plane becomes extremely low in underdoped samples. Furthermore, the *d*-wave superconducting gap of the inner CuO_2 plane is enhanced to an unprecedentedly large value of nodal gap $\Delta_0 \sim$ 80-100 meV, and persisted up to $\sim 1.5T_c$ without the appearance of a Fermi arc, indicating a robust *nodal metal*. We attribute the nodal-metallic behavior to the unique local environment of the inner CuO_2 plane in the triple-layer cuprates, sandwiched by optimally-doped two outer CuO_2 planes and hence subject to strong proximity effect from both sides. Such a situation is realized only in triple-layer cuprates, and explains why the T_c reaches the maximum at $n = 3$ in every cuprate family [1].

[1] S. Ideta *et al.*, Nat. Commun. **16**, 9470 (2025).

O33 - Observation of saddle-loop band structure in Pt(Bi,Se)2 by high-resolution ARPES

Correlated Materials

Yusei Morita[1]
Kosuke Nakayama[1], Naohiro Ito[2], Takemi Kato[3], Tomonori Nakamura[4], Hongyun Zhang[3, 5], Xiao Tang[5], Tianyun Lin[5], Koki Yanagizawa[1], Seigo Souma[3, 6], Sebun Masaki[7], Takumi Ikushima[7], Yuto Moriyasu[7], Kenta Hagiwara[8], Fumihiko Matsui[8, 9], Kiyohisa Tanaka[8, 9], Kenichi Ozawa[10], Daisuke Shiga[11], Hiroshi Kumigashira[11], Masaki Maeda[7], Yasuhiro Niimi[7, 12], Takanori Kida[13], Masayuki Hagiwara[13], Timur K. Kim[14], Cephise Cacho[14], Takashi Takahashi[1], Yoshinori Okada[4], Shuyun Zhou[5], Takashi Koretsune[1], Kazutaka Kudo[7, 12], Takafumi Sato[1, 3, 6, 15, 16]
[1] Department of Physics, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan
[2] Toyota Central R&D Labs., Inc., Nagakute 480-1192, Japan
[3] Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, Sendai 980-8577, Japan
[4] Okinawa Institute of Science and Technology Graduate University, Okinawa 904-0495, Japan
[5] State Key Laboratory of Low Dimensional Quantum Physics and Department of Physics, Tsinghua University, Beijing 100084, P. R. China
[6] Center for Science and Innovation in Spintronics (CSIS), Tohoku University, Sendai 980-8577, Japan
[7] Department of Physics, Graduate School of Science, Osaka University, Toyonaka 560-0043, Japan
[8] UVSOR Synchrotron Facility, Institute for Molecular Science, Okazaki 444-8585, Japan
[9] School of Physical Sciences, The Graduate University for Advanced Studies (SOKENDAI), Okazaki 444-8585, Japan
[10] Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki 305-0801, Japan
[11] Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Sendai 980-8577, Japan
[12] Institute for Open and Transdisciplinary Research Initiatives, Osaka University, Suita 565-0871, Japan
[13] Center for Advanced High Magnetic Field Science, Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan
[14] Diamond Light Source, Harwel Science and Innovation Campus, Didcot, Oxfordshire OX11 0QX, UK
[15] International Center for Synchrotron Radiation Innovation Smart (SRIS), Tohoku University, Sendai 980-8577, Japan
[16] Mathematical Science Center for Co-creative Society (MathCCS), Tohoku University, Sendai 980-8578, Japan

Abstract text: Exploiting electronic singularities to drive emergent quantum phenomena is a key basis in condensed matter physics, yet this powerful strategy has been largely limited to two dimensions, leaving the potential of three-dimensional materials often inaccessible. A “saddle-loop” singularity—a one-dimensional ring of saddle points—has been proposed as a way to extend the concept of van Hove singularities to three-dimensional electron systems (Fig. 1), but has remained experimentally elusive. Here, we provide the direct experimental evidence for the saddle-loop singularity in $Pt(Bi_{1-x}Se_x)_2$, using angle-resolved photoemission spectroscopy. We also demonstrate its functional role by showing that the superconducting critical temperature is maximized when the

saddle loop is tuned to the Fermi level. Furthermore, our advanced theoretical calculations reveal that the saddle loop originates from inter-orbital hybridization, establishing a generalizable design concept. Our findings demonstrate a viable mechanism for realizing singular electronic states in three-dimensional electron systems, providing a platform to investigate correlation-driven phenomena in three dimensions.

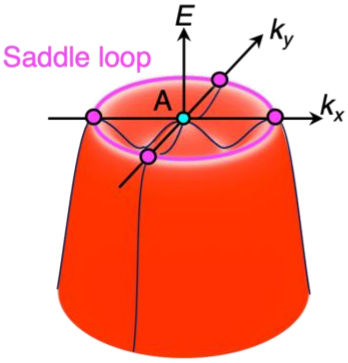


Fig. 1 : Band dispersion in the k_x-k_y plane, featuring the saddle-loop structure (magenta line/point) identified in this study.

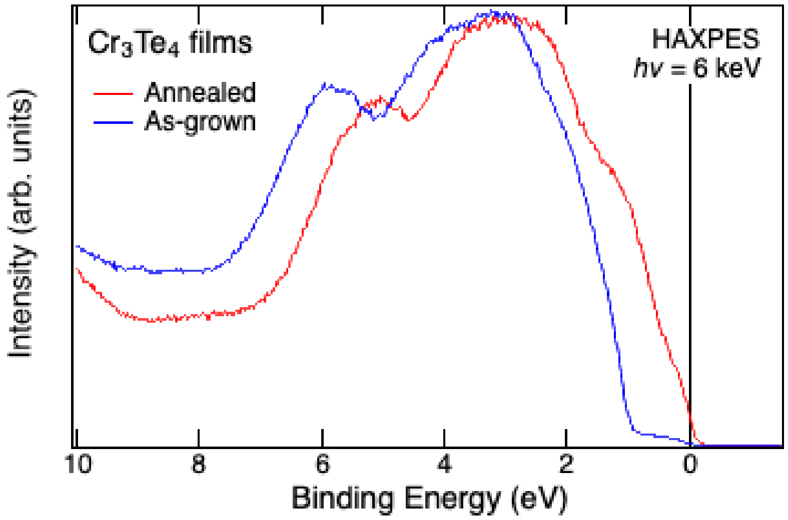
When: 2026-06-23, 15:45 - 16:05, Where: Heinz-Otto Kreis

O34 - p-d Hybridized Valence-Band Structure Induced by Intercalation Ordering in van der Waals Ferromagnet Cr3Te4

Correlated Materials

Masaki Kobayashi[1]
Kanta Endo[2], Kosuke Takiguchi[1], Tom Ichibha[3], Kenta Hongo[3, 4], Yoshitaka Taniyasu[1], Masaki Nakano[5]
[1] Basic Research Laboratories, NTT, Inc.
[2] Department of Applied Physics, the University of Tokyo
[3] School of Information Science, JAIST
[4] Research Center for Advanced Computing Infrastructure, JAIST
[5] College of Engineering, Shibaura Institute of Technology

Abstract text: Van der Waals ferromagnet $Cr_{1+\delta}Te_2$ consists of layered $CrTe_2$ with additional self-intercalated Cr ions. Its magnetic properties strongly depend on the intercalation concentration d and the ordering of intercalated Cr ions. In particular, post-growth annealing of an as-grown Cr_3Te_4 ($\delta = 1/2$) thin film alters the magnetic easy axis from perpendicular to in-plane directions, where the annealing is expected to evaporate excess Te and increase the degree of ordering of the intercalant. In this study, we have performed hard X-ray photoemission spectroscopy (HAXPES) to elucidate the electronic states of Cr_3Te_4 thin films with varying annealing temperature (T_A). With increasing T_A, the peak positions of the Te core-level spectra show blue shifts, while those of the Cr spectra remain nearly unchanged. While the valence-band spectrum of the as-grown sample has weak density of states near the Fermi level (E_F), the band width of the valence band that is mainly comprised of Te 5*p* orbital becomes drastically wider with increasing T_A above 400°C. The valence bands of the annealed films cross E_F with relatively large density of states to that with the as-grown film. Density functional theory (DFT) calculation reveals that the density of states near E_F mainly arises from the Cr 3*d* band and the Te 5*p* band shows blue shift with increasing the dimensionality of CrTe compounds. Based on the findings, the modification of the valence-band structure is attributed to the hybridization between the Te 5*p* band and intercalated Cr 3*d* orbital induced by the intercalation ordering.



When: 2026-06-23, 15:20 - 15:45, Where: Heinz-Otto Kreis

O35 - Phase transitions in VO2 and related compounds: surprises and resolutions

Correlated Materials

D. D. Sarma[1, 2]
[1] Solid State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru 560012, India
[2] Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Abstract text: Materials in which sudden changes in conductive properties can be induced by external stimuli have attracted attention for decades under the broad heading of metal-insulator transition. An iconic example is vanadium dioxide, VO_2. Its metal-insulator transition at $T_c = 340$ K has been rationalized in terms of the accompanying structural transition (rutile-to-monoclinic, R-M1) below which all vanadium atoms pair into dimers, and electronic correlations promote a non-local spin-singlet insulating state. It is also known that the structural aspects and phase transition of pure VO_2 can be intriguingly influenced by small (<10%) doping with various elements, such as Al, Cr, and Fe. In addition, VO_2 can also exist in many polymorphs besides the most commonly occurring form of R and M1 mentioned above. Together, these VO2-derived variants encompass a fascinating range of physical phenomena that challenge our understanding of structure-property relationships and metal-insulator transitions. Following an introduction to what we already know, I shall present some of our recent works that underline the surprises of this family of compounds and explain our attempts to understand them.

When: 2026-06-25, 10:20 - 10:40, Where: Heinz-Otto Kreis

O36 - Single domain spectroscopic signatures of a magnetic Kagome metal

Correlated Materials

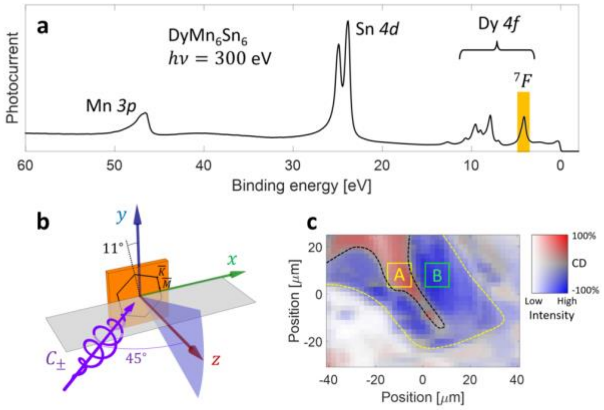
L. Plucinski[1]
G. Bihlmayer[1], Y. Mokrousov[1], Yishiu Zhou[1], Yixi Su[1], A. Bostwick[2], C. Jozwiak[2], J. Denlinger[2], E. Rotenberg[2], D. Usachov[3], C. M. Schneider[1]
[1] Forschungszentrum Juelich GmbH, Juelich, Germany
[2] LBNL, Berkeley, United States
[3] DIPC, San Sebastian, Spain

Abstract text: Spin- and orbital-resolved access to the electronic bands is necessary to establish key properties of quantum materials such as the quantum-geometric tensor. Despite the recent revival of interest in magnetic Kagome compounds, no spectroscopic access to their magnetic properties has been available so far due to small domain sizes and the lack of appropriate techniques. Furthermore, their real-space magnetic texture is often complex and temperature-dependent.

We investigate the magnetic Kagome metal $DyMn_6Sn_6$ using high-resolution micro-focused circular-dichroic angle-resolved photoemission (μ-CD-ARPES) to probe its magnetic and electronic properties. By tuning the kinetic energy to various features of the Dy *4f* multiplet, we resolve magnetic domains in samples cryo-cooled down to 20 K. Smaller, but clear, signatures are also detected in the Mn *3p* levels. The behavior of both Dy *4f* and Mn *3p* features is in remarkable agreement with our modeling based on the Hartree–Fock method, revealing ferrimagnetic alignment of Dy and Mn local moments and further strengthening our interpretation.

Adjusting the energy to the Mn *3d*-dominated valence bands reveals signatures that we relate to the orbital magnetization through comparison with *ab initio* electronic structure calculations. Our study establishes spectroscopic access to a single magnetic domain in a Kagome metal and demonstrates μ-CD-ARPES as a direct probe of magnetic domain properties, opening the way for spatially resolved studies of complex magnetic phases in quantum materials.

Reference: arXiv:2507.12085 (2025); accepted for publication in Nature Communications.



a XPS spectrum of $DyMn_6Sn_6$ at $h\nu = 300$ eV at 20K. **b** Experimental geometry. **c** Micrograph of the cleaved surface highlighting magnetic domains A and B, using circular dichroism at the ^7F feature of the Dy *4f* multiplet. Data measured at the nanoARPES branch of the MAESTRO beamline at ALS.

When: 2026-06-25, 09:55 - 10:20, Where: Heinz-Otto Kreis

O37 - Spin and charge order as contrast mechanism in space and time.

Correlated Materials

Martin Beye[1, 2]
Anton Harrer[1], Safiya Ahsan[1], Simon Marotzke[2, 3], Anton Tremsin[4], Jörg Schwenke[5], Christian Schüssler-Langeheine[6]
[1] Fysikum, Stockholm University, Stockholm, Sweden
[2] Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany
[3] Universität Kiel, Kiel, Germany
[4] Space Science Laboratory, University of California, Berkeley, USA
[5] MAX IV Laboratory, Lund, Sweden
[6] Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Abstract text: Functionality of complex quantum materials can be found in local order of fundamental degrees of freedom, like spin, charge and orbital occupation. Such order can be exquisitely probed by resonant soft X-ray scattering (RSXS). Using RSXS as contrast mechanism for real-space imaging as well as for X-ray photon correlation spectroscopy (XPCS) opens avenues to connect real-space structures, domains and pinning sites with domain dynamics and phase transition behaviour.

In this presentation, I will show recent results using XPCS on different samples with a new Timepix-based detector to achieve nanosecond temporal resolution of domain dynamics, limited only by the coherent flux of current X-ray sources. Using transmission zone plates as lens elements allows to image domains in real-space and I demonstrate results with resolutions far below the micrometer regime, which resolves domain patterns and shows the relation to pinning induced by surface preparation or sample growth. Correlating both modalities allows for a deeper understanding of materials and opportunities to tune the functionality for specific needs.

When: 2026-06-25, 11:15 - 11:40, Where: Heinz-Otto Kreis

O38 - Ultrafast dynamics in charge density wave materials studied by optical and photoemission spectroscopy techniques at the T-ReX facility

Correlated Materials

Wibke Bronsch[1]
Manuel Tuniz[2], Denny Puntel[2], Francesco Sammartino[2], Fulvio Parmigiani[1, 2], Federico Cilento[1]
[1] Elettra-Sincrotrone Trieste S.C.p.A., Trieste, Italy
[2] Department of Physics, Università degli Studi di Trieste, Trieste, Italy

Abstract text: The combination of time-resolved optical and photoemission spectroscopy techniques allows for gaining complementary insights in a materials response to optical excitation. In striving towards a better understanding of the fundamental processes underlying the physics of charge density wave (CDW) systems, this combination of techniques turns out to be a powerful tool. In CDW systems periodic lattice distortions and electronic structure modifications are simultaneously occurring below a critical temperature. Whereas with optical spectroscopy we are getting access to the investigation of the phonon modes related to the CDW phase, angle-resolved photoemission allows us to map the samples band structure. In this talk I am aiming for introducing the T-ReX user facility for ultrafast table-top time-resolved spectroscopies [1-4] developed at FERMI, Elettra-Sincrotrone Trieste, while discussing recent results acquired on different CDW systems [5-7].

[1] https://www.elettra.eu/labs/t-rex.html
[2] S. Peli *et al.*, J. Electron Spectrosc. Relat. Phenomena **243**, 146978 (2020).
[3] R. Cucini *et al.*, Structural Dynamics **7**, 014303 (2020).
[4] M. Perlangeli *et al.*, Optics Express **28**, 8819 (2020).
[5] W. Bronsch *et al.*, Faraday Discussions **237**, 40 (2022).
[6] W. Bronsch *et al.*, Phys. Rev. B **111**, 125102 (2025).
[7] M. Tuniz *et al.*, Commun. Mater. **6**, 243 (2025).

When: 2026-06-25, 12:05 - 12:25, Where: Heinz-Otto Kreis

O39 - Visualizing strain-tuned insulator-metal transition in 1T-TaS2 using micro-ARPES

Correlated Materials

Shuto Suzuki[1], Kosuke Nakayama[1], Koki Yanagizawa[1], Katsuaki Sugawara[1, 2, 3], Seigo Souma[3, 4], Kenichi Ozawa[5], Syunichi Takano[1], Takashi Takahashi[1], Tsutomu Nojima[2, 6], Keiji Ueno[7], Takafumi Sato[1, 3, 4, 8, 9]
[1] Department of Physics, Graduate School of Science, Tohoku University, Sendai, Japan
[2] Precursory Research for Embryonic Science and Technology (PRESTO), Japan Science and Technology Agency (JST), Tokyo, Japan
[3] Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, Sendai, Japan
[4] Center for Science and Innovation in Spintronics (CSIS), Tohoku University, Sendai, Japan
[5] Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), Tsukuba, Japan
[6] Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
[7] Department of Chemistry, Saitama University, Saitama, Japan
[8] International Center for Synchrotron Radiation Innovation Smart (SRIS), Tohoku University, Sendai, Japan
[9] Mathematical Science Center for Co-creative Society (MathCCS), Tohoku Universit, Sendai, Japan

Abstract text: The nature of the insulating state in the layered dichalcogenide 1T-TaS_2, which is long regarded as a correlation-driven Mott insulator, has recently been reinterpreted as a band insulator arising from interlayer dimerization. This shift in understanding highlights the critical role of stacking order and raises a fundamental question: can we engineer novel electronic phases by actively tuning interlayer coupling?

In this study, we address this by visualizing the strain-tuned electronic phases in 1T-TaS_2 using micro-focused angle-resolved photoemission spectroscopy (micro-ARPES) combined with first-principles calculations. Figure 1(a) shows the band dispersion of unstrained 1T-TaS_2 measured in the low-temperature charge density wave (CDW) phase ($T = 40$ K). At higher binding energies, we observe S 3p-derived hole bands centered at the Γ point, alongside multiple Ta 5d-derived bands near the Fermi level (E_F). These Ta 5d bands form an energy gap at E_F, reflecting the insulating nature of the system. Upon applying uniaxial strain, our measurements reveal that this energy gap collapses and the Ta 5d bands cross E_F [Fig. 1(b)], directly demonstrating a strain-induced insulator-to-metal transition.

We demonstrate that this emergent metallic phase is driven by a strain-induced rearrangement in the interlayer stacking of the Star-of-David charge order, effectively disrupting the interlayer dimerization. Our micro-ARPES study thus establishes uniaxial strain as a powerful tool for manipulating interlayer coupling, opening new pathways for exploring hidden quantum phases in two-dimensional materials.

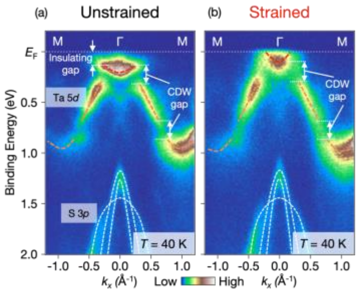


Fig. 1: ARPES intensity of 1T-TaS_2 measured at $T = 40$ K for the unstrained (a) and strained (b) phases, respectively.

Energy materials

When: 2026-06-22, 16:05 - 16:25, Where: Sonja Lyttkens

O40 - Combining experimental design and software based image recognition for op-erando APXPS electrode/electrolyte interface potential probing

Energy materials

Qianhui Liu[1]
Laura King[1], Helena Wagner[2], Tove Ericson[1], Robert Temperton[3], Maria Hahlin[1, 2]
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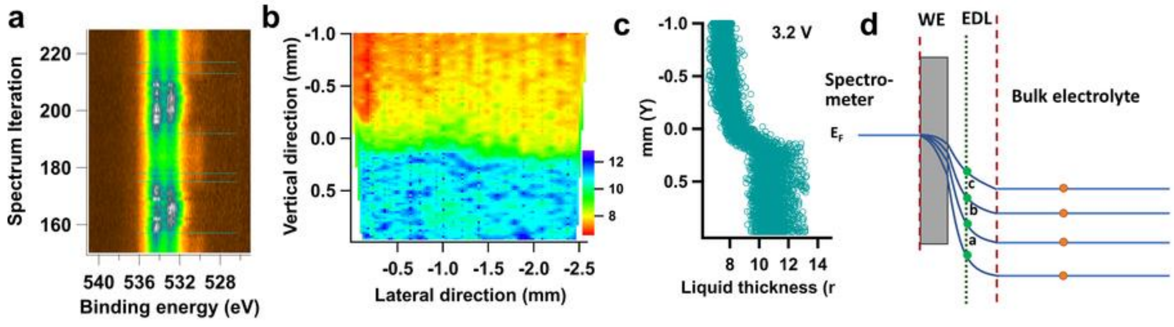
Abstract text: Probing the electrode/electrolyte interface with operando ambient pressure X ray photoelectron spectroscopy in the dip-and-pull setup remains large challenges on 1) mataining stable electrolytes under their vapor pressure, 2) probing an interface region with a liquid layer thinner than the XPS probing depth, in the meantime, with sufficient electrochemical acitivity. Apart from the fundamental challenges, the temporal and spatial variation of liquid layer, and irradiation effect amplifies the difficulties of the eperiements.

In this work, an efficient interface probing methodology is realized through experimental design combined with advanced data processing. Scanning APXPS is employed with programmed route periodically probing across the dry-wet boundary near the top edge of the liquid layer to capture the interface spectroscopic feature (Figure 1a). To distinguish and select the interface-featured spectra from the mixed signals, software based spectroscopic recognition are developed including 1) intensity attenuation recognition which distinguish the interface-featured spectra from the intensity attenuation pattern of the electrode/electrolyte peaks, and 2) potential recognition which distinguishes the BE shift pattern over the height in the meniscus. Further by translating the relative spectral intensities into liquid thickness, a spectro-microscopic image of the liquid distribution (Figure 1b, c) with topographical resolution is obtained. Combining with the spectral energies and chemical distribution information, it sees strong correlation between the energetics and the liquid layer thickness of the probing position, which is suggested to do with the EDL potential drop (Figure 1d). In addition, the lithiation/delithiation of the electrode further affects the BE shifts in the spectra.



When: 2026-06-26, 09:55 - 10:15, Where: Sonja Lyttkens

O41 - Enantio-differentiation and observation of parity-breaking electronic hybridization in chiral ferroelectric oxide NbOI2

Energy materials

Keisuke Fukutani[1, 2]
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Abstract text: A broken-symmetry state of matter, called chirality, has recently been shown to manifest itself in a wide spectrum of novel properties, leading to the renewed fundamental understandings on the electronic properties and structural dynamics of matters. In particular, the chiral structural asymmetries are shown to induce distinct orbital-angular-momentum textures in electronic systems and pseudo angular momentum in phononic systems. The former can lead to the emergence of chiral fermions, as well as so-called orbital Hall effects, and the latter, known as chiral phonons, have been reported to participate in novel interplay with electronic spins as well as photon helicities.

In this study, we utilize angle-resolved photoemission circular dichroism (CD-ARPES) to probe the impacts of broken symmetry in a chiral ferroelectric oxide $NbOI_2$. As shown in Fig. 1, our results demonstrate that even sub-angstrom atomic displacements in this material give rise to pronounced enantio-specific circular dichroisms in a manner fully consistent with the theoretical expectations, thereby demonstrating its strong sensitivity in differentiating the handedness of chiral crystals. Furthermore, we demonstrate that the electronic chirality, generated by the parity-breaking hybridization can be quantified by the intensity-normalized photoemission circular dichroism, which serves as an order parameter for small symmetry breaking. Our findings not only demonstrate the strength of CD-ARPES as an effective tool for unambiguous enantio-differentiation, but also provides a methodology for quantifying the electronic symmetry breaking leading to materials' chirality.

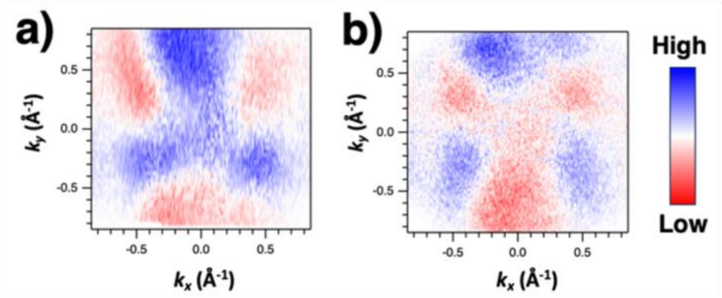

Figure 1: Results of our CD-ARPES measurements for two samples of $NbOI_2$ shown in (a) and (b). The equienergy surface was sliced at the binding energy of 1.85 eV, near the valence band maximum. The measurements were performed at UVSOR BL5U with $h\nu = 54$ eV at $T = 300$ K

When: 2026-06-22, 14:25 - 14:45, Where: Sonja Lyttkens

O42 - Ni doped NbSe2 Nanosheets as Effective Catalyst for Electrochemical Urea Oxidation Reaction (UOR)

Energy materials

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Sameer Sapra[1]
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[2] Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Abstract text: Modulating the electronic structure of transition metal dichalcogenides (TMDs) through heteroatom doping is a promising strategy to enhance their catalytic performance. In this context, nickel (Ni) serves as an ideal dopant owing to its ability to exist in stable higher valent oxidation states and to provide catalytically active species for the urea oxidation reaction (UOR). In this work, we report Ni doping in $NbSe_2$ nanosheets resulting in formation of $Ni_xNb_{1-x}Se_2$ NSs with x = 0, 0.05, and 0.10 successfully synthesized via a hot injection colloidal route. Structural analysis using X ray diffraction (XRD) and Raman spectroscopy reveals lattice distortion arising from the substitutional incorporation of Ni into Nb sites, which is further corroborated by X ray absorption spectroscopy (XAS) collected at the Nb K-edge. X ray photoelectron spectroscopy (XPS) studies confirms the formation of additional intrinsic defects upon Ni doping, in agreement with electron paramagnetic resonance (EPR) results. The electrocatalytic performance of the $Ni_xNb_{1-x}Se_2$ nanosheets was evaluated for the urea oxidation half-cell reaction. Pristine $NbSe_2$ exhibits limited UOR activity, whereas Ni incorporation markedly enhances catalytic efficiency. This improvement is attributed to the synergistic effect between Ni dopants and high valent Nb species, which collectively facilitate charge transfer and increase the density of active sites. The study demonstrates that controlled Ni doping is an effective strategy to modulate the electronic structure and catalytic performance of $NbSe_2$ based transition metal dichalcogenides for energy conversion applications.

When: 2026-06-22, 15:45 - 16:05, Where: Sonja Lyttkens

O43 - Pentacene-like Frontier Orbitals : revisiting NEXAFS exploitation

Energy materials

Nadine Witkowski[1], Noemi Vannucchi[1, 2], Fredrik O. L. Johansson[2], Ludovic Salvagnac[3], Jean-Baptiste Doucet[3], Ruslan Ovsyannikov[4], Erika Giangrisostomi[4], Mathieu G. Silly[5], Isabelle Séguy[3], Andrej Jancarik[6]
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[6] Centre de Recherche Paul Pascal,CRPP ,UMR5031,Université de Bordeaux, CNRS,F-33600 Pessac, France

Abstract text: In the present study, we unveil the electronic structure of the highest occupied and lowest excited unoccupied molecular frontier orbitals of semiconducting bisacene thin films elaborated from a liquid ink. Thin films of angular fused bisacenes, namely pentaceno-pentacene, pentaceno-hexacene and hexaceno-hexacene are obtained after the thermal conversion of the spin coated thin films prepared from highly concentrated ink of precursor molecules. Thus, by a combination of electron spectroscopies, namely valence band photoemission and near edge X-ray absorption fine structure spectroscopy, we are able to characterize the occupied and excited unoccupied density of state of the molecular frontier orbitals. We demonstrate that, under specific assumption, it is possible to combine valence band spectra and absorption spectra relatively to the Fermi level and derive the transport gap of angular fused bisacene films relatively to that of pentacene. Both, the electronic structure of the frontier orbitals and the transport gap of a pentaceno-pentacene film are found alike as evaporated pentacene film. This demonstrates that, in thin film, the delocalized character of the electrons along the angular fused bisacene is limited to the acene sub-unit and adopt the pentacene electronic structure. Because of the high solubility of the bisacene precursors, it can be forseen as a promising alternative for pentacene precursor which exhibits poor solubility.

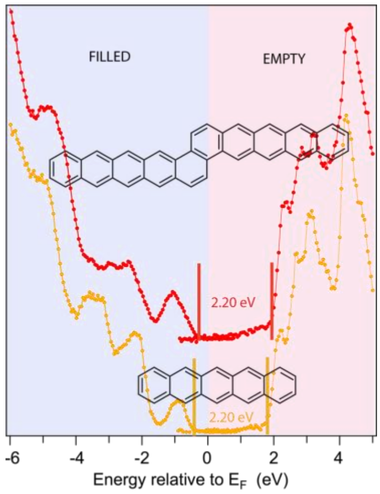

Fig.: Combined valence band photoemission spectra (filled states) and NEXAFS spectra (empty states) plotted relatively to Fermi energy

When: 2026-06-22, 14:00 - 14:25, Where: Sonja Lyttkens

O44 - Shining a Light on the Dynamic Surface State of Cu-based Single-Atom Alloys Using Ambient Pressure X-ray Photoelectron Spectroscopy

Energy materials

Iradwikanari Waluyo[1]
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Abstract text: Single-atom catalysts (SACs) have recently attracted significant attention due to their excellent catalytic properties combining the atomic efficiency of isolated active sites with unique chemical and electronic properties that distinguish them from conventional bulk or nanoparticle counterparts. A type of SAC called single-atom alloy (SAA) is composed of a dilute amount of a catalytically active noble metal (e.g. Pd, Pt, Rh) atomically dispersed in the surface of a more inert host metal (e.g. Cu, Ag, Au). The synergistic interactions between the dopant and host metal atoms result in bifunctional catalysts that deviate from the typical scaling relationships that govern catalytic activity. Synchrotron-based ambient pressure X-ray photoelectron spectroscopy (AP-XPS) experiments have revealed how the surface chemical state of Cu-based SAA model systems with Pt and Rh dopants dynamically evolve under reaction conditions, thus revealing property-structure-reactivity relationships important in catalysis. Pt and Rh dopants interact differently with CO molecules, resulting in starkly different adsorption configurations and CO-induced atomic mobility. We also found significant differences in how Pt and Rh either promote or hinder O_2 dissociation and H_2 activation depending on the structural arrangements of the dopant with respect to the host. In addition, structural heterogeneities of the Cu host metal surface were found to significantly impact the dopant alloying sites, which subsequently alter surface chemical reactivity. Our in-situ research using AP-XPS revealed how such a small amount of dopant metal can have an outsize impact on reactivity, with important implications in various catalytic reactions.

When: 2026-06-26, 10:15 - 10:35, Where: Sonja Lyttkens

O45 - Studying Laser Induced Ion Migration In Perovskite Single Crystals Using X-Ray Photoelectron Spectroscopy

Energy materials

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[3] Department of Chemistry, University of A Coruña, A Coruña, Spain

Abstract text: Lead halide perovskites have shown tremendous potential within photovoltaic applications, due to their multifunctional properties as well as the tunability of the bandgap through compositional change of the material. However, these materials have also shown to succumb to degradation when exposed to external stress, such as heat and illumination, which includes migration of ions. Thus, for these materials to be commercially applicable in for example solar cells, these challenges need to be addressed.

In this presentation I will show how we use X-ray Photoelectron Spectroscopy (PES) at synchrotron facilities to study the ion movement in mixed halide perovskites under illumination. By using an X-ray beam with low enough flux, we could ascertain that the X-rays themselves were not inducing any changes to the materials. Thus, we could perform PES, while additionally applying a 515 nm laser to see how visible light induces ion migration.

Studying $MAPbI_3$, $MAPbBr_3$, $MAPbBr_{3-x}I_x$ and $MAPbBr_{3-y}I_y$ single crystals (where x and y indicate different ratios of the two halides) using the above-mentioned setup, we saw that the laser induces ion migration of the two halides over time, indicating that bromide migrates toward the surface of the material, while iodide moves toward the bulk. This process is partially reversible when the laser is turned off, indicating a level of self-healing within the perovskite.

When: 2026-06-26, 11:55 - 12:15, Where: Sonja Lyttkens

O46 - Understanding corrosion of TiCN in acidic and alkaline environments: a route to produce corrosion resistant coatings

Energy materials

Chaimaa Fikry[1]
Varun Raj Damerla[1], Juliana Kessler[2], Erik Lewin[2], Leif Nyholm[2], Rebecka Lindblad[1]
[1] X-Ray Photon Science, Department of Physics and Astronomy, Uppsala University, Sweden
[2] Inorganic Chemistry, Department of Chemistry, Uppsala University, Sweden

Abstract text: Titanium carbonitride (TiCN) can play a significant role as a coating material for bipolar plates (BP) in fuel cells, due to its high corrosion resistance and conductivity. These components are situated between Membranes Electron Assembly (MEA), where the oxido-reduction reactions take place. This harsh environment makes it difficult for BP to ensure their performance over time, hence the need of a corrosion resistant protective coating. For this purpose, further information on the corrosion of TiCN are needed. In this study, we accelerate the corrosion reaction via electro-chemical treatement in acidic and alkaline conditions, to simulate the harsh environment in a MEA.

By performing electrochemical and XPS measurements using the dip-and-pull method within the same ambient-pressure chamber, we have followed the evolution of the passive film over a de-fined potential range. Each current step can be directly correlated with a corresponding oxidation state. Results from in-vacuo measurements at the HIPPIE beamline (MAX IV) show differencies in the evolution of the oxide layer when the sample is exposed to acidic (fig.1) and alkaline solution (fig.2). A reduction of the native oxide is observed in the N1s core level spectrum after simple exposure to both acidic and alkaline solution (OCP – fig. 1b,2b). However, in alkaline conditions, a nitrogen oxidation starts already at -0.19V vs Ag/AgCl, indicating the formation of a new passive film (fig. 2a,b). Whereas in acidic solution, this increase is observed only at potentials above +1.00 V vs Ag/AgCl (fig. 1a,b). Further interpretation of other core-levels spectra will be presented.

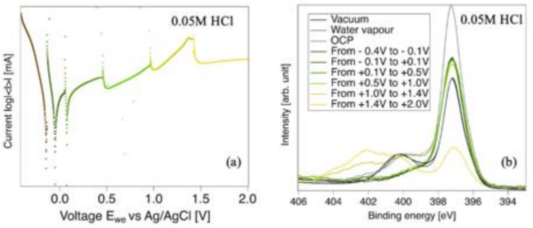

Figure 1 (a) Potentiodynamic curve of TiCN in 0.05M HCl. (b) N1s core level spectrum before and after electrochemical treatment.

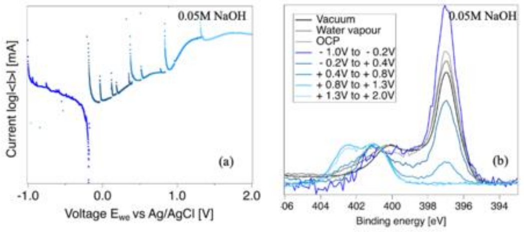

Figure 2 (a) Potentiodynamic curve of TiCN in 0.05M NaOH. (b) N1s core level spectrum before and after electrochemical treatment.

When: 2026-06-22, 14:45 - 15:05, Where: Sonja Lyttkens

O47 - Understanding the donor-acceptor interaction at the m-MTDATA-PPT interface

Energy materials

Cesare Grazioli[1]
Luca Schio[1], Monica de Simone[1], Luca Floreano[1], Marcello Coreno[2], Ambra Guarnaccio[2], Tingting Wang[3], Quanzhen Zhang[3], Teng Zhang[3], Davide Piva[4], Roberto Costantini[4], Iulia Emilia Brumboiu[5], Rokaya Osama[6], Barbara Ressel[6], Fredrik Johansson[7], Elin Cartwright[7], Carla Puglia[7]
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[3] Beijing Institute of Technology, 100081 Beijing, People's Republic of China
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Abstract text: Donor-acceptor (D-A) molecular interfaces govern key charge transfer processes in next generation organic optoelectronics. Here, we investigate the electronic interaction at the m-MTDATA/PPT interface, exploiting the elemental and interface sensitivity of VUV and soft X ray spectroscopies to elucidate charge delocalization mechanisms in complex organic systems. This study is part of a broader research effort spanning gas phase AMO characterization of molecular building blocks and extensive theoretical collaboration for electronic structure modelling.
We employ PES, NEXAFS, and ResPES to characterize m-MTDATA, a π conjugated donor based on a TPA moiety, together with the ambipolar acceptor PPT. NEXAFS measurements reveal that the unoccupied electronic structure of m-MTDATA is highly environment dependent: states in the gap region evolve distinctly when the molecule is isolated, adsorbed on Au(111), or deposited on PPT. In the latter case, these modifications reflect genuine donor-acceptor hybridization and highlight direct D-A coupling at a buried organic-organic interface. ResPES data further confirm this interaction through the suppression of a characteristic C K edge resonance, indicative of ultrafast electronic delocalization within the core hole lifetime.
We distinguish substrate induced effects from intrinsic D-A interactions by analysing different adsorption schemes: isolated layers, D on A deposition, and coverage variations. Preliminary HHG/VUV pump-probe measurements are also being explored to extend the study into the time domain and assess possible ultrafast population changes in the system, providing a complementary route to investigate charge-transfer processes.
Our multidisciplinary approach provides an integrated picture of electronic processes at the m-MTDATA/PPT interface.

When: 2026-06-26, 11:15 - 11:35, Where: Sonja Lyttkens

O48 - Using Photoelectron Spectroscopy to Study Energetic Alignment and Interfacial Chemistry in Perovskite Solar Cells

Energy materials

Karen Radetzky[1]
Alberto García Fernández[2], Birgit Kammlander[1], Rahul Varma[1], Evelyn Johannesson[1], Brian Rydgren[1], Julia Prumbs[1], Håkan Rensmo[1], Ute Cappel[1]
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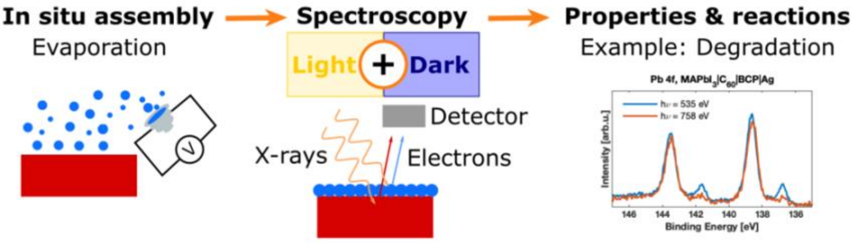
Abstract text: Organic-inorganic lead halide perovskites are used as absorbers in solar cell devices, which promise to deliver affordable and sustainable energy. However, challenges remain in optimizing the device interfaces which are crucial to effective charge extraction but also present sites for charge recombination and chemical reactions. These processes limit device performance and long-term stability and therefore need to be understood before device commercialization. Insights can be gained with photoelectron spectroscopy (PES) as the quantitative and qualitative information contained in the PE spectra can be related to the electronic structure and composition of solid samples.[1]

In this talk, I will present high-quality synchrotron-based PES data measured on a well-defined model system. As a substrate, a perovskite single crystal was used to study fundamental material properties.[2,3] During the experiment, electron extracting layers of C_{60}, bathocuproine (BCP), and silver were evaporated in situ while PE measurements were performed after each deposition step. Via this approach, each interface could be characterized individually. Moreover, PES was used study the impact of operating conditions on the solar cell. Here, the interfaces were investigated under Laser illumination to examine additional photo-induced effects. I will show how we discovered unfavorable energy alignment at the perovskite /C_{60} interface, device degradation through ion migration, and decomposition reactions via analysis of PE spectra.

The talk demonstrates how PES can be used to reveal interfacial energy alignment and degradation pathways in PSCs. The permeability of the electron transporting layers to perovskite ions is identified as a key target for future material design.



When: 2026-06-22, 16:25 - 16:45, Where: Sonja Lyttkens

O49 - Utilizing time-resolved photoelectron spectroscopy to investigate ultrafast charge-carrier dynamics in solar cells

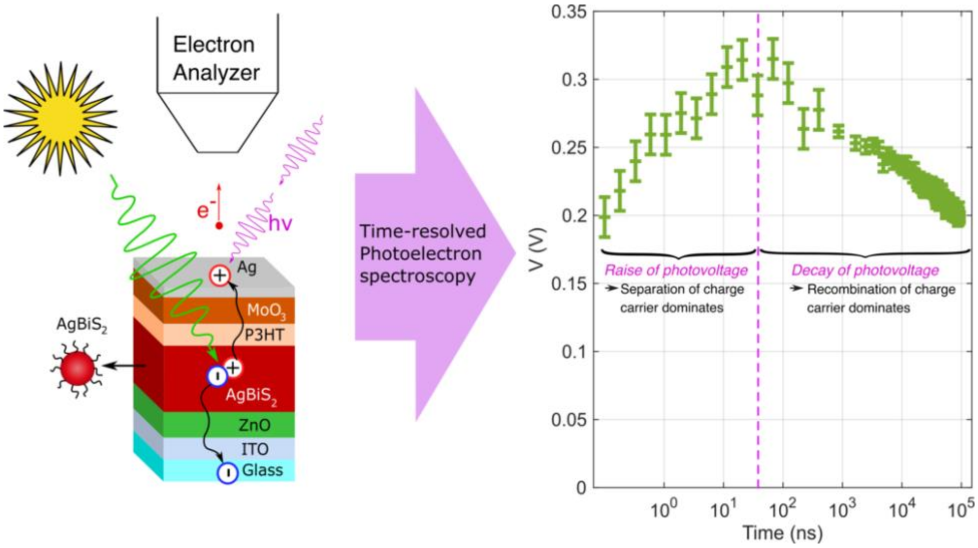
Energy materials

Julia Prumbs[1], Fiona Treber[2], Karen Radetzky[1], Brian Rydgren[1], Birgit Kammlander[1], Ute Cappel[1]
[1] Department of Physics and Astronomy, Uppsala Universitet, Lägerhyddsvägen 1, 751 20 Uppsala
[2] Department of Chemistry, Uppsala Universitet, Lägerhyddsvägen 1, 751 20 Uppsala

Abstract text: Solar cells are among the most promising renewable energy technologies today. Currently, research focuses on thin-film solar cells, in which the absorbing material is sandwiched between selective contacts. The performance of such devices critically depends on efficient charge separation at the interfaces, making a detailed understanding of the dynamics and energetics of the charge-carrier transport within the solar cell essential for developing higher-efficiency devices. Since these processes occur on ultrafast timescales, time-resolved measurements are required to directly study the underlying mechanisms within the solar cell to identify factors that might limit device efficiency.

In this presentation, I will show how we employ time-resolved X-ray photoelectron spectroscopy (PES) to probe the ultrafast dynamics of charge-carrier generation and recombination in $AgBiS_2$ quantum dot solar cells. The method is based on a pump–probe set-up in which a visible laser pulse, operating at a lower repetition rate, excites the sample, while synchronized X-ray pulses at a higher repetition rate probe the resulting excited states. This enables measurement of the rapid generation of charge carriers (photovoltage) with picosecond resolution, as well as charge-carrier recombination in the millisecond regime within a single experiment.

Therefore, this approach probes processes from picoseconds to microseconds and enables direct investigation of how device architecture influences charge transport and recombination. By measuring different sample architectures, individual contributions from the different layers can be identified. The method is feasible for different types of solar cells and provides a powerful tool for understanding the ultrafast dynamics.



HHG/VUV

When: 2026-06-23, 10:20 - 10:40, Where: Eva von Bahr

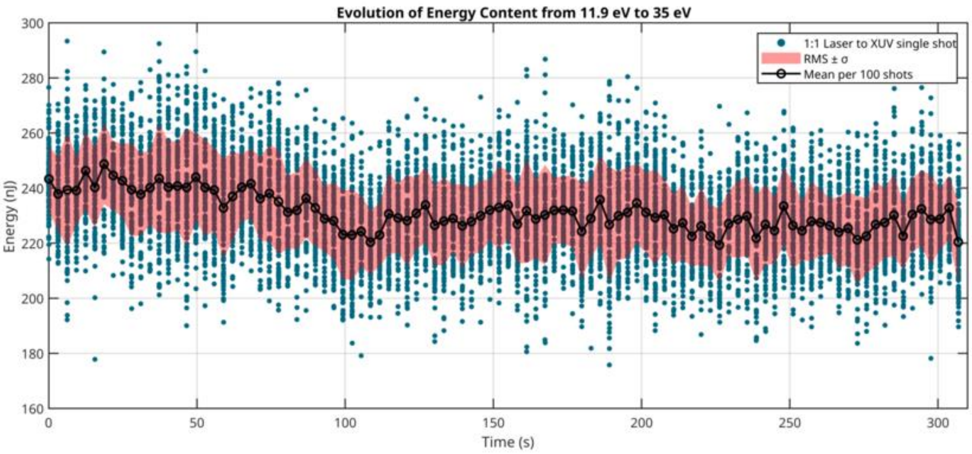
O50 - A continuously operating kHz source of high-intensity relativistic high-order harmonics

HHG/VUV

Andre Kalouguine[1]
Antoine Cavagna[1], Christian Cabello[1], Jaismeen Kaur[1], Stefan Haessler[1], Rodrigo Lopez-Martens[1]
[1] Laboratoire d’Optique Appliquée (LOA), CNRS, École polytechnique, ENSTA, Institut Polytechnique de Paris, Palaiseau, France

Abstract text: We report on the generation of high-power relativistic high-order harmonics at 1-kHz repetition rate using the SalleNoire2.0 installation [1] at LOA. A CEP-stable 4 fs, 2.5 mJ driving pulse is tightly focused onto a colliding-jets liquid-leaf target, producing coherent broadband radiation spanning the visible to XUV range (1.5 eV to 35 eV) [2].
XUV energy measurements exceed 200 nJ in the 12-35 eV photon energy range (see figure), corresponding to an IR-to-XUV conversion efficiency of around 10^{-4}, among the highest reported for tabletop systems. The characterised stability of the spectral and spatial characteristics of the relativistic HHG emission underpins its potential as a powerful secondary source. Simulations indicate that the emitted radiation is nearly chirp-free and could be refocused into an isolated attosecond pulse.
The continuous (minutes to hours, see figure) kHz-operation of the source represents a breakthrough for relativistic laser-plasma interactions and enables its use as a stable driver for attosecond experiments requiring very high pulse intensities. Calculations predict that refocused intensities above 10^{15} W/cm^2 are achievable, opening the way to strong-field studies in the XUV regime. The talk will also present the plans for the experiments aiming to obtain a usable refocused attosecond pulse.

[1] M. Ouillé et al., ‘Relativistic-intensity near-single-cycle light waveforms at kHz repetition rate’, Light Sci Appl, vol. 9, no. 1, p. 47, Mar. 2020, doi: 10.1038/s41377-020-0280-5.
[2] A. Cavagna et al., ‘Continuous relativistic high-harmonic generation from a kHz liquid-sheet plasma mirror’, Opt. Lett., OL, vol. 50, no. 1, pp. 165–168, Jan. 2025, doi: 10.1364/OL.545912.



When: 2026-06-23, 09:55 - 10:20, Where: Eva von Bahr

O51 - All-attosecond transient absorption spectroscopy in atoms, molecules and solids

HHG/VUV

Bernd Schütte[1]
[1] Max-Born-Institut

Abstract text: A longstanding goal in attosecond science is the ability to perform attosecond-pump attosecond-probe spectroscopy (APAPS). Pioneering experiments have been performed using HHG and FEL sources. All-attosecond transient absorption spectroscopy (AATAS) is a particularly attractive technique, as it combines an extremely high temporal resolution in both the pump and the probe steps with an excellent spectral resolution.

Here I will present our first results on AATAS in atoms, molecules and solids. In a first series of experiments, we studied electronic coherences in atoms. Fig. 1a shows an AATAS map recorded in Ar, where the broadband blue features are dominated by the depletion of neutral atoms. The narrowband white and red features are attributed to resonant absorption in the generated Ar^+ ions. Clear oscillating features with a period of 23 fs are observed (see also Fig. 1b), which are the result of generating these ions in a superposition of their ground-state and excited-state spin-orbit manifolds.

In addition, I will show how AATAS allows us to investigate nonadiabatic dynamics in organic molecules that occur e.g. at conical intersections. The high stability of our setup further enables us to study electronic dynamics in solids on attosecond to femtosecond timescales.

When: 2026-06-26, 11:15 - 11:40, Where: Heinz-Otto Kreis

O52 - Do we really understand attosecond interferometry in molecules?

HHG/VUV

Giuseppe Sansone[1]
[1] University of Freiburg

Abstract text: Pioneering experiments involving attosecond interferometry in atoms based on table-top sources have played a key role in measuring the time it takes for a photoelectron wave packet to be emitted after the absorption of an extreme ultraviolet photon. However, applying this approach to molecules raises fundamental questions about the information that can be extracted from the experimental data. This is due to the complex energy structure of molecular systems, whereby photoelectrons of the same energy can be emitted via several different pathways. In this work, I present evidence that analysing the amplitude and phase of photoelectron wave packets generated by two-colour photoionisation provides information on dynamics driven in the ion by the near-infrared field used in the attosecond interferometry approach. These dynamics can significantly impact the photoionisation time delays observed in the experiment. The ability to observe effects connected to dynamics induced in ions relies heavily on measuring angle- and energy-resolved photoelectron distributions in conjunction with specific ionic species.

When: 2026-06-23, 11:40 - 12:00, Where: Eva von Bahr

O53 - Efficient high harmonic generation driven by pulses with energies below one microjoule

HHG/VUV

Maria Carla Lupu[1]
Filchito Renee Bagsican[1], Tatsunosuke Hanano[1], Michael Man[1], Julien Madéo[1]
[1] OIST

Abstract text: The process of High Harmonic Generation (HHG) has enabled coherent table-top sources of XUV radiation with various applications such as attosecond science [1]. The scale invariance of nonlinear optical processes in gases has provided a framework where HHG could be downscaled to the paraxial limit and driven by nJ-class systems [2,3,4]. However, there is an ambiguity on the validity of this law down to this limit as no experiment has demonstrated the expected conversion efficiency (10^{-6} – 10^{-5} with a NIR driver [3,5,6]). Here, we demonstrate that the scale invariance still holds close to the paraxial limit. We used a 2 MHz 800 nJ NIR driver focused to a ~4 µm focal spot into bar-level 25 µm gas target and obtained a flux up to 10^{12} photons/s at 34 eV, with a conversion efficiency of 3×10^{-6}. A 1D HHG model including focusing geometry agrees with the experiment indicating operation in the absorption-limited regime. Demonstrating efficient HHG near the paraxial limit provides a pathway toward compact, high-repetition-rate XUV sources driven by nJ-class laser systems.

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When: 2026-06-26, 10:20 - 10:40, Where: Heinz-Otto Kreis

O54 - Extreme ultraviolet transient reflectivity of semiconductor-metal interfaces

HHG/VUV

Emmanouil Kechaoglou[1]
Fransesco Corazza[1], Peter Michael Kraus[1, 2]
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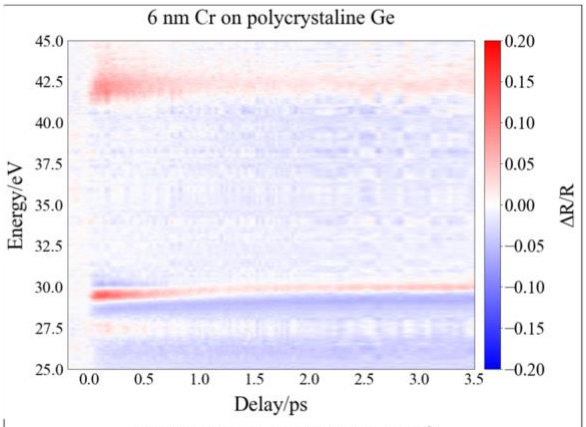
Abstract text: Interface-driven physics underpins next-generation electronics and photovoltaics, yet the relevant ultrafast processes in buried layers remain difficult to access with current metrology. Here we use transient XUV spectroscopy to provide element- and layer-resolved access to ultrafast interface dynamics, establishing a route to functional ultrafast metrology for novel materials.

The transient optical behavior of bilayer structures of Ge with both a thin (6 nm) or thick (75 nm) Cr layer has been recorded. The initial photoexcitation of the samples is achieved by 800 nm 35 fs laser pulses while the probe arm consists of High Harmonics generated in Argon, allowing the observation of the M-edge transient reflectivity (ΔR/R) of both materials in a single measurement ($\theta = 47^o, 57^o$ & 70^o from the surface normal). The implementation of Kramers–Kronig constrained variational analysis [1] effectively translates absolute reflectivity to both parts of the dielectric function based on fundamental causality relations for every time delay used between pump and probe beams.

The time-dependent evolution of the dielectric function is linked to carrier excitation and subsequent relaxation with observed spectroscopic features linked to electron, hole and phonon dynamics. Different energy dissipation pathways among bulk materials and interfaces are recorded and their relation to quantitative carrier mobility between the layers could act as a local conductivity proxy for these structures. Future implementation of the method to atomically thin materials and more complex structures could elucidate the ultrafast behavior of materials in realistic technological applications.

[1] A.B. Kuzmenko, Rev. Sci. Instrum. 76, 083108 (**2005**)



Transient reflectivity of the bilayer at $\theta_{AOI} = 57^o$

When: 2026-06-26, 09:55 - 10:20, Where: Heinz-Otto Kreis

O55 - High-intensity attosecond beamline for nonlinear XUV measurements

HHG/VUV

Laszlo Veisz[1]
Sajjad Vardast[1], Alexander Muschet[1], N. Smijesh[1, 2], Mohammad Rezaei-Pandari[1], Fritz Schnur[1], Robin Weissenbilder[3], Elisa Appi[3], Jan Lahl[3], Sylvain Maclot[3, 4], Per Eng-Johnsson[3], Anne L'Huillier[3]
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[2] Laboratory for Attosecond Sciences, Light and Matter Physics, Raman Research Institute, Bangalore, 560080, India
[3] Lund University, Department of Physics, Lund, 22100, Sweden
[4] Université Caen Normandie, ENSICAEN, CNRS, CEA, Normandie Univ, CIMAP UMR6252, Caen, F-14000, France

Abstract text: The field of attosecond physics has grown rapidly in recent years; however, experimental platforms enabling attosecond pump-attosecond probe spectroscopy remain scarce. Here, we present a newly developed beamline for the generation and application of high-energy, isolated attosecond pulses in the extreme ultraviolet (XUV) and soft X-ray spectral ranges. The approach is based on upscaling high-harmonic generation (HHG) in a gas medium to higher intensities.

The fundamental properties of the generated HHG radiation (including pulse energy, beam profile, spectral distribution, and divergence) are systematically characterized and optimized. The source delivers pulse energies of up to 55 nJ within the zirconium transmission window (65-150 eV), with high stability and a divergence of 0.1 mrad. Numerical simulations are performed to identify optimal operating conditions, showing excellent agreement with the experimental observations.

Temporal super-resolution of the driving laser field is implemented, resulting in a significantly broadened spectral continuum. The beamline further incorporates a split-and-delay stage, enabling pump-probe experiments. The HHG radiation is focused to a spot size below 6 μm using two distinct focusing optics. Spatially resolved ion microscopy is employed to characterize ion generation at the focal region.

Overall, the presented beamline provides a versatile platform for nonlinear XUV and soft X-ray studies using isolated attosecond pulses.

When: 2026-06-25, 11:40 - 12:05, Where: Sonja Lyttkens

O56 - New advances in Attosecond Chemistry

HHG/VUV

Fernando Martin[1, 2]
[1] Departamento de Química, Universidad Autónoma de Madrid, 28049 Madrid, Spain
[2] Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA-Nano), Cantoblanco, 28049 Madrid, Spain

Abstract text: Since the first attosecond pump-probe experiments performed in molecules [1,2], the field has grown exponentially, leading to the new discipline of attochemistry [3]. As a result, it is nowadays possible to follow in real time the motion of the "fast" electronic motion in molecules, mostly in the gas phase, and understand how this motion affects the "slower" motion of atomic nuclei and vice versa. There are, however, new scenarios [4] that will allow one to extend the range of applications to more complex molecular systems [5] and to overcome some of the limitations of current attosecond technologies. In addition, the role of pulse-induced coherences in the ensuing molecular dynamics is receiving a considerable attention, since they may offer new opportunities to control chemical reactions or open new scenarios for quantum information technologies [6].

In this talk, I will describe some of the new theoretical developments aiming at supporting ongoing experimental efforts along some of the above-mentioned directions, thus illustrating the high potential of attochemistry to uncover new phenomena in chemistry and the need for such theoretical developments to guide the experimental efforts.

[1] G. Sansone et al, *Nature* **465** 763 (2010).
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[3] M. Nisoli et al, *Chem. Rev.* **117**, 10760 (2017).
[4] F. Calegari and F. Martín, *Commun. Chem.* **6**, 184 (2023).
[5] F. Vismarra et al, *Nature Chemistry* **16**, 2017(2024).
[6] L. M. Koll et al, *Nature* **652**, 82 (2026).

When: 2026-06-23, 09:00 - 09:45, Where: Eva von Bahr

O57 - Shaping the Future of Ultrafast: Power, Precision, and Simplicity through Yb-Doped Lasers and Dual-Combs

HHG/VUV

Ursula Keller[1]
[1] ETH Zurich, Department of Physics, Switzerland

Abstract text: Ultrafast laser science has undergone a remarkable transformation since the first femtosecond dye lasers. After 1990, the “revenge of the solid state” enabled performance scaling by orders of magnitude in pulse duration, average power, pulse energy, repetition rate, and full frequency-comb stabilization. Although passive modelocking was first demonstrated in a solid-state Nd:glass laser in 1966, Q-switching instabilities limited its potential; in 1976, Hermann A. Haus identified relaxation oscillations as a fundamental obstacle to stable passive modelocking. This challenge was overcome in 1992 with semiconductor saturable absorber mirror (SESAM) modelocking, establishing a robust platform for ultrafast solid-state lasers and enabling broad scientific and industrial deployment.

Key advances enabled by the ultrafast solid-state laser technology includes power and repetition-rate scaling, frequency-comb stabilization, and the generation of optical-cycle-scale pulses directly from modelocked oscillators. These developments enabled carrier-envelope-offset phase control, transformed frequency metrology, supported single-attosecond pulse generation, and opened new routes to attosecond measurements such as the attoclock technique.

The talk will highlight the transition from Ti:sapphire to Yb-doped ultrafast lasers, which offer higher power, higher repetition rates, greater robustness, and few-cycle pulse generation through efficient external compression. Finally, I will discuss SESAM-based dual-comb modelocking from a single laser cavity, which requires no active stabilization and transfers pump-probe measurements and Fourier-transform spectroscopy into the electronic domain without mechanical delay lines. Single-cavity dual-comb lasers generate two frequency combs with a precisely controlled, small difference in repetition rate and are now commercially available for diverse applications.

When: 2026-06-24, 15:45 - 16:05, Where: Sonja Lyttkens

O58 - Subwavelength imaging of nanoscale magnetic domain walls during ultrafast demagnetization with a table-top extreme ultaviolet source

HHG/VUV

Hung-Tzu Chang[1]
Sergey Zayko[1], Timo Schmidt[2], Ofer Kfir[3], Murat Sivis[1, 4], Johan H. Mentink[5], Manfred Albrecht[2], Claus Ropers[1, 4]
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[2] Institute of Physics, University of Augsburg, 86135 Augsburg, Germany
[3] School of Electrical & Computer Engineering, Tel Aviv University, Tel Aviv 69978, Israel
[4] 4th Physical Institute, University of Goettingen, 37077 Goettingen, Germany
[5] Radboud University, Institute for Molecules and Materials, Nijmegen, 6525 AJ, The Netherlands

Abstract text: Understanding the behavior of photoexcited magnetic domain walls is crucial to ultrafast manipulation of spin textures. However, direct observation of such phenomena require femtosecond real-space imaging at nanometer scales, which is challenging due to the extreme spatial and temporal resolution required simultaneously. Extreme ultraviolet light pulses produced by high-harmonic generation not only provide temporal resolution down to attoseconds but also enable imaging of nanoscale objects. Here we present femtosecond subwavelength imaging of magnetic domains in TbCo and Co/Pd thin films at the Co $M_{2,3}$ edge (20.8 nm or ~60 eV) during photoinduced demagnetization. With spatial resolution down to 13.5 nm, we extract the properties of domain walls in real space with experimental precision of <2 nm. Contrary to previous reports which inferred domain wall broadening and motion during reversible demagnetization from indirect, reciprocal space measurements, we show that the width and position of domain walls remain invariant down to our experimental precision. For optical excitation inducing >50% demagnetization, stochastic, irreversible switching of domains occurs. Our results establish an upper limit for domain wall motion and lateral spin transport across the domain walls after homogeneous optical excitation. The imaging technique can be readily generalized for nanometer, spatially-resolved studies of ultrafast carrier, phonon, and spin dynamics in solids.

References:

[1] Chang et al. arxiv: 2504.17917.
[2] Zayko et al. Nat. Commun. 12, 6337 (2021)
[3] Kfir et al. Sci. Adv. 3, eaao4641 (2017)
[4] Pfau et al. Nat. Commun. 3, 1100 (2012)
[5] Jangid et al., Phys. Rev. Lett. 131, 256702 (2023)

When: 2026-06-23, 11:15 - 11:40, Where: Eva von Bahr

O59 - Towards a monochromatized-photon-excitation dispersed-photon-emission map for all singly excited states of H2

HHG/VUV

Arno Ehresmann[1]
Philipp Schmidt[1, 2], Johannes Viehmann[1], Peter Baumgärtel[3], Dana Bloß[1], Niklas Golchert[1], Emilia heikura[1], Catmarna Küstner-Wetekam[1], Lutz Marder[1], Yusaku Terao[1], Andreas Hans[1], Adrian Krone[1]
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[3] Helmholtzzentrum für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Abstract text: H_2 has always been the testbed for advancements in fundamental molecular physics, being investigated for well more than 100 years. As H_2 is the most abundant molecule in space it is a useful probe for astrophysical processes, necessitating quantitative data on its photon absorption and emission. Since H_2 is homonuclear, transitions between rovibrational levels of the same electronic potential are dipole-forbidden, causing no (or very weak quadrupolar) features in the infrared spectral region. Consequently, the major absorption or emission features are caused by transitions between rovibronic levels of the electronic ground state and those of the singly-excited states, lying in the vacuum ultraviolet (VUV) or far ultraviolet (FUV) spectral range. We are currently working on recording a complete two-dimensional (monochromatized) photon-excitation (dispersed) photon-emission (PhexPhem) map of H_2 in the excitation energy range between 11 and 18eV and the fluorescence wavelength range between 75 and 180 nm. Among other features, this enables the observation of complete systems of its Condon diffraction bands, which originate from spontaneous radiative dissociation of individual bound electronically excited rovibronic levels, one of the most relevant processes for the destruction of H_2 in space. These bands are extremely sensitive to relative shapes and positions of the involved potential energy curves and can be used to accurately test theoretical approximations. For the B-X system of electronic states, we show that specific measured spectral characteristics of individual bands are extremely sensitive to the internuclear distance difference of the two involved potential energy curves.

When: 2026-06-24, 15:20 - 15:45, Where: Sonja Lyttkens

O60 - Ultrafast relaxation of XUV-excited and photoionized helium nanodroplets

HHG/VUV

Marcel Mudrich[1]
[1] University of Kassel

Abstract text: Helium nanodroplets are quantum fluid clusters that feature extraordinary properties such as ultralow temperature and superfluidity. They are mostly used as inert nanometer-sized cryo-matrices for isolating molecules and for aggregating molecular complexes and nanostructures that are hard or impossible to form by other means. However, when helium nanodroplets are photo-excited or ionized, they turn into highly reactive species that feature intriguingly complex relaxation and reaction dynamics.

Using new extreme light sources such free-electron lasers (FEL) and high-harmonic generation (HHG) sources, we experimentally probe the ultrafast relaxation dynamics of pure and doped helium nanodroplets triggered by ultrashort VUV pulses. In this way, we obtain information about how a superfluid reacts to impulsive perturbations in time. It turns out that helium nanodroplets are excellent model systems to study fundamental radiochemical processes such as secondary electron production, elastic and inelastic electron scattering, and intermolecular transfer of energy and charge. As special features of helium nanodroplets, resonant excitation leads to the migration of excited atoms to the droplet surface and along the surface, and the transfer of energy and charge between helium atoms and `dopant´ atoms or molecules attached to the droplets.

In my talk, I will present a few recent results including ultrafast [1] and ultraslow ICD [2] of pairs of He* excitations which we probe by measuring electron spectra or fluorescence spectra emitted by the helium nanodroplets after strong-field ionization.

[1] A. C. LaForge et al., Phys. Rev. X 11, 021011 (2021)
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When: 2026-06-23, 12:00 - 12:20, Where: Eva von Bahr

O61 - Unraveling the dynamics of solvated (di-)electrons in sodium-doped ammonia clusters

HHG/VUV

Grite L. Abma[1]
Dominique P. Borgeaud dit Avocat[1], Angela L. Spadea[1], Sebastian Hartweg[2], Bruce L. Yoder[1], Ruth Signorell[1]
[1] Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich, Switzerland
[2] Institute of Physics, University of Freiburg, Freiburg, Germany.

Abstract text: Solvated electrons were first observed in solutions of alkali metals in liquid ammonia. Since that discovery, these solutions have been widely employed as powerful reducing agents in industrial-scale chemical processes [1]. Solvated electrons have also been recognized as crucial intermediates in radiation chemistry, particularly in aqueous environments [2]. Despite their importance, the mechanisms of electron-induced reactions are yet to be completely understood, partially due to the challenges associated with conducting controlled experiments with low-energy electrons in bulk liquid phases. Clusters represent a valuable alternative here. We report initial time-resolved results on photo-induced relaxation dynamics of low-energy solvated electrons in sodium-doped ammonia clusters. The clusters are photoexcited using a VUV pulse and the dynamics are probed using a UV pulse, where photoionization competes with autoionization processes. The decay mechanisms for the sodium-ammonia system have previously been observed only in small clusters (<20 molecules) [3], but the lifetime of the states remains unobserved experimentally. Characterizing the ultrafast dynamics of solvated electrons and di-electrons in the presence of valence vacancies could provide new insight into their high reactivity and may have direct implications for understanding electron-driven processes in radiation chemistry.

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[2] Garrett, B. C. et al. Chem. Rev. 105, 355-390 (2005)
[3] Hartweg, S. et al. Science 380, 6650 (2023)

Instrumentation

When: 2026-06-22, 11:50 - 12:10, Where: Heinz-Otto Kreis

O62 - Advanced Single-Hemisphere Photoelectron Momentum Microscopy with Time-of-Flight Detection at the Diamond Light Source

Instrumentation

Olena Tkach[1], Deepnarayan Biswas[2], Matthias Schmitt[3], Jieyi Liu[2], Tien-Lin Lee[2], Olena Fedchenko[1, 4], Michael Sing[3], Hans-Joachim Elmers[1], Gerd Schönhense[1]
[1] Institute of Physics, Johannes Gutenberg University, Mainz, Germany
[2] Diamond Light Source Ltd., Didcot, United Kingdom
[3] Physikalisches Institut, Universität Würzburg, Würzburg, Germany
[4] Goethe University Frankfurt, Frankfurt am Main, Germany

Abstract text: Soft X-ray photoelectron momentum microscopy is a novel approach to ARPES, which maps electronic bands in $(E,\boldsymbol{k})$ across the full Brillouin zone. The fixed sample geometry eliminates any modulation of the matrix element due to a change in angle of incidence as needed in the classical approach. We introduce a new endstation [1] at the soft-X-ray branch of beamline I09 [2] at the Diamond Light Source, UK. The photon energy ranges from $h\nu$=110eV to 2keV, with circular polarization available for $h\nu$>145eV. The key component is a single hemispherical analyzer combined with time-of-flight (ToF) detection [3]. Energy and momentum resolutions are 10meV and 0.01Å^{-1}, with potential for further improvement. The large angular filling of the entrance lens allows k-field diameters up to 8Å^{-1}. As an example, the figure presents 4D intensity (a-d) and circular dichroism (f-i) tomography of the Cu Fermi surface. The 3D Fermi surface was concatenated from 20 k_x-k_y sections as shown in (a-d). A k_x-k_z section is displayed in (e), showing the region between the 'belly' and 'neck'. Here we use the terminology of deHaas-vanAlphen experiments; the theoretical Fermi surface is shown in (j). The circular dichroism in the angular distribution (CDAD) exhibits a rich structure, panels (f-i); color code: red and blue for positive and negative CDAD. This is unexpected for a *sp*-band. Results for a Kagome metal [4] demonstrate the efficiency of the combined dispersive and ToF energy analysis.

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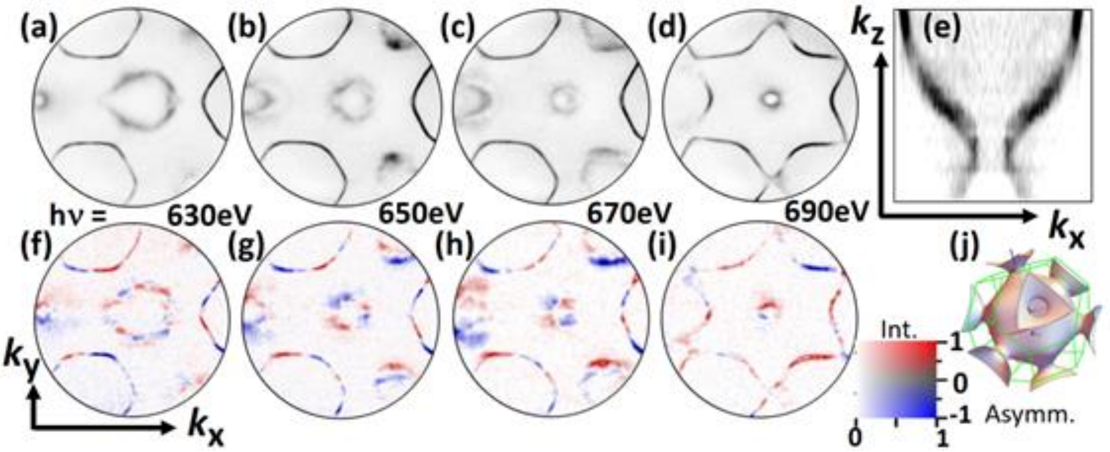

When: 2026-06-22, 16:10 - 16:30, Where: Eva von Bahr

O63 - Angle-resolved Photo-Emission Spectrometers for Non-Invasive Photon Diagnostics at the European X-Ray Free Electron Laser

Instrumentation

Joakim Laksman[1]
Florian Dietrich[1], Theophilos Maltezopoulos[1], Jia Liu[1], Danilo Enoque Ferreira de Lima[1], Jan Grünert[1]
[1] European X-Ray Free-Electron Laser Facility GmbH

Abstract text: Angle-resolved photo-emission spectrometers with microchannel plate detectors and fast electronics are versatile and powerful devices for providing non-invasive single-shot photon diagnostics at MHz repetition rate X-ray free-electron lasers. In this contribution, we demonstrate the performance and characteristics of our two operational spectrometers for the applications of spectral diagnostics and polarimetry at both soft X-rays and hard X-rays. In particular hard X-ray operation imposes specific design challenges due to poor photoionization cross-sections and very high photoelectron velocities. Additionally, we describe the adaptations and further developments required to enable temporal profiling with angular streaking for sub-fs X-Ray pulses. Furthermore, new automation tools and online data analysis that enable continuous support for machine operators and instrument scientists has been developed. Customized software provide real-time monitoring of photon beam polarization and spectral distribution both in single-color and two-color operation. Also, recent advancements in machine learning enable resolution enhancement by training the photoelectron spectrometer together with an invasive high-resolution spectrometer, which generates a response function model.

When: 2026-06-24, 11:40 - 12:05, Where: Heinz-Otto Kreis

O64 - Coherent Soft X-Ray Imaging and Fluctuation Spectroscopy for Magnetic and Electronic Disorder

Instrumentation

Sophie A. Morley[1]
[1] Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, USA

Abstract text: Many of the world’s synchrotrons are completing upgrades to fourth generation sources this decade which provides a huge boost in coherence. Methods such as ptychographic imaging and X-ray photon correlation spectroscopy (XPCS) are set to benefit tremendously. I will discuss the recent developments in these techniques at the soft x-ray C*Oherent Scattering and MICroscopy (COSMIC)* Beamline (7.0.1) at the Advanced Light Source and provide an outlook for after our upgrade.

XPCS allows the study of dynamics in materials at the micro to atomic scale, dependent on the energy of the x-rays. When coherent light scatters from a sample it forms an interference pattern on a two-dimensional detector known as speckle. Measuring speckle patterns as a function of time is the basis of XPCS and characteristic fluctuation times of a sample can be extracted and connected to spatial features such as defect motion using theory and modelling [1]. In this way XPCS provides insight into the temporal and spatial evolution of material properties, from diffusion and relaxation processes to phase transitions and non-equilibrium phenomena [2,3]. Imaging these same systems can also help aid the interpretation of XPCS. Ptychography is a type of microscopy where the coherence of the technique removes the resolution restriction placed on the imaging system by the optics. We have recently demonstrated 30 nm resolution in reflection ptychography in the soft x-ray regime [4]. We anticipate this opening up a new pathway to the imaging of complex magnetic, charge and orbital orders in the future.

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When: 2026-06-25, 15:35 - 15:55, Where: Sonja Lyttkens

O65 - Commissioning of the High-Resolution Nano-PES Beamline (ID41) at HEPS: Probing Localized Charge Dynamics in 2D Materials

Instrumentation

Teng ZHANG[1]
Chen LIU[2], Jiaou WANG[2], Yeliang WANG[1]
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[2] High Energy Photon Source, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China

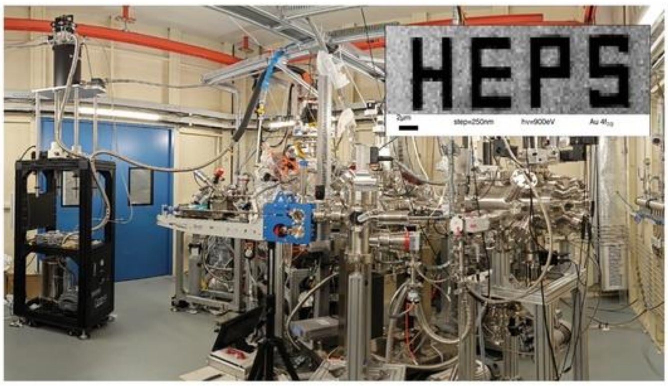
Abstract text: The newly established High Energy Photon Source (HEPS) in Beijing, China, features the ID41 High-resolution Nano Electronic Structure Spectroscopy (HiNESS) beamline, a state-of-the-art facility designed for sub-micron operando characterization. Supported by the high brightness of this diffraction-limited storage ring light source, ID41 delivers a spatial resolution better than 200 × 200 nm and an energy resolution below 20 meV in the soft X-ray regime. In this contribution, we present the instrumentation advancements, endstation capabilities, and commissioning results of the ID41 nano-XPS beamline.

To validate the beamline’s performance, we conducted preliminary nano-PES experiments on two-dimensional Indium Selenide (InSe) on Si/SiO2 substrates. InSe serves as a stringent test system due to its pronounced sensitivity to local charging and non-uniform carrier distributions. Utilizing an incident photon energy of 900 eV, we achieved rapid large-area screening followed by targeted, high-spatial-resolution mapping of micro/nano-islands. High-quality *in situ* In 3d fine spectra precisely captured localized charging effects and resolved core-level shifts induced by carrier concentration variations.

These results demonstrate the system’s robust capability to trace micro-local charge transport. As a scanning soft X-ray nano-PES facility, ID41 delivers high-resolution spectral quality that naturally complements existing full-field imaging and ambient-pressure techniques. Ultimately, ID41 enables researchers to decouple complex mechanisms including band bending and potential barrier evolution under multi-field operando conditions, establishing the beamline as a powerful new tool for advanced nanoelectronics research.

Selected references

High Energy Photon Source (HEPS), Beijing, China



ID41 HiNESS beamline endstation and commissioning performance validation

When: 2026-06-24, 15:20 - 15:40, Where: Heinz-Otto Kreis

O66 - Development of a Soft X-ray Magneto-ARPES Technique at NanoTerasu

Instrumentation

Hideaki Iwasawa[1, 2, 3]
Fumi Nishino[2], Miho Kitamura[2], Taichi Okuda[3], Koji Horiba[2]
[1] Synchrotron Radiation Research Center, National Institutes for Quantum Science and Technology
[2] NanoTerasu Center, National Institutes for Quantum Science and Technology
[3] Research Institute for Synchrotron Radiation Science, Hiroshima University

Abstract text: Angle-resolved photoemission spectroscopy (ARPES) under external fields has recently emerged as a powerful approach for probing electronic states while actively tuning the physical properties of materials. In particular, ARPES under applied magnetic fields has attracted increasing attention as an advanced technique that extends the capability of conventional ARPES measurements [1, 2]. However, the Lorentz force acting on low-kinetic-energy photoelectrons significantly distorts electron trajectories, which has been a major obstacle for reliable measurements under magnetic fields. To address this issue, we have been developing a magneto-ARPES technique using soft X-ray excitation at the micro-ARPES beamline BL06U of NanoTerasu [3]. The higher kinetic energy of photoelectrons in the soft X-ray regime substantially reduces magnetic-field-induced trajectory distortions, enabling more robust ARPES measurements under magnetic fields. We report the instrumental development of this system, including a sample manipulator equipped with four electrical contacts and a customized sample holder with an integrated coil system that enables the application of magnetic fields up to approximately 100 mT at the sample position. Representative magneto-ARPES measurements obtained with this setup will also be presented. Our results demonstrate that soft X-ray ARPES provides a practical platform for magneto-ARPES experiments and opens new opportunities for studying magnetic and spin-related electronic phenomena in quantum materials.

[1] S. H. Ryu *et al.*, J. Electron Spectrosc. Relat. Phenom. **266**, 147357 (2023).
[2] J. Huang *et al.*, Rev. Sci. Instrum. **94**, 093902 (2023).
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When: 2026-06-24, 12:05 - 12:25, Where: Heinz-Otto Kreis

O67 - Development of Spin-Resolved Photoemission Microscopy at NIMS

Instrumentation

Koichiro Yaji[1, 2, 3]
Shunsuke Tsuda[1]
[1] Center for Basic Research on Materials, National Institute for Materials Science (NIMS)
[2] Unprecedented-scale Data Analytics Center, Tohoku University
[3] Photon Science Innovation Center (PhoSIC)

Abstract text: Understanding electronic states near the Fermi level is essential for developing new materials and enhancing their performance, as these states directly influence material properties. In recent years, there has been an increasing demand for techniques capable of probing electronic structures within sub-micrometer regions. Spin-resolved photoemission spectroscopy (SARPES) is a powerful method for investigating spin-polarized electronic structures. However, conventional SARPES instruments typically employ a single-channel spin detector, which requires point-by-point measurements in momentum space and results in extremely long data acquisition times.

Recent advances in instrumentation have enabled the development of momentum microscopes equipped with multi-channel spin detectors. Based on an imaging concept, these detectors enable simultaneous acquisition of spin information across a wide region of momentum space, dramatically improving the efficiency of spin-resolved measurements.

Here, we report the development of an imaging-type spin-resolved photoemission microscope based on a momentum microscope equipped with a multi-channel spin detector and a 10.9 eV VUV laser. In real-space mode, the system achieves spatial resolutions of approximately 400 nm for spin-resolved imaging and 30 nm for spin-integrated imaging. We demonstrate its performance through spin-polarization imaging of polycrystalline Fe and spin-resolved Fermi-surface mapping of Bi(111).

In addition, we are developing a complementary spin-resolved photoemission system using soft X-rays at NanoTerasu. These approaches open new opportunities for investigating microscopic materials, including polycrystalline, powdered, and combinatorial samples that are difficult to study using conventional SARPES.

When: 2026-06-24, 15:40 - 16:00, Where: Heinz-Otto Kreis

O68 - High Throughput and High Resolution: Pushing Detector Technology for Soft X-ray RIXS

Instrumentation

Viktoria Hinger[1], Anna Bergamaschi[1], Ashish Bisht[2], Maurizio Boscardin[2], Maria Carulla[1], Matteo Centis Vignali[2], Nuno Duarte[3, 4], Francesco Ficorella[2], Loïc Le Guyader[3], Omar Hammad Ali[2], Shuqi Li[1], Aldo Mozzanica[1], Giovanni Paternoster[2], Marco Ramilli[3], Sabina Ronchin[2], Justine Schlappa[3], Andreas Scherz[3], Bernd Schmitt[1], Saverio Silletta[1], Monica Turcato[3], Jiaguo Zhang[1]
[1] Paul Scherrer Institute, Villigen PSI, Switzerland
[2] Fondazione Bruno Kessler, Trento, Italy
[3] European XFEL GmbH, Schenefeld, Germany
[4] CERN, Geneva, Switzerland

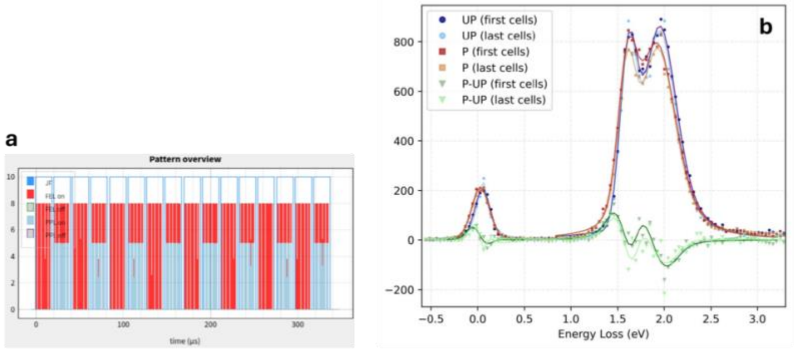
Abstract text: With advancing light sources, Resonant Inelastic X-ray Scattering (RIXS) increasingly targets higher throughput, multidimensional scans, and time-resolved studies. In many cases, detector performance limits efficiency. CCD cameras and CMOS image sensors provide excellent sensitivity but are constrained by low frame rates and limited active areas.

Hybrid pixel detectors offer an attractive alternative, combining high frame rates, large detector areas, and robust operation. While they are widely used for hard X-rays, their application below 1 keV has been limited by low quantum efficiency and insufficient signal-to-noise ratio.

In a collaboration between the Paul Scherrer Institute and Fondazione Bruno Kessler, we have developed sensors with internal signal amplification that enable hybrid pixel detectors optimized for soft X-rays, achieving quantum efficiencies above 85% at 250 eV [1] and a signal-to-noise ratio greater than five for single photons down to 390 eV [2].

We present our development of hybrid pixel detectors for soft X-ray RIXS and discuss the performance in recent experiments and upcoming improvements. To meet the spatial-resolution requirements of RIXS spectrometers, we employ a rectangular pixel design that enables charge-sharing-based position interpolation, achieving sub-pixel resolution better than 3 µm in the dispersive direction. A proof-of-concept RIXS experiment at the European XFEL at the Cu L-edge (930 eV) demonstrated a record frame rate of 47 kHz [3], significantly increasing data acquisition speed and enabling intra-train pump-probe measurements.

[1] Carulla et al., Sensors 24(3), 942 (2024).
[2] Zhang et al., JINST 17, C22011 (2022).
[3] Duarte et al., arXiv:2511.12314 (2025).



a. XFEL filling pattern with overlaid detector gates, effective image frequency of 47 kHz. The pump-probe laser (PPL) is alternated between Off and On status in the same pattern as the detector gates.

b. RIXS spectra of a CuO sample at 928.5 eV acquired 1 ps after PPL excitation (P) and without (UP) and their difference spectra (P-UP). Different shades show signal variations between the first half (first cells) and the second half (last cells) of an XFEL pulse train [3].

When: 2026-06-22, 10:45 - 11:10, Where: Heinz-Otto Kreis

O69 - High-transmission soft x-ray spectroscopy for operando studies of chemical bonding in applied material systems

Instrumentation

Lothar Weinhardt[1, 2, 3]
[1] Department of Chemistry and Biochemistry, University of Nevada Las Vegas (UNLV), Las Vegas, USA
[2] Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany
[3] Institute for Chemical Technology and Polymer Chemistry (ITCP), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Abstract text: Material and device development crucially depend on an in-depth characterization of the electronic and chemical properties of the involved materials and their interfaces. Traditionally, x-ray spectroscopy techniques are very powerful tools for probing these properties. Instrumental advances have been achieved over the last decades, mostly focusing on high-resolution (and unavoidably low-transmission) instruments, which are particularly important for fundamental studies of well-defined systems. In contrast, real-world devices require highly sensitive (high-transmission) probes that are able to measure trace elements, minimize the x-ray dose, and are applicable in an *in situ/operando* environment. At the same time, the most relevant materials questions concern the chemical bonding present in the materials and how they react to changes in processing or operating conditions, which does not require the highest possible energy resolution. In our efforts, we focus on developing x-ray spectroscopy techniques and the necessary experimental setups for this type of applications, which has led to the development of the SALSA (Solid and Liquid Spectroscopic Analysis) experimental station operated at the Advanced Light Source, Lawrence Berkeley National Laboratory, novel soft x-ray spectrometer concepts and the X-SPEC beamline at the KIT Light Source.

This presentation discusses the recent development of experimental setups and x-ray spectroscopy tools, in particular soft x-ray emission spectroscopy (XES) and resonant inelastic (soft) x-ray scattering (RIXS), for applied materials research. Using selected examples, it will be shown how XES and RIXS reveal bonding interactions in solids and solutions and how this is used in *operando* studies.

When: 2026-06-25, 15:15 - 15:35, Where: Sonja Lyttkens

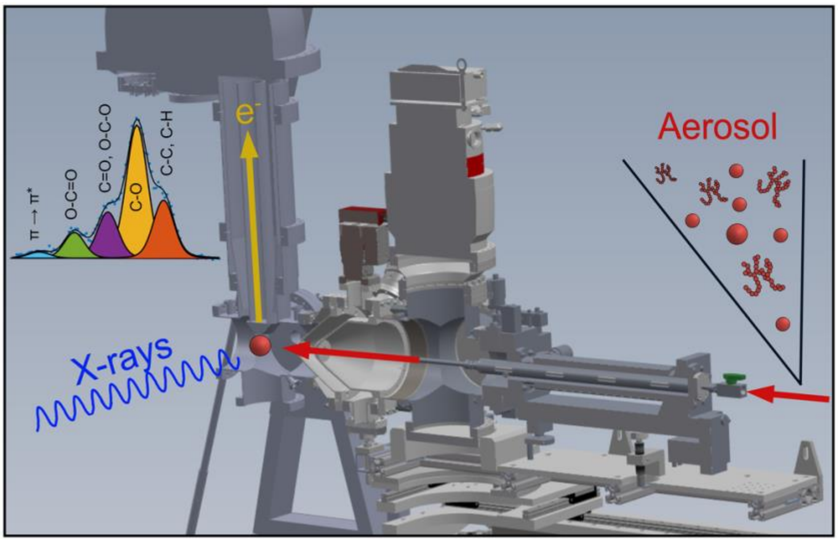
O70 - In-flight surface characterization of aerosol particles at the MAX IV synchrotron radiation facility

Instrumentation

Calle Preger[1]
Jenny Rissler[2], Antti Kivimäki[1], Axel C. Eriksson[2], Noelle Walsh[1]
[1] MAX IV Laboratory, Lund University, Lund, Sweden
[2] Ergonomics and Aerosol Technology, Lund University, Lund, Sweden

Abstract text: The chemical surface properties of aerosol particles are of utmost importance, as they govern their reactivity and toxicology. Thus, the surface properties of aerosol particles are relevant for their health effects, their impact on climate, and development of new materials. To enable direct surface investigation of aerosols, a dedicated aerosol sample-delivery system (ASDS) has been developed at the MAX IV synchrotron radiation facility in Lund, Sweden [1]. The ASDS combines an aerodynamic lens with differential pumping stages and is optimized for in-flight X-ray photoelectron spectroscopy (XPS). It continuously transports aerosols from atmospheric pressure into vacuum, enabling their analysis only seconds after formation. This rapid, substrate-free approach minimizes radiation damage, avoids artefacts associated with particle collection, and allows characterization of truly unsupported aerosols. Additionally, gas molecules propagating with the particle beam can be exploited for energy calibration and gas–particle studies. Since its inclusion into standard user calls in spring 2023, the ASDS has been applied to a wide range of aerosol types, including soot, sea salt, secondary organic aerosol, and engineered nanoparticles. MAX IV provides basic instrumentation for aerosol generation and characterization, and users have the option of bringing their own unique aerosol generation systems to enable comprehensive in-flight XPS of lab-generated aerosols.

[1] C. Preger *et al.*, *J. Synchrotron Rad*. 31 (2024) 1382.



When: 2026-06-24, 09:55 - 10:20, Where: Heinz-Otto Kreis

O71 - Multidimensional Nanoscale Spectromicroscopy at ALS-U To Observe Materials At Work

Instrumentation

Hendrik Ohldag[1, 2, 3]
Alexander Ditter[1], Morgan Ericksen[1], Joseph Tocci[1], James Nasiatka[1], David Shapiro[1]
[1] Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA USA
[2] Department of Materials Science, Stanford University, Stanford, CA USA
[3] Department of Physics, University of California Santa Cruz, Santa Cruz, CA USA

Abstract text: The Advanced Light Source has been operating as a third-generation light source for more than 30 years and Scanning Transmission X-ray Microscopy has been an integral part of the user program ever since. The first part of this talk will review the current state of the program, including in-operando chemistry, heavy element chemistry, magnetic imaging and ptychography. Over the course of the next few years the accelerator will be upgraded to a diffraction limited light source (ALS-U). With the expected increase in intensity comes the ability to acquire data much faster than today, which will enable our user community to address scientific questions that remain unanswered today, in particular how materials change over various timescales.

Dwell times may be as short as a few microseconds per pixel. This will require to develop faster scanning hardware to efficiently acquire full STXM images in much less than a second. Together with detection electronics that are able to count and register single x-ray pulses from the synchrotron we will cover time scales from nanoseconds to seconds at ALS-U and thus being able to observe transient processes over a wide range of relevant time and length scales with chemical and magnetic sensitivity.

When: 2026-06-22, 11:10 - 11:30, Where: Heinz-Otto Kreis

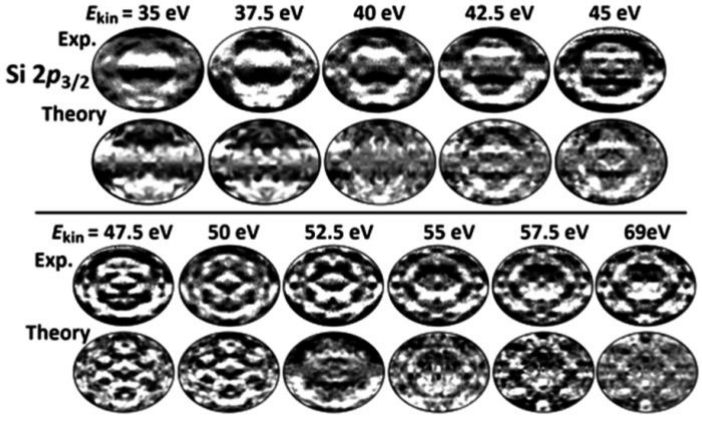
O72 - Recording Photoelectron Diffraction at Very Low Kinetic Energies

Instrumentation

Gerd Schönhense[1]
Olena Tkach[1], Trung-Phuc Vo[2], Deepnarayan Biswas[3], Jieiy Lee[3], Tien-Lin Lee[3], Olena Fedchenko[1,4], Jan Minár[2], Hans-Joachim Elmers[1]
[1] Institute of Physics, Johannes Gutenberg University, Mainz, Germany
[2] University of West Bohemia, Czech Republic
[3] Diamond Light Source Ltd., Didcot, United Kingdom
[4] Goethe University Frankfurt, Frankfurt am Main, Germany

Abstract text: Photoelectron diffraction (PED) is an exciting technique providing a direct, element-specific, 3D view of the local atomic structure. It can distinguish between chemically non-equivalent atoms without requiring long-range surface order. We introduce a new recording technique of PED here. $I(E_{\mathrm{kin}},k_x,k_y)$ diffractograms are captured by k_x,k_y momentum imaging and E_{kin} variation via the photon energy. This approach maximizes the information obtained from the PED experiment. It combines the '*large-solid-angle mode*' [1] with the *'scanned-energy mode'*[2,3]. First experiments were performed using the combined hemispherical & time-of-flight momentum microscope[4] at beamline I09 at the Diamond Light Source. This instrument is equipped with a novel multimode front lens[5]. Photoelectrons from the selected core level are recorded in a large solid angle (2p at low energies). This approach was benchmarked on the model systems Si and Ge (Si-2*s*,-2*p*, Ge-3*p*,-3*d*) down to 35eV. Despite the fact that the inelastic mean free path is only a few interatomic distances, all PED patterns show a rich structure, see example rows 1&3 in Fig.1 (all images show CDAD contrast). The PED patterns for Ge-3*d* and-3*p*, as well as Si-2*s* and-2*p* show significant differences, emphasizing the influence of the initial state. One-step photoemission calculations[6] agree well with experimental data (rows2&4 in Fig.1) and predict PED structures down to the photoemission threshold. These calculations bridge the gap between classical PED analysis and electronic structure investigations.

[1] Fadley & Bergstrom, *Phys.Lett.*A,**35**,375(1971)
[2] Kevan,Shirley et al., *Phys.Rev.Lett.***41**,1565(1978)
[3] Woodruff & Bradshaw, *Rep.Prog.Phys*.**57**,1029(1994)
[4] Schmitt & al.,*Ultramicroscopy,* **276**,14169(2025)
[5] Tkach & Schönhense,*Ultramicroscopy,* **276**,14167(2025)
[6] Vo et al., *npj Comput.Mater*.,**11**,159(2025)



When: 2026-06-25, 14:55 - 15:15, Where: Sonja Lyttkens

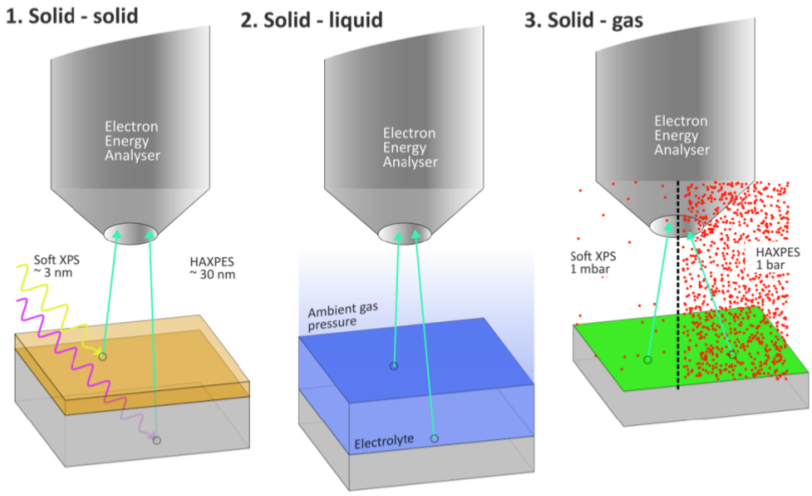
O73 - SpectroMAX: A New Hard X-ray Photoelectron Spectroscopy Beamline at MAX IV Laboratory

Instrumentation

Robert Temperton[1]
Esko Kokkonen[1], Andrey Shavorskiy[1], Louisa Pickworth[1], Marcus Agåker[2], Andreas Lindblad[2]
[1] MAX IV Laboratory, Lund University, Fotongatan 2, 224 84 Lund, Sweden
[2] Department of Physics and Astronomy, Uppsala University, Regementsvägen 1, 75237 Uppsala, Sweden

Abstract text: MAX IV recently completed a technical design report (TDR) for a possible new tender-to-hard X-ray beamline dedicated to operando HAXPES studies of advanced materials and devices in action. The TDR, funded by the Wallenberg Initiative Materials Science for Sustainability, proposes a beamline and a suite of instruments to investigate the interfaces between solids, liquids, and gases of relevance to areas including catalysis, energy storage, corrosion, photovoltaics, advanced electronics, the green hydrogen economy, and more. The increased probing depth of HAXPES (compared to standard XPS) opens up possibilities to study the chemical properties of solid-solid buried functional interfaces, solid-liquid and solid-gas interfaces at pressures of several atmospheres. Such properties can then be investigated as a function of temperature, pressure, bias, and illumination.

This talk presents the outcome of the TDR: a state-of-the-art beamline providing X-ray photon energies from 2.1 up to 15 keV with a tuneable beam size between ~2 and ~200 µm. This enables both spatial mapping of heterogeneous surfaces and also beam-damage control for sensitive samples. Two focal points allows for a diverse selection of sample environments: A UHV-HAXPES setup will be permanently installed in the upstream focal point of the beamline. The downstream focal point will be a flexible port where one can switch between two *operando* AP-HAXPES instruments, one optimised for solid-liquid and the other for solid-gas interfaces (at gas pressures up to 1 bar), or alternatively to host user-provided instruments. Together, this would provide Sweden with a flexible and world-leading platform for studies of functional interfaces.



When: 2026-06-24, 10:20 - 10:40, Where: Heinz-Otto Kreis

O74 - Time-resolved XAS in the range from nanoseconds to seconds to probe rearrangements around catalytic centers induced by light.

Instrumentation

Grigory Smolentsev[1], Thomas Huthwelker[1], Raphael Jay[2], Philippe Wernet[2], Cheshta Chopra[1, 3], Silvia Grandi[4], Stefano Caramori[4], Abhimanyu Bharade[1], Thomas Schmidt[1, 3],Maarten Nachtegaal[1, 3]
[1] Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland
[2] Uppsala University, 75120, Uppsala, Sweden
[3] ETH Zürich, CH-8093 Zürich, Switzerland
[4] University of Ferrara, 44121 Ferrara, Italy

Abstract text: An overview of recent developments and applications of light-initiated time-resolved X-ray absorption spectroscopy at the Swiss Light Source (SLS) synchrotron will be presented. This includes the development of a pump–probe instrument covering time scales from 100 ps to a few microseconds using tender X-rays. The instrument is unique among synchrotrons and complementary to setups available at X-ray Free Electron Lasers such as SwissFEL. We demonstrate its application to carbon–hydrogen bond activation by a Rh complex[1]. Two intermediate states—alkane complexation at the Rh center and the oxidative addition step—were captured using pump–probe XAS at the Rh L_3 edge. This enabled construction of a molecular-level picture of C–H activation with orbital resolution.

Pump–probe XAS in the hard X-ray range, particularly on nanosecond to microsecond time scales, has also been used at SLS to investigate photocatalytic and luminescent materials[2]. Slower processes in the millisecond regime, relevant for working photoelectrodes, can be studied using modulated light excitation combined with time-resolved X-ray fluorescence detection. Such capabilities are also available at ESRF. As a recent example, we investigate structural changes around Co in oxygen-evolving photoelectrodes consisting of a CoPi catalyst on a Fe_2O_3 light absorber. By comparing transient XAS spectra with simulations based on different mechanistic models, the role of Co centers—whether in hole accumulation or as catalytic sites in the rate-limiting step—is clarified.

Finally, new opportunities for pump–probe XAS and XES enabled by the SLS2.0 upgrade will be discussed.

[1]Jay et al. *Science* **2023**, 380, 955.
[2]M. Vogt, G. Smolentsev *ChemPhotoChem* **2022,** 6, e202100180

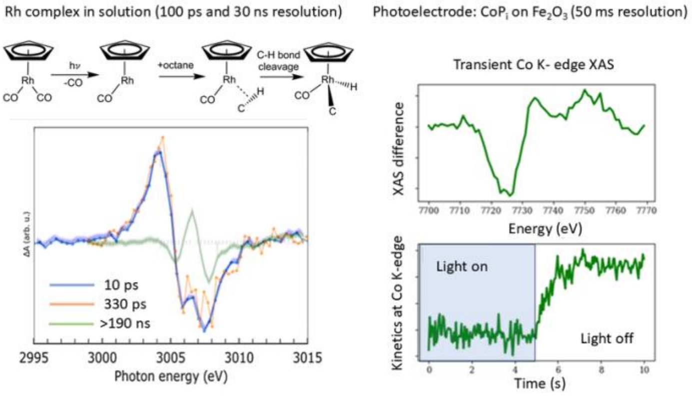


Figure 1. Left: Pump-probe XAS at Rh L3-edge corresponding to C-H bond activation. Right: Transient XAS at Co K-edge for CoPi-Fe_2O_3 photoelectrode.

Liquids

When: 2026-06-25, 11:15 - 11:40, Where: Eva von Bahr

O75 - Attosecond spectroscopy of electronic decoherence in liquid water

Liquids

HUGO MARROUX[1]
[1] Université Paris - Saclay, CEA, LIDYL, Gif-sur-Yvette, 91191, France.

Abstract text: Electron scattering dynamics in liquid water play a central role in fields ranging from ultrafast chemistry to radiolysis. Currently, comparisons of photoelectron angular distributions (PADs) measured in gas and liquid phases are the primary experimental approach for characterizing elastic and inelastic mean free paths in water. Reported values are typically below 10 nm for photoelectrons with kinetic energies under 100 eV, corresponding to scattering times on the atto to few-femtosecond scale. Attosecond spectroscopy therefore offers a promising complementary approach.
Here, we perform reconstruction of attosecond beating by two-photon transitions (RABBIT) measurements on gas- and liquid-phase water over a kinetic energy range of 30–60 eV. RABBIT is an electron interferometry technique based on two-photon transitions induced by an IR dressing field overlapped with an XUV attosecond pulse train, producing oscillatory photoelectron interferograms as a function of IR–XUV delay. The oscillation phase encodes photoionization dynamics, while the contrast reflects the coherence of the electronic wavepacket.

We observe a strong reduction of the oscillation contrast from 0.6 in the gas phase to 0.2 in the liquid phase. Control experiments and simulations allowed us to clearly identify elastic scattering in the liquid environment as the dominant source of decoherence. To interpret these observations, we developed a stochastic model of liquid-phase RABBIT spectroscopy linking decoherence to electron mean free paths and scattering phases. These results demonstrate, for the first time, the use of RABBIT spectroscopy to probe electronic decoherence in liquids.

O76 - How Surfactants Control the Work Function of Aqueous Solutions

Liquids

Qi Zhou[1]
Dominik Stemer[1], Clemens Richter[1], Etienne Rouquet[1], Michele Pugini[1], Rémi Dupuy[1, 2], Tillmann Buttersack[1], Florian Trinter[1], Uwe Hergenhahn[1], Hendrik Bluhm[1], Stephan Thürmer[3], Gerard Meijer[1], Bernd Winter[1]
[1] Department of Molecular Physics, Fritz-Haber-Institut der Max Planck Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany
[2] Sorbonne Université, CNRS, Laboratoire de Chimie Physique - Matiere et Rayonnement, LCPMR, F-75005 Paris Cedex 05, France
[3] Department of Chemistry, Graduate School of Science, Kyoto University, Kitashirakawa-Oiwakecho, Sakyo-Ku, Kyoto 606-8502, Japan

Abstract text: Recent developments in liquid-jet photoelectron spectroscopy (LJ-PES) enable the determination of absolute electron binding energies (BEs) [1]. Utilizing this technique, we previously observed up to 0.7 eV BE shifts of water's spectral features in solutions containing surfactant tetrabutylammonium iodide [2], mainly attributed to changes in the solutions' work function as a function of concentration, due to the build-up of an interfacial dipole layer. Understanding the effect of charge distribution and interfacial orientation of a surfactant molecule on the work function and ionization energy is of great importance in atmospheric chemistry, where complex mixtures are present at aerosol interfaces.

We explored benzoic acid, octanoic acid, and their fluorinated derivatives, which exhibit different dipole moment orientations relative to the solution surface. Here, we observe that a reversal in dipole orientation leads to spectral shifts of water's lowest-BE feature in opposite directions, with the magnitude depending on the dipole moment component normal to the interface. For a useful comparison of the different surfactants, we correlate PES results to interfacial molecule concentrations as assessed via concentration-dependent surface-tension measurements. Our results demonstrate how even small chemical modifications of a surfactant molecule may strongly alter the interfacial potential, i.e., how easily electrons can cross the aqueous-phase interface. In an atmospheric chemistry context, work functions affect charge exchange between aerosols and gaseous species, formation of reactive species, and the reactivity of water surfaces.

References

[1] Thürmer *et al.*, *Chem. Sci.*, **12**, 10558-10582 (2021).
[2] Credidio *et al.*, *Phys. Chem. Chem. Phys.*, **24**, 1310-1325 (2022).

When: 2026-06-22, 11:10 - 11:35, Where: Sonja Lyttkens

O77 - Intermolecular Decay of X-Ray-Irradiated Solvated Ions studied by coincidence spectroscopy

Liquids

Dana Bloß[1]
[1] Universität Kassel

Abstract text: The investigation of liquid samples by X-ray induced electron spectroscopy has made tremendous progress throughout the last decades through the development of the liquid microjet technique. One of the main remaining challenges is the study of secondary non-local ionization mechanisms such as intermolecular Coulombic decay (ICD) and electron-transfer-mediated decay (ETMD). Due to the low energy of the emitted electrons, their signal is often hidden in an enormous background of slow electrons produced by scattering effects. The coincident detection of multiple electrons emitted from liquids after their exposure to ionizing radiation is a promising approach to overcome this challenge by significant suppression of the background. We describe a magnetic bottle electron spectrometer for coincident multi-electron detection from liquid samples and present results on ICD and ETMD processes from Auger final states in prototypical solvated Mg^{2+} and Ca^{2+} ions. In Mg^{2+}, X-ray ionization of the K-shell and following Auger decay triggers a rich cascade of ICD and ETMD processes, some of which could be identified experimentally. Remarkably, they leave the ions finally in their initial state and can be regarded as catalysts for X-ray induced production of slow electrons and water cations. In Ca^{2+}, we use resonant excitation and subsequent resonant Auger decay for driving ICD. In this scenario, the emission of slow electrons and production of water cations is site- and energy-selective, with potential implications in radiation damage contexts.

When: 2026-06-22, 10:45 - 11:10, Where: Sonja Lyttkens

O78 - Liquid-Jet Photoelectron Spectroscopy of Aqueous Solutions: Electron Scattering and Interfacial Properties

Liquids

Bernd Winter[1]
[1] Fritz-Haber-Institut, Faradayweg 4-6, 14195 Berlin, Germany

Abstract text: Liquid-jet photoemission spectroscopy (LJ-PES) is a well-established technique for directly probing electronic structure, molecular and solute organization, and interfacial properties in aqueous solutions. By precisely referencing the kinetic energies of both primary and secondary electrons to the vacuum and Fermi levels, LJ-PES provides a direct bridge between surface science and electrochemical descriptors.

In this presentation, I examine the capability of PES to resolve solute distributions at the solution–vacuum interface, with particular emphasis on the absolute electron probing depth into solution. This analysis is grounded on quantifying associated inelastic and elastic electron scattering lengths, over a wide range of electron energies, fully based on experiment.

The talk concludes by addressing key challenges in studying near-ionization-threshold processes, where photoelectron signals are significantly perturbed by quasi-elastic electron scattering. A notable example is aqueous-phase photoelectron circular dichroism (PECD), which requires highly specialized experimental setups and motivates the development of more efficient future electron detection schemes.

When: 2026-06-25, 12:00 - 12:20, Where: Eva von Bahr

O79 - Local Electronic Structure of Methylammonium in Solid, Solution, and Gas Phase Probed by Resonant Inelastic (Soft) X-ray Scattering

Liquids

Dirk Hauschild[1, 2, 3], Constantin Wansorra[1, 2], Stephen Faussett[2], Ralph Steininger[1], Wanli Yang[4], Clemens Heske[1, 2, 3], Lothar Weinhardt[1, 2, 3]
[1] Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT), Kaiserstraße 12, 76131 Karlsruhe, Germany
[2] Department of Chemistry and Biochemistry, University of Nevada, Las Vegas (UNLV), 4505 Maryland Parkway, Las Vegas, NV 89154-4003, USA
[3] Institute for Chemical Technology and Polymer Chemistry (ITCP), Karlsruhe Institute of Technology (KIT), Kaiserstraße 12, 76131 Karlsruhe, Germany
[4] Advanced Light Source (ALS), Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Abstract text: Methylammonium (MA$^+$, $CH_3NH_3^+$) is the prototype organic cation in hybrid halide perovskite-based solar cells. Its local electronic structure and hydrogen-bonding interaction critically influences the optoelectronic properties and long-term stability of the devices. To understand their electronic structure, soft x-ray emission spectroscopy (XES) and resonant inelastic (soft) x-ray scattering (RIXS) provide a local (i.e., atom-specific) probe of the occupied and unoccupied states.

In our contribution, we determine the local electronic structure of MACl, MABr, and MAI salts in the solid state, in aqueous solutions at low and high pH values (i.e., with protonated and deprotonated amine groups), in dimethyl sulfoxide (DMSO), and in the gas phase. The experimental data is complemented by density functional theory (DFT) spectra calculations (Fig. 1). In the solid state, a strong influence of nuclear dynamics on the time scale of the RIXS process is found, which is anion-dependent. In aqueous solution and in DMSO, the characteristic N K NH_3^+ fingerprint is retained, but distinct spectral differences to the solid state indicate strong solvent–solute interactions. Methylamine in aqueous solution at high pH and in the gas phase shows a characteristic NH_2 spectral signature. The strong spectral changes will be discussed in view of the local chemical and electronic structure and across the different MA environments.

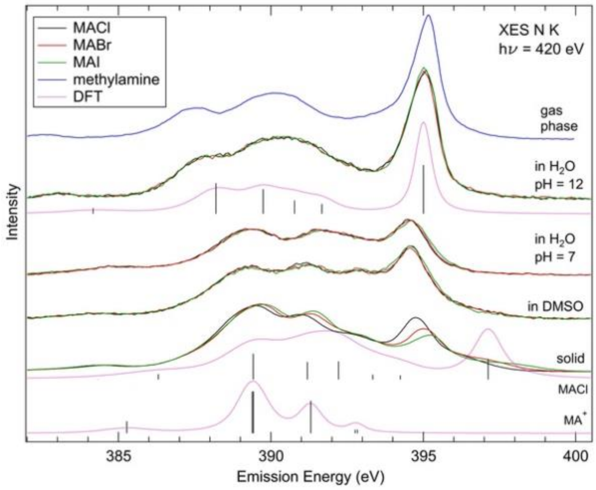


Fig. 1: N K XES spectra of MACl (black), MABr (red), MAI (green), and methylamine (blue). DFT-calculated x-ray emission intensities (black bars) and the corresponding broadened spectra (magenta) are shown. From bottom to top: solid state, in DMSO, in aqueous solution (low and high pH), and in gas phase.

When: 2026-06-25, 11:40 - 12:00, Where: Eva von Bahr

O80 - Modulation of Amino Acid Interfacial Behavior by Inorganic Salts in Aqueous Solutions

Liquids

Ricardo R. T. Marinho[1], Vincenzo Carravetta[2], Alexandra Mocellin[1], Caroline Leck[3], Christophe Nikolas[4], Debora Vasconcelos[5], Joel Anderson[6], Sirin Gholami[4], Ouassim Hocine[5], Michele Pugini[4], Florian Trinter[4], Eva Muchova[7], Rebecca Ingle[8], Marta Berholts[5], Iyas Ismail[9], Victoria Kabanova[5], Gunnar Öhrwall[10], Olle Björneholm[5], Hans Ågren[5, 11], **Arnaldo Naves de Brito**[6]
[1] Institute of Physics, University of Brasilia, Brasilia, Brazil
[2] Institute of Chemical and Physical Processes, Pisa, Italy
[3] Department of Meteorology, Stockholm University, Stockholm, Sweden
[4] Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
[5] Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden
[6] Institute of Physics Gleb Wataghin, University of Campinas, Campinas, Brazil
[7] Department of Physical Chemistry, University of Chemistry and Technology,Prague, Czech Republic
[8] Department of Chemistry, University College London, London, United Kingdom
[9] Sorbonne Université, CNRS, Paris, France
[10] MAX IV Laboratory, Lund University, Lund, Sweden
[11] Faculty of Chemistry, Wroclaw University of Science and Technology, Wroclaw, Poland

Abstract text: Cloud activation and related interfacial processes are strongly influenced by the partitioning of organic solutes between the bulk and the surface of aqueous salt solutions. Building on our previous research on the surface propensity of amino acids in aqueous solutions [1], we investigate how inorganic salts modify the interfacial behavior of three representative amino acids—valine, serine, and glycine—using a combination of surface-sensitive spectroscopy and molecular simulations. We focus on how varying ionic strength and cation identity affect the relative accumulation or depletion of these amino acids at the solution–vapor interface under near-neutral conditions.

We employ X-ray photoelectron spectroscopy to quantify the interfacial enrichment of each amino acid in the presence of different salts, and classical molecular dynamics simulations to interpret the observed trends in terms of molecular orientation and hydration patterns. The experiments reveal a clear hierarchy in surface propensity among the three amino acids and show that added electrolytes can selectively enhance the interfacial presence of the more amphiphilic species, particularly in solutions containing divalent cations. The simulations provide a microscopic picture that links this behavior to salt-induced changes in hydration and the energetic balance governing hydrophobic side-chain exposure at the interface.

These results identify a concrete mechanism by which common seawater ions modulate the surface activity of amino acids, with implications for organic enrichment at marine interfaces and potential downstream effects on aerosol formation and cloud droplet nucleation.

Reference: 1] Björneholm, O., Öhrwall, G., de Brito, A. N., Ågren, H., & Carravetta, V. *Accounts Chem. Res.* **55**, 3285–3293 (2022).

O81 - Soft X-ray Views of Molecular Dynamics in Complex Environments

Liquids

Zhong Yin[1]
[1] Tohoku University

Abstract text: Light–matter interactions are fundamental processes that govern much of the natural world. The initial absorption of light by a system triggers a cascade of ultrafast dynamics within a complex environment. Understanding each step of this intricate pathway at the molecular level remains one of the central challenges in modern science, largely due to the extreme timescales involved and the strong coupling between electronic and nuclear motion.[1,2]
In this talk, I will present experimental examples that exploit the power of X-ray spectroscopy to investigate chemical systems in their natural environment: the liquid phase. X-ray spectroscopy is an element-, site-, and orbital-specific technique that acts as a highly localized probe of molecular electronic structure.[3] This unique capability makes it an indispensable tool for unraveling the complex interplay between chemical systems and their surrounding environment.
The presented work combines "water-window" photon sources[4] and endstations at large-scale light-source facilities,[5,6] These approaches open new opportunities for studying molecular dynamics, solvation effects, and nonequilibrium processes in complex environments with unprecedented resolutions.[7-9]

References

[1] J.R. Dwyer, et al. PTRS. A, 364, 741 (2006). [2] C. Bostedt et al, RMP 88, 015007 (2016) [3] T. Fransson et al. Chem. Rev. 116, 7551 (2016) [4] A.R. Attar et al, Science 356, 54 (2017) [5] J. Schlappa et al. JSR 32, 29 (2025) [6] M. Agåker et al. JSR 32, 1328 (2025) [7] Z. Yin et al Nature, 619, 749 (2023) [8] Y.P. Chang et al Nature Physics, 21, 137 (2025) [9] Z. Yin et al. JACS 147, 9190 (2025)

When: 2026-06-22, 11:35 - 11:55, Where: Sonja Lyttkens

O82 - Spin states of myoglobin heme iron in aqueous solutions at room temperature probed from porphyrins using nitrogen K-edge X-ray absorption spectroscopy

Liquids

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Abstract text: We conducted X-ray absorption spectroscopy (XAS) measurement for myoglobin dissolved in water (1 mM) at the nitrogen K-edge using a transmission-type liquid cell [1] at the soft X-ray beamline BL3U at the UVSOR-III Synchrotron [2]. In the XAS spectra of myoglobin, peaks associated with the C=N π* orbitals were identified in positions lower than the peak associated with the polypeptide. We then calculated inner-shell excitation energies for with or without coordinated oxygen molecule as well as different oxidation numbers of the heme iron (Fe^{2+}/Fe^{3+}) with the time-dependent density functional theory (TDDFT) [3] considering the scalar relativistic effect by the Douglas–Kroll–Hess (DKH) transformation [4]. The comparison clarified that oxymyoglobin, which consists of myoglobin (Fe^{2+}) and an oxygen molecule, is in the lowest spin state ($S = 0$). It also clarified that deoxymyoglobin, which is myoglobin (Fe^{2+}) without oxygen, is in spin fluctuation between $S = 2$ and 1, while metmyoglobin (Fe^{3+}) is in spin fluctuation between $S = 5/2$ and 3/2. The present work shows capability of XAS at the porphyrin ring to identify the spin state of myoglobin in solutions influenced by physiological conditions such as temperature and the protein structure [5].

References

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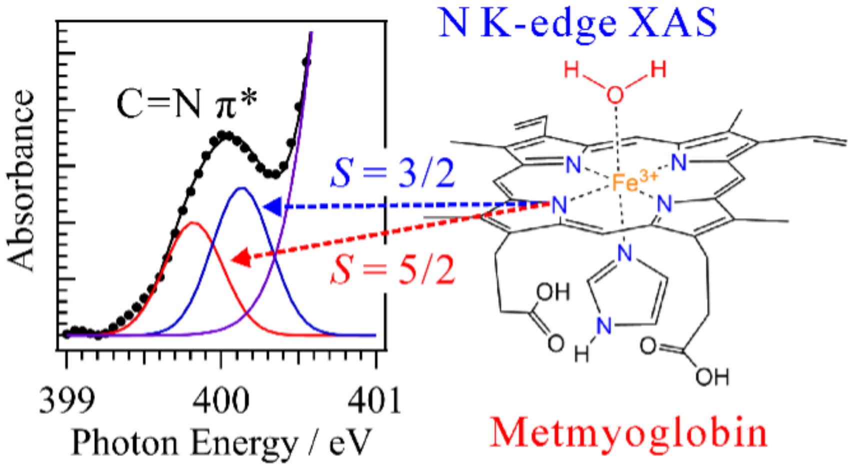

When: 2026-06-25, 09:55 - 10:20, Where: Eva von Bahr

O83 - Stability and Reactivity of Aromatic Radical Anions in Solution

Liquids

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Abstract text: Radical anions of aromatic hydrocarbons are key intermediates in reactions spanning organic, inorganic and organometallic chemistry. A well-known example is the Birch reduction, in which the aromaticity of arenes is disrupted to form nonconjugated cyclohexadiene. We investigate the electronic structure of aromatic radical anions in the solution phase employing a combination of liquid-jet (LJ) photoelectron (PE) spectroscopy measurements and electronic structure calculations. Specifically, we characterised the pure solvent tetrahydrofuran (THF) using LJ-PE measurements alongside initio molecular dynamics simulations and G_0W_0 calculations.

Next, we determined the electronic structure of the neutral molecules naphthalene (Np) and benzophenone (Bp), as well as their radical anion counterparts, Np^{-} and Bp^{-}, in THF. Wherever feasible, we performed orbital assignments of the measured PE features of the aromatic radical anions, comparing them to UV–vis absorption spectra of the corresponding neutral molecules to help rationalise the assignments. Analysing the differences in electronic structure between the neutral species and their anionic counterparts provides insight into the electrostatic stabilisation of the radical anions in solution.

Finally, we achieve excellent agreement between the reduction potentials extracted from the present LJ-PES measurements of Np^{-} and Bp^{-} in THF and previous electrochemical data obtained from cyclic voltammetry measurements. In this context, we discuss how the choice of solvent significantly impacts the optimisation of conditions for the Birch reduction process, in which aromatic radical anions play a crucial role as reactive intermediates. Furthermore, we give an outlook on how we aim to increase the reactivity of these radical anions employing photo-excited states.

When: 2026-06-25, 10:20 - 10:40, Where: Eva von Bahr

O84 - Tender X-ray RIXS Studies of Intermolecular Charge Transfer in Aqueous Solutions

Liquids

Iyas ISMAIL[1]
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Abstract text: Charge transfer between ions and the surrounding solvent plays a central role in aqueous chemistry, governing processes such as electron solvation, intermolecular coupling, and chemical reactivity. Core-level spectroscopies provide a powerful way to probe these processes because the excitation starts from localized orbitals and the subsequent decay occurs on ultrafast timescales.

I will first present the MOSARIX multi-crystal spectrometer developed by our group and installed at the GALAXIES beamline of the SOLEIL synchrotron. This instrument enables efficient tender X-ray emission and resonant inelastic X-ray scattering (RIXS) measurements in the 2–12 keV range and allows experiments on liquid jets under bulk-sensitive conditions.

Using this setup, we investigate two directions of charge transfer between ions and solvent /ligand.

First, we study intermolecular radiative decay (IRD), a non-local relaxation process in which a core hole on a solvated ion is filled by an electron originating from neighboring solvent molecules or ligands. This process corresponds to charge transfer from the solvent to the ion, and the emitted photon reflects the electronic structure of the first solvation shell. Measurements on aqueous Ca^{2+} systems show that IRD provides a chemically selective probe of the local coordination environment, revealing changes associated with chelation by EDTA and ion pairing.

We then investigate charge-transfer-to-solvent (CTTS) excitations in aqueous iodide. The L_3 RIXS maps display a crossover from Raman-like dispersive emission to fluorescence-like emission near the ionization threshold. We show that the ultrashort core-hole lifetime (~200 as) limits electron delocalization, so that the observed CTTS states retain an exciton-like character.

When: 2026-06-22, 11:55 - 12:15, Where: Sonja Lyttkens

O85 - X-Ray-Induced Charge-Transfer-Processes in Solution

Liquids

Olle Björneholm[1]
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Abstract text: X-ray-induced core excitation and decay dynamics of isolated atoms is nowadays relatively well understood. How are such processes affected by an aqueous environment? I will discuss some recent studies on how water molecules may participate in non-local processes involving charge transfer, such as Intermolecular Coulombic Decay (ICD) [1], Electron Transfer Mediated Decay (ETMD) [2], and Intermolecular Radiative Decay (IRD) [3] in various stages of the core-hole excitation and decay. These processes are relevant for issues connected to radiation damage in an aqueous environment, and they also openthe possibility to probe the local environment of solutes, and ultrafast solute-solvent electron dynamics.

Exciting or ionizing core levels to induce these processes provides chemical selectivity and the possibility to probe ultrafast processes. Chemical selectivity comes from the core-levels being atomic-like and localized, which enables selective probing of chemically inequivalent species. The core-holes have typically a lifetime of a few femtoseconds, which is used in core-hole-clock techniques to probe ultrafast processes from tens of femtoseconds down to a few hundred attoseconds. I will introduce these processes, and present recent results that exemplify some types of phenomena in solution that can be studied, and what can be learned.

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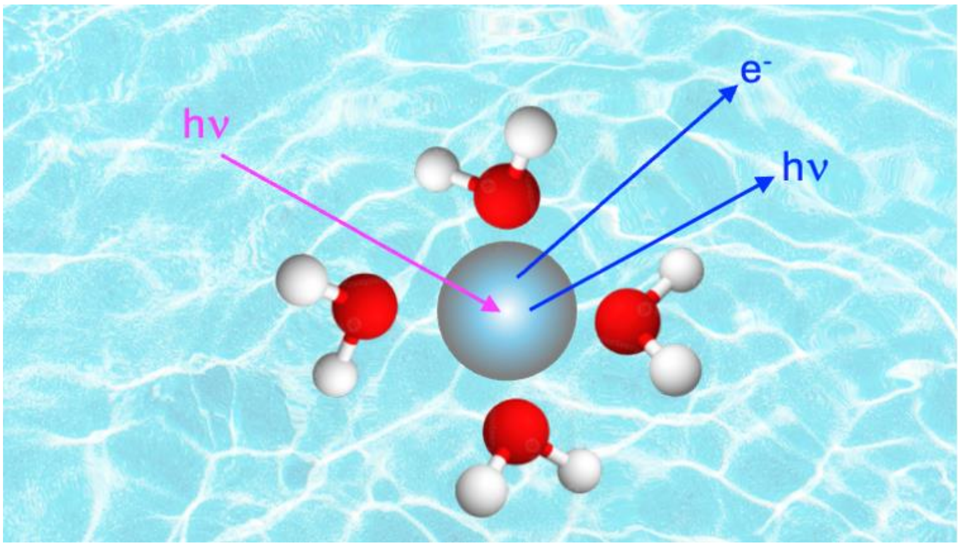

RIXS

O86 - Lattice Coupling of Trapped O_2 in Battery Cathodes Probed by O K-edge Resonant Inelastic X-ray Scattering and Benchmarked Against O_2 Implanted in Gold

RIXS

Pontus Törnblom[1], Moritz Hirsbrunner[1], Johan Oscarsson[2], Mauricio Sortica[2], Sahil Tippireddy[3], Ke-Jin Zhou[3], Mirian Garcia-Fernandez[3], Robert House[4], Daniel Primetzhofer[2], Håkan Rensmo[1], Laurent Duda[1]

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[3] Diamond Light Source, Harwell Science and Innovation Campus, Didcot, United Kingdom
[4] Department of Materials, University of Oxford, Oxford, United Kingdom

Abstract text: Certain battery cathodes form trapped molecular O_2. Whether this is an electrochemical effect or x-ray beam induced is debated in literature. If it indeed occurs during charge and becomes reincorporated back into lattice oxygen upon discharge it offers a reversible mechanism for storing additional charge. Regardless of the production mechanism, little is known about the local environment of this trapped O_2, about how it couples to the surrounding lattice and the formation/dissolution processes. Therefore we applied high-resolution resonant inelastic x-ray scattering (RIXS) at the O K-edge to charged lithium-ion (LR-NMC) and sodium-ion (NMMO) cathodes, alongside a reference model system of O_2 implanted in gold (O-in-Au) that confines O_2 in a chemically inert host.

By analysing the scattering-angle-dependent parity-forbidden transitions of O_2 and by simulating the vibrational-progression envelope with Morse potentials, we find that the cathodes exhibit substantially larger parity-forbidden spectral weight than free O_2, consistent with inversion-symmetry breaking at inequivalent trapping sites. The simulations reveal a weakened ground-state bond and a strongly perturbed intermediate-state potential with increased lifetime broadening. NMMO and LR-NMC show clear signatures of lattice-molecule coupling, with NMMO indicating a more strongly interacting environment, while these signatures are only weak in the more gas-phase-like O-in-Au.

Together, these results show that trapped O_2 in charged cathodes is not an inert spectator but is measurably modified by coupling to the transition-metal-oxide framework. Looking ahead, we are developing in-situ and operando O K-edge RIXS capabilities to track the formation and reincorporation of trapped O_2 in real time during electrochemical cycling.

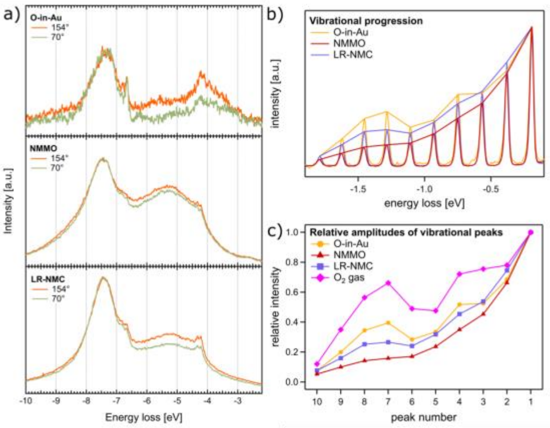

Figure 1. O K-edge RIXS spectra measured at 531 eV in a) displaying the intenisty increase of the parity forbidden transitions between energies -7 to -4 eV in energy loss as the scattering angle becomes more backscattered for the battery cathodes and O-in-Au. In b) and c) the vibrational envelope is traced for the same samples as well as for free O_2 gas.

When: 2026-06-25, 14:00 - 14:45, Where: Eva von Bahr

O87 - Magnetically Coupled Excitons in van der Waals Quantum Materials

RIXS

Mark P. M. Dean[1]
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Abstract text: Recent advances in resonant inelastic x-ray scattering (RIXS) have revealed a new class of excitonic quasiparticles in magnetic van der Waals materials, where electronic and spin degrees of freedom are intrinsically intertwined. I will present an overview of dispersive excitons across antiferromagnetic $NiPS_3$, ferromagnetic CrI_3, and anisotropic semiconductor CrSBr. In $NiPS_3$, we demonstrate that the exciton is a Hund's exciton whose formation is governed by local Hund's exchange and whose propagation closely mirrors double-magnon dynamics, establishing a direct link between exciton motion and spin exchange processes[1]. Extending this framework to ferromagnetic CrI_3, we identify sharp, spin-flip dark excitons that disperse with bandwidths comparable to magnetic excitations and exhibit strong temperature dependence across the magnetic transition, highlighting their magnetic origin and long lifetimes[2]. Finally, in CrSBr, we uncover an anisotropic dark exciton with unexpected two-dimensional propagation coexisting with quasi-one-dimensional electronic structure, pointing to exchange-mediated hopping mechanisms distinct from conventional band-like excitons[3]. Together, these results establish a general paradigm in which exciton dispersion in correlated magnets is governed by spin interactions rather than purely electronic band structure. This emerging class of magnetically coupled excitons opens new avenues for controlling energy and information transport in quantum materials.

W. He et al., Magnetically propagating Hund's exciton in van der Waals antiferromagnet $NiPS_3$, Nature Communications 15, 3496 (2024).
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When: 2026-06-22, 11:35 - 11:55, Where: Eva von Bahr

O88 - Matrix dependent modulation of parity selective RIXS channels in molecular oxygen

RIXS

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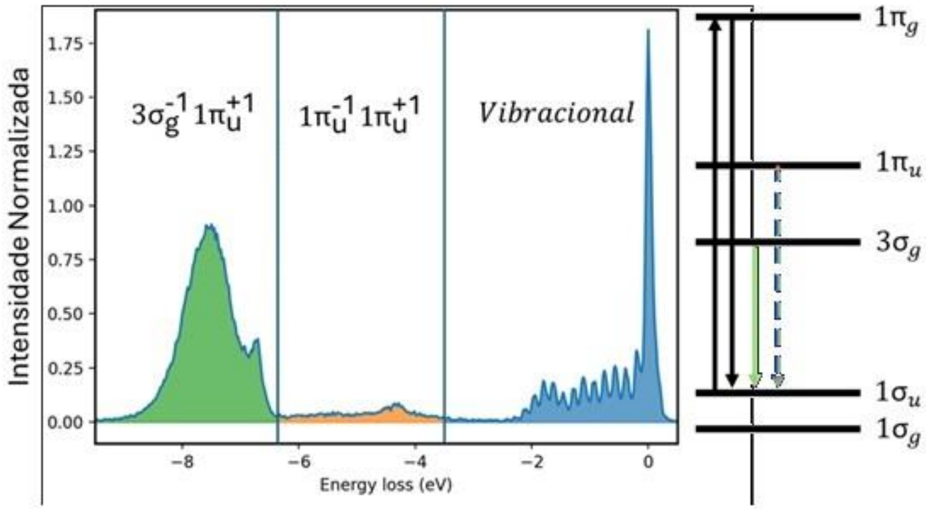
Abstract text: Resonant inelastic soft X-ray scattering at the O K edge of molecular oxygen provides direct access to parity selective decay channels following excitation at the 1s → π* resonance. In gas phase O_2, Söderström et al. demonstrated that the spectral region from 3.95 to 6.35 eV is dominated by parity forbidden ungerade final states, mainly $A'^3\Delta u$, $A^3\Sigma_u^+$ and $B^3\Sigma_u^-$, whereas the 6.35 to 9.55 eV region is dominated by the parity allowed gerade $B'^3\Pi g$ final state. They further showed that the low/high intensity ratio is an operational measure of the forbidden to allowed balance and that this ratio is sensitive to interference effects and parity violation in O_2 RIXS. Here, we use this same spectral framework to compare pure O_2 and O_2 diluted in a cryogenic Ar matrix. Our data show that the low/high ratio decreases from 0.105 for pure O_2 to 0.054 for $Ar:O_2$, corresponding to an approximately twofold reduction of the low energy contribution under matrix isolation. This result indicates that the surrounding argon environment measurably alters the balance between parity forbidden and parity allowed channels. This behavior is consistent with a modification of the symmetry sensitive interference conditions that govern the final state distribution in O K edge RIXS. These results establish the forbidden to allowed spectral ratio as a sensitive probe of environmental perturbation in molecular oxygen and support the use of parity selective RIXS observables to investigate weak confinement and symmetry breaking effects in condensed and matrix isolated systems.



When: 2026-06-25, 15:15 - 15:35, Where: Eva von Bahr

O89 - Nonlocal resonant inelastic X-ray scattering

RIXS

Ji-Cai Liu[1]
Faris Gel’mukhanov[2], Victor Kimberg[2], Jian Wang[1], Marcus Agåker[3, 4], Joseph Nordgren[3], Johan Forsberg[4], Victor Ekholm[4], Conny Såthe[4], Olle Björneholm[3], Arnaldo Naves de Brito[5], Takashi Tokushima[4], Anirudha Ghosh[4], Jan-Erik Rubensson[3], Johan Söderström[3]
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Abstract text: Resonant X-ray and Auger scattering of symmetric molecules is a nice tool to study a fundamental quantum mechanical effect – Young’s double slit scattering [1-4]. In the description of resonant inelastic X-ray scattering (RIXS) from inversion-symmetric molecules the small core-level splitting is typically neglected. However, the spacing Δ between the gerade and ungerade core levels in homonuclear diatomic molecules can be comparable to the lifetime broadening Γ of the intermediate core-excited state. We show that when $\Gamma \sim \Delta$, the scattering becomes nonlocal in the sense that X-ray absorption at one atomic site is followed by emission at the other site [5]. This is manifested in an unusual dependence of the RIXS cross section on the sum of the momenta of incoming and outgoing X-ray photons $k + k'$, contrary to the normal $k - k'$ dependence in the conventional local RIXS theory. The nonlocality of the scattering strongly influences the scattering-angle and excitation-energy dependence of the intensity ratio between parity forbidden and allowed RIXS channels [5]. Numerical simulations for N_2 show that the nonlocal RIXS process can readily be observed at present-day X-ray radiation facilities, and we discuss recent experimental results.

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[2] A. Revelli, et al, Sci. Adv. **5**, 2375 (2019)
[3] F. Gel’mukhanov, et al., Rev. Mod. Phys. **93**, 035001 (2021)
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[5] F. Gel’mukhanov, et al., Phys.Rev.A. **108**, 052820 (2023)

When: 2026-06-25, 14:55 - 15:15, Where: Eva von Bahr

O90 - Probing bond covalency in M2UO2Cl4 (M = Rb, Cs) with O K resonant inelastic soft x-ray scattering

RIXS

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Natalia Palina[4], Harry Ramanantoanina[4], Kurtis Stanistreet-Welsh[5], Ralph Steininger[1], Constantin Wansorra[1, 3], Dirk Hauschild[1, 2, 3], Andy Kerridge[5], Clemens Heske[1, 2, 3], Tonya Vitova[4], Lothar Weinhardt[1, 2, 3]
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Abstract text: Uranium(VI), specifically U(VI)O_2^{2+}, plays a crucial role in the mobilization behavior of uranium in its environment and is thus highly relevant to the long-term safety assessment of nuclear waste repositories in geological formations. New and deeper insights into the U(VI)O_2^{2+} electronic structure and bonding properties require novel experimental and theoretical spectroscopic approaches. In this contribution, we apply O K resonant inelastic soft x-ray scattering (RIXS) to study bond covalency in $M_2UO_2Cl_4$ (M = Rb, Cs). We collected O K RIXS maps using our high-transmission spectrometer of the X-SPEC beamline at the KIT Light Source. The experimental data is compared to calculations using time-dependent density functional theory and restricted active space self-consistent field (RASSCF) theory simulations. Features in the experimental O K RIXS maps and x-ray absorption spectroscopy (XAS) data are consistent with the calculated spectra. In the XAS spectra, peaks corresponding to electronic transitions from O 1s to molecular orbitals consisting of a mix of O 2p, U 5f, and 6d orbitals demonstrate a covalent U-O bonding interaction. We find the absorption edge at higher energies for $Rb_2UO_2Cl_4$ as compared to $Cs_2UO_2Cl_4$; a detailed analysis of this finding and of the O K RIXS and XAS data will be presented, providing a comprehensive picture of the electronic and chemical structure in $M_2UO_2Cl_4$ (M = Rb, Cs) from the perspective of the O atoms.

When: 2026-06-22, 10:45 - 11:10, Where: Eva von Bahr

O91 - Recent progress at the beamline for resonant inelastic soft X-ray scattering at the Canadian Light Source

RIXS

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Abstract text: The techniques available at the REIXS beamline at CLS to probe the electronic structure of novel materials are soft X-ray absorption, X-ray emission, Resonant inelastic X-ray scattering, and X-ray excited optical luminescence.

The talk will focus on Eu-doped nitride and oxide semiconductors used for lighting applications. The research presents direct measurements of rare earth energy levels, critical to the color, efficiency, and performance of LED phosphors. Modern phosphors use the $5d^1$ to $4f^{n+1}$ transition of Eu^{2+} (Ce^{3+}), which is an excited state since Eu^{2+} has no 5d electrons in the ground state. These 5d states are very sensitive to the surrounding crystal and therefore key Eu^{2+}luminescence parameters like wavelength and efficiency can be tailored by the choice of host lattice.

We experimentally directly determine the energetic separation of the Eu 5d state and the conduction band. We also directly observe conduction to valence band and 4f to valence band transitions in X-ray excited optical luminescence spectra of a series of cutting-edge phosphors [1-5].

In a series of new nitride semiconductors, intraband states caused by defects are monitored by luminescence and the measurements are compared to our density functional theory calculations.

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[2] T.M. Tolhurst et al., Chem. Mat. **29**, 7976-7983 (2017)
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When: 2026-06-24, 16:00 - 16:20, Where: Heinz-Otto Kreis

O92 - RIXS Studies on Altermagnets

RIXS

Di-Jing Huang[1, 2]
Hsiao-Yu Huang[1], Jun Okamoto[1], Ganesha Channagowdra[1], Amol Singh[3], Chung-Yu Mou[2], Mizuki Furo[4], Atsushi Hariki[4], Bin Gao[5, 6], Pengcheng Dai[5, 6], Evgenia V. Komleva[7], Sergey V. Streltsov[7], Atsushi Fujimori[1, 2], Sang-Wook Cheong[8]
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Abstract text: Resonant inelastic X-ray scattering (RIXS) is a powerful, symmetry-sensitive probe of electronic excitations in strongly correlated quantum materials. Here, we present RIXS studies revealing bi-antermagnetism of $Fe_2Mo_3O_8$ [1] and altermagnetic boosting of chiral phonons in Mn-doped Ni2TeO6 [2]. These results demonstrate how RIXS can be used to investigate altermagnetism and chirality.

An altermagnet is a recently identified class of magnets that exhibit zero net magnetic moment but break symmetry under the combined operations of parity and time reversal. We use circular dichroism (CD) in RIXS to identify a new form of altermagnetism, namely bi-altermagnetism, in the correlated insulator $Fe_2Mo_3O_8$, which comprises two altermagnetic sublattices. We reveal the emergence of CD in this achiral, zero-magnetization system, thereby probing mirror-symmetry breaking associated with altermagnetic order. Our findings showcase the use of RIXS-CD as a probe of magnetic sublattices in systems with zero net magnetization.

Second, to explore the possible connection between chiral phonons and magnetic chirality, we investigat the crystallographically polar and chiral compound (Mn,Ni)3TeO6, which hosts three distinct states: a paramagnetic state, a helical spin state with magnetic chirality, and a collinear spin state without magnetic chirality. We observe an approximately tenfold enhancement of chiral-phonon coupling in the helical spin state along the screw axis, compared with both the paramagnetic and collinear spin states. These results identify a new route to amplify chiral phonons through an altermagnetic effect arising from non-relativistic spin splitting.

Reference:

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When: 2026-06-22, 09:30 - 10:15, Where: Eva von Bahr

O93 - Studying Chemical Reactions with Ultrafast Elastic and Inelastic X-ray Scattering

RIXS

Simone Techert[1]
[1] Deutsches Elektronen-Synchrotron DESY

Abstract text: When studying the mechanisms of chemical reactions, we – nearly intuitively – sketch energy landscapes as a function of reaction coordinate, and explain them by well-defined transition states, Hammond's principle, intermediates' populations, reaction volumes, the energetics etc. When extending spectroscopic investigations to ultrafast studies, we add to Polanyi's (potential) energy surfaces wave packet propagations since we observe chemical reactions – still - in energy dimensions.

Ultrafast, high-flux elastic X-ray studies performed at synchrotrons or free-electron lasers, allow us to determine atomic positions as a function of time. We Fourier-transform elastic X-ray scattering pattern collected as a time-series of X-ray snapshots, from the reciprocal to real space. From the Polanyi surface perspective, we turn the classical chemical reaction coordinates by projecting along the energy coordinate, and expressing "traditional" reaction coordinates as time-dependent atomic coordinate changes. Within, we directly deduce physicochemical parameters, which are otherwise buried under the total energy surface; we study disorder-driven reactions and rationalize their reaction properties while they otherwise violate common "structure-function" principles.

Continuing research at high flux X-ray sources, but coming back to the reaction energetics, ultrafast inelastic soft X-ray scattering / X-ray emission spectroscopy completes chemical mechanistic information we miss within the ultrafast elastic X-ray scattering approach. I will present selected results of our ultrafast time-resolved and/or in-situ/operando inelastic X-ray scattering of catalytic reactions (like the oxygen evolution reaction). The reactions are selected such that they violate the so-called scaling law by their disorder properties - bringing us back to the full circle to the studied chemical reactions.

When: 2026-06-24, 14:55 - 15:20, Where: Heinz-Otto Kreis

O94 - The RIXS Beamline at Sirius: Instrumentation Advances, and First User Science

RIXS

Tulio Rocha[1]
[1] Brazlilian Synchrotron Light Laboratory (LNLS), Brazilian Center for Research in Energy and Materials (CNPEM), Campinas, Brazil.

Abstract text: Resonant Inelastic X-ray Scattering (RIXS) is a rapidly evolving technique for probing low-energy excitations in condensed matter and molecular systems. The IPÊ beamline at Sirius, Brazil’s 4th generation synchrotron light source, was designed as a dedicated platform for high-resolution soft X-ray XAS and RIXS experiments. In this talk, I will present an overview of the beamline development, including its conception, commissioning progress, instrumentation advances, and first user experiments. I will discuss recent developments in sample environments, acquisition systems, and online data-processing interfaces that have enabled new experimental capabilities and significantly improved the user experience. I will also highlight preliminary scientific results from early user proposals on condensed matter and materials physics, as well as the role of the beamline in fostering a growing RIXS community in Brazil and Latin America. Finally, I will present commissioning results obtained after the installation of a new full-length undulator, including a substantial increase in photon flux and perspectives for further improvements in overall beamline performance.

When: 2026-06-22, 14:45 - 15:05, Where: Eva von Bahr

O95 - Time-resolved Resonant Inelastic X-ray Scattering reveals how Orbital Symmetry Alignment Enables C–H Activation

RIXS

Timo Dederichs[1], Ambar Banerjee[2], Victoria Kabanova[1], Robert Stefanuik[1], Antonia Freibert[3], Emma V. Beale[4], Florian Dworkowski[4], Rebecca G. Castillo[5], Philip J. M. Johnson[4], Claudio Cirelli[4], Nils Huse[4], Camila Bacellar[4], Raphael M. Jay[1], Philippe Wernet[1]
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[2] Research Institute for Sustainable Energy (RISE), TCG Centres for Research and Education in Science and Technology (TCG-CREST), Kolkata, 700091 India
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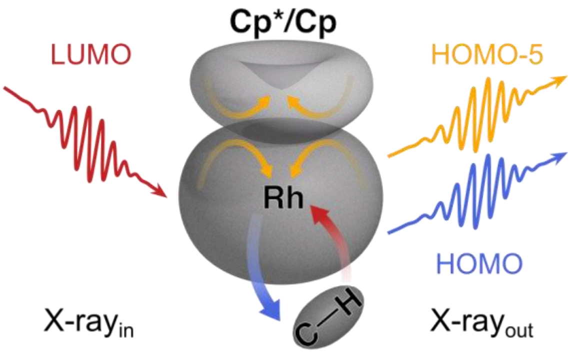
Abstract text: The selective activation and transformation of C–H bonds, one of the most ubiquitous yet inert bonds in nature, has been a long-standing goal of organic and organometallic chemistry. C–H functionalization of alkanes enables streamlined synthetic routes by avoiding prefunctionalized substrates and multi-step procedures. A promising strategy for C–H bond activation under mild conditions involves photo-triggered transition metal complexes, which often activate C–H bonds through formation of metal–alkane σ-complexes. In these intermediates, the metal coordinates to a C–H σ-bond that is subsequently cleaved through synergistic donation and back-donation interactions. Because these σ-complexes are short-lived transient intermediates, their direct experimental characterization is challenging, and limited access to their transient electronic structure has constrained understanding of their reactivity. Here, we demonstrate how optical pump/X-ray probe spectroscopy reveals key electronic-structure effects in C–H-activating σ-complexes. Starting from three Rh carbonyl precursors, we photochemically generate three Rh–alkane σ-complexes and locally probe their electronic structure at the Rh centers. Femtosecond time-resolved X-ray absorption spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS) at the Rh L_3-edge provide orbital-level sensitivity to interactions between the Rh center, ancillary ligands, and alkane C–H σ-bonds that modulate metal–alkane donation and back-donation, thereby influencing reactivity toward C–H activation. Supported by theoretical calculations, our results reveal specific occupied molecular orbitals of defined symmetry that regulate reactivity by channeling electron density to and from the coordinated C–H bond via the metal center. Elucidating these electronic factors establishes a foundation for rational ligand design aimed at enhancing the efficiency of metal-mediated C–H activation.



When: 2026-06-22, 11:10 - 11:35, Where: Eva von Bahr

O96 - Ultrahigh-Resolution 2D-RIXS and RIXS Microscopy at NanoTerasu

RIXS

Jun Miyawaki[1]
[1] National Institutes for Quantum Science and Technology

Abstract text: The characterization of subtle elementary excitations in quantum materials requires pushing the limits of both energy and spatial resolution. At NanoTerasu, a new 3-GeV synchrotron radiation facility in Japan, we have developed and commissioned the "2D-RIXS" spectrometer at BL02U, designed to meet these demanding requirements. This instrument achieves world-leading energy resolution in the soft X-ray regime [1], offering unique capabilities for investigating the electronic and magnetic ground states of complex systems.

I will describe the 2D-RIXS optical design, which has been optimized for high throughput and ultrahigh resolution [2,3]. A notable achievement is the successful realization of a RIXS microscopy system with 1-μm spatial resolution through fine-tuning and commissioning [4]. This development opens new opportunities for studying inhomogeneous electronic states and microscopic magnetic domains in functional materials.

I will highlight recent results on Yttrium Iron Garnet (YIG), a prototypical material in the fields of spintronics and magnonics. By utilizing the ultrahigh resolution of the 2D-RIXS, we have successfully resolved fine low-energy excitations that were previously challenging to observe. These results demonstrate the spectrometer's capability to provide fundamental insights into the collective excitations of magnetic insulators. Finally, I will discuss future prospects and how this combination of spectroscopy and microscopy will facilitate more detailed studies of diverse quantum materials.

[1] K. Yamamoto *et al.*, J. Phys.: Conf. Series **3010**, 012115 (2025). [2] J. Miyawaki *et al.*, J. Phys.: Conf. Series **2380**, 012030 (2022). [3] J. Miyawaki, arXiv:2601.07889. [4] K. Yamamoto *et al.*, J. Synchrotron Rad. **33**, (2026).

When: 2026-06-25, 15:35 - 15:55, Where: Eva von Bahr

O97 - Uniaxial strain effects on PrNiO2 thin films revealed by RIXS

RIXS

Marli Dos Reis Cantarino[1]
Francesca Martino[1, 2], Mathieu Flavenot[3], Francesco Rosa[2], Yiran Liu[4], Hoshang Sahib[3], Flora Yakhou-Hariis[1], Daniele Preziosi[3], Nicholas B. Brookes[1]
[1] European Synchrotron Radiation Facility, Grenoble, France
[2] Dipartimento di Fisica, Politecnico di Milano, Milano, Italy
[3] IPCMS, Université de Strasbourg, Strasbourg, France
[4] Max Planck Institute for Solid State Research, Stuttgart, Germany

Abstract text: Hydrostatic pressure is a powerful parameter to induce high-temperature superconductivity (SC), but alternative tuning strategies are required to approach ambient conditions. In infinite-layer (IL) nickelates $R\mathrm{NiO_2}$, obtained by reducing thin films of the perovskite $R\mathrm{NiO_3}$ phase, the removal of apical oxygen modifies the Ni electronic configuration toward a cuprate-like state. Additionally, biaxial epitaxial strain influences the IL phase stabilization and can strongly affect magnetic and electronic properties and SC transition temperatures (T_C) [1,2]. Notably for bilayer nickelates, strain can simulate bulk high-pressure effects, with a T_C of 40 K in $La_3Ni_2O_{7-d}$ thin films [3,4], compared to 80 K in bulk samples under hydrostatic pressure. It is therefore of great interest to decouple externally applied mechanical stress from epitaxial strain and to investigate its impact on the electronic excitations. 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 strain cell. We found that uniaxial tensile strain increases magnon energies compared to as-grown samples, and induces a shift in the dd peaks, pointing to a crystal-field environment change. We conclude that uniaxial strain can effectively enhance the magnetic exchange interaction, and that the route for transferring strain from the substrate to the film warrants further exploration in thin-film materials.

[1]Q. Gao *et al.*, Nat Commun **15**, 5576 (2024)
[2]H. Sahib *et al.*, Advanced Materials **37**, 2416187 (2025)
[3]E.K. Ko *et al.*, Nature **638**, 935 (2025)
[4]G. Zhou *et al.*, Nature **640**, 641 (2025)

Sources

When: 2026-06-24, 11:15 - 11:40, Where: Heinz-Otto Kreis

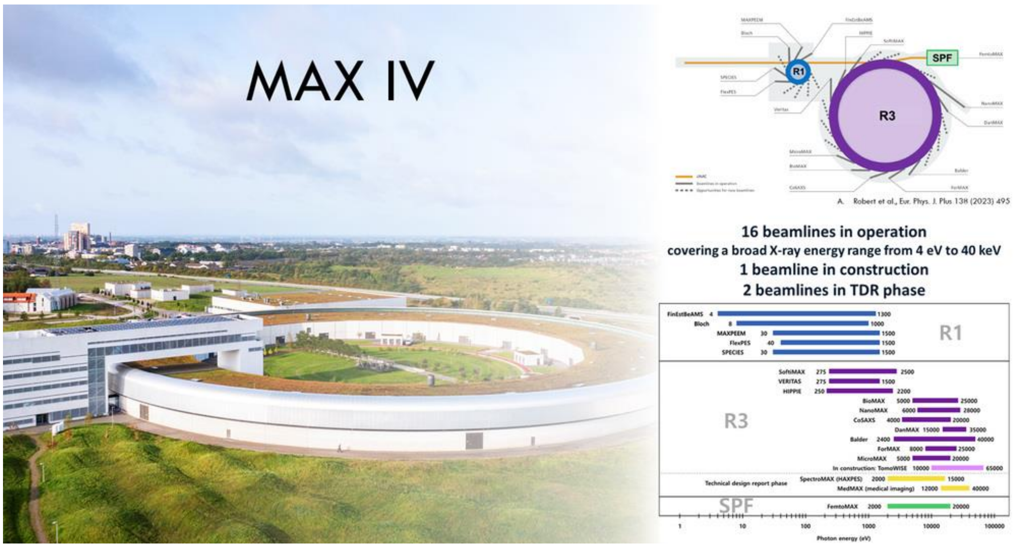
O98 - Opportunities and developments at the MAX IV Laboratory, the Swedish national synchrotron light source

Sources

Joachim Schnadt[1]
[1] MAX IV Laboratory

Abstract text: The MAX IV Laboratory in Lund is Sweden's national synchrotron radiation facility. Each year, it serves more than two thousand users from Sweden, the Nordic countries, Europe and the entire world. It features a linear accelerator and two electron storage rings, one with an electron energy of 1.5 GeV and one with an energy of 3 GeV – the latter is the world's first fourth-generation synchrotron light source. Since the inauguration of MAX IV in 2016, a portfolio of 16 beamlines within spectroscopy, diffraction/scattering and imaging has been brought into full user operation. A beamline for tomographic imaging, TomoWISE, has received funding and is in the construction phase, while two more beamlines – one for HAXPES and one for medical imaging – are in the technical design report phase. MAX IV is now preparing for an upgrade of the 3 GeV storage ring, called MAX4^U, and at the same time it is discussing strategies for its portfolio development in both the soft and hard x-ray ranges, on all its light sources.

In the presentation, the offerings of and opportunities at MAX IV will be discussed. Particular, but not exclusive, emphasis will be put on soft x-rays and spectroscopy. Future developments, including ongoing investments, will be outlined to provide a picture of the future state of MAX IV, both in a near-term and a long-term perspective. Besides technical advancements also new opportunities in terms of, e.g., access modes will be presented.



A. Robert et al., Eur. Phys. J. Plus 138 (2023) 495

16 beamlines in operation
covering a broad X-ray energy range from 4 eV to 40 keV
1 beamline in construction
2 beamlines in TDR phase

When: 2026-06-22, 11:30 - 11:50, Where: Heinz-Otto Kreis

O99 - The MAX 4U Accelerator Design

Sources
Eshraq Al Dmour[1], Murilo Barbosa Alves[1], Åke Andersson[1], Marco Apollonio[1], Francis Cullinan[1], Henrique O. C. Duarte[1], Marek Grabski[1], Robert Lindvall[1], Stephen Malloy[1], Aashoo Sharma[1], Magnus Sjöström[1], Hamed Tarawneh[1], Pedro Fernandes Tavares[1], Sara Thorin[1], Karl Åhnberg[1], Erik Mansten[1], Joachim Schnadt[1], Aymeric Robert[1], **Olof Karis**[1]
[1] MAX IV Laboratory, Lund university, Box 118, 221 00 Lund, Sweden

Abstract text: The MAX IV 3 GeV storage ring in Lund, Sweden, was the first implementation of a multibend achromat (MBA) lattice fourth-generation light source worldwide. Since it started delivery of light in 2016, several others have been built or are being planned or commissioned, capitalizing on the MBA concept and expanding it to push the brightness and coherence performance even further.

To continue to offer the Swedish and international scientific communities competitive tools beyond the end of this decade, MAX IV Laboratory launched in 2024 the conceptual design of MAX 4^U, an upgrade of its 3 GeV storage ring initially aiming at an emittance below 100 pm.rad. This performance boost is to be achieved through a minimum-interference upgrade in which localized interventions in selected subsystems and components are carefully chosen to provide the maximum performance increase with minimum cost and, equally important, minimum dark time for the MAX IV user community. The main conclusion of the conceptual design report (CDR), published in December 2025 was the decision to further enhance the performance of the upgrade aiming now at an emittance below 75 pm rad in the technical design phase. This contribution describes the latest developments in accelerator physics and engineering aspects of the MAX 4^U design.

Theory

When: 2026-06-23, 14:55 - 15:20, Where: Sonja Lyttkens

O100 - Non-local decay investigated by X-ray photoemission: the neon-argon system

Theory

Alan Guilherme Falkowski[1]
Arnaldo Naves de Brito[1]
[1] Universidade Estadual de Campinas

Abstract text: X-ray photons possess sufficient energy to excite or ionize core electrons in materials, creating a core hole. Beyond simple ionization, secondary processes occur, such as Auger-Meitner decay and fluorescence. Considering weakly bonded systems, a less dominant process called interatomic (or intermolecular) Coulombic decay (ICD) could occur. Discovered by Cederbaum *et al.*, the ICD consists of a non-local energy or electron transfer between entities in weakly bound matter [1]. However, the ICD process involves electron emission from the system. This raises a fundamental question: can non-local decay (NLD) occur via photon emission instead? A recent study of solvated magnesium and sodium ions provided affirmative evidence [2]. Motivated by this finding, we performed a theoretical investigation of the diatomic neon-argon (NeAr) to study NLD following core ionization of the neon 1s orbital, i.e., the probability of electron decay from argon into the core hole of neon. We employed the restricted active space self-consistent field (RASSCF) method [3], as implemented in the OpenMolcas quantum chemistry package [4], to calculate the relevant electronic states. Preliminary results reveal a NLD from the 3p orbital of argon to the core-hole of neon. The probability of this process may increase with the addition of further argon atoms to the system.

[1] L. S. Cederbaum *et al.*, Phys. Rev. Lett. **79**, 4778 (1997).
[2] J. Söderström *et al.*, Nat. Commun. **16**, 10046 (2025).
[3] P. A. Malmqvist *et al.,* J. Phys. Chem. **94**, 5477 (1990).
[4] G. Li Manni *et al.*, J. Chem. Theory Comput. **19**, 6933 (2023).

When: 2026-06-24, 12:05 - 12:25, Where: Sonja Lyttkens

O101 - Relaxation dynamics of suddenly created electron-nuclear states

Theory

Hans Ågren[1]
Jicai Liu[1], Svyatoslav Blinov[1], Vincenzo Carravetta[1], Victor Kimberg[1], Faris Gelmukhanov[1]
[1] Uppsala University

Abstract text: We address the fundamental X-ray problem formulated by Rolf Manne [1]: What is the relaxation time of the electron subsystem due to a sudden creation of a core hole? However, when we ask how fast the electron subsystem is rearranged in the field of a suddenly created core hole, we face the problem with physical meaning of this rearrangement and how to measure this relaxation dynamics which according to Manne [1] proceeds in the atto-second region. One is often faced with a rather naive view on this problem, that the energy of the suddenly created core-hole state should gradually evolve to the energy of the fully relaxed core-hole state. Governed by this idea some experimental groups even try to measure the corresponding relaxation time. We show that this nave picture is not correct. To shed light on this problem we investigate the relaxation dynamics of electron-nuclear systems in the field of suddenly created core- or -valence holes considering three qualitatively different techniques: X-ray absorption/ionization by using X-ray pulses with varying pulse duration; time resolved UV + X-ray pump-probe spectroscopy with varying delay time between the pulses; and RIXS with variable scattering duration. Using a wave packet approach we analyze the general scenario of the relaxation dynamics and the region of applicability of Manne's time.

*Dedicated to the memory of Rolf Manne

References [1] R. Manne, The Lifetime of the Koopmans-theorem state in core photoelectron spectroscopy. An estimate based upon the sudden approximation, Chem. Phys. Lett., 104, 378 (1984)

When: 2026-06-24, 14:55 - 15:20, Where: Sonja Lyttkens

O102 - Theory of Attosecond Processes: From XUV Metrology to Quantum Light in Strong Fields

Theory

Johannes Feist[1]
[1] Universidad Autónoma de Madrid

Abstract text: We present theoretical work on two aspects of attosecond and strong-field physics. First, full-dimensional ab-initio simulations are used to benchmark and predict attosecond correlated electron dynamics experiments. In the context of RABBIT-based attosecond metrology, these calculations reveal the limits of standard approximations used to extract the Wigner delay from measured sideband phases. For two-photon double ionisation of H2, full-dimensional simulations uncover the decisive role of nuclear motion, which induces strong electron-electron-nuclei correlations and leaves clear signatures in the photoelectron angular distributions. Second, we examine possibilities of exploiting quantum driving fields within strong-field physics. General time-bandwidth uncertainty bounds for multimode quantum states clarify when nonclassical light can offer an advantage, and a temporal-mode treatment of high-harmonic generation establishes under what conditions, and in what systems, genuine quantum effects in strong-field processes might become observable.

When: 2026-06-23, 15:40 - 16:00, Where: Sonja Lyttkens

O103 - Vibrationally resolved Photoionizing delays in H2O

Theory

Prateek Pranjal[1]
Jesus Gonzalez-Vazquez[2], Roger Yulier Bello Romero[3], Fernando Martín[1, 2]
[1] IMDEA Nanoscience, Madrid, Spain
[2] Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, Madrid, Spain
[3] Departamento de Química Física Aplicada, Universidad Autónoma de Madrid, Madrid, Spain

Abstract text: Attosecond science has had a meteoric rise in the past two decades thanks to advances in the ultra-fast laser technology. This has allowed for controlling and observing electron dynamics in atoms and molecules in real time and allowing the study of phenomena happening on their natural time scales. In particular, the attosecond photoionization time delay has motivated a large number of studies in both atomic and molecular systems.

In the present work, we use the XCHEM methodology in full-dimensionality (including nuclear degrees of freedom) to simulate RABBITT spectra and calculate the corresponding photoionization time delays in H2O. The XCHEM approach includes electron correlation in both the target and neutral states, as well as correlation of the outgoing electron with those of the target and has been shown to work well for water in the one-photon ionization case. This is necessary to properly describe the multi-electron targets. The RABBITT spectra and photoionization time delays for each polarization direction are presented up to an electron kinetic energy of 40 eV, where comparison with experimental results is possible.

The extracted two-photon ionization delays do not vary monotonically with photon energy, can either increase or decrease along the different vibrational progressions, and show strong selectivity of the laser-photoelectron interaction with respect to the final vibrational mode, which is the consequence of geometrical changes associated with such modes. Thus, the importance of including nuclear motion for such calculations is underlined.

[1] Pranjal, J. Gonzalez-Vazquez, R. Y. Bello, F. Martin, Physical Review Letters, 2025, 135, 223202.

When: 2026-06-24, 11:40 - 12:05, Where: Sonja Lyttkens

O104 - X-ray fingerprints of proton transfer

Theory

Michael Odelius[1]
[1] Department of Physics, Stockholm University, Stockholm, Sweden

Abstract text: The sensitivity of X-ray spectroscopy to hydrogen bonding and proton transfer is discussed against the background of spectrum simulations [1-3]. X-ray spectroscopy is an element-specific probe, which allows for investigations of the local electronic structure in complexes systems. In the context of molecular orbital (MO) theory, X-ray absorption probes excitations into virtual MOs and their associated strong dependence on (hydrogen-)bonding through the anti-bonding character of the virtual MOs. Monitoring fluctuations in protonated water complexes, we can determine the influence of changes in covalent bonds and electrostatics on electronic structure and X-ray spectrum. Valence-excitations open new unoccupied orbitals which give distinct spectral features and allow us to follow excited state dynamics and proton transfer.

Complementary to X-ray absorption, the occupied MOs can be probs in X-ray fluorescence at the decay of the core-ionized or core-excited state yielding X-ray emission or resonant inelastic X-ray scattering, respectively. Thereby a solid link to electronic structure calculations can be created. Furthermore, absorption of the X-ray photon creates a core-hole strongly perturbing the electronic system and it can result in proton transfer as an intrinsic spectroscopic effect, which can be utilised in resonant inelastic X-ray scattering to study the ground state energy landscape. Simulations of X-ray spectra are required to separate the influence of proton transfer in different electronic states.

[1] M. Ekimova, et al. Angew. Chem. Int. Ed. 61 e202215119 (2022)
[2] S. Eckert et al., Angew. Chem. Int. Ed. 61 e202200709 (2022)
[3] V. Vaz da Cruz et al., Nat. Commun. 10 1013 (2019)

XFEL

When: 2026-06-26, 11:40 - 12:05, Where: Eva von Bahr

O105 - Coherent sub-femtosecond X-ray radiation: single-spike pulses and mode-locked frequency combs

XFEL

Eduard Prat[1]
[1] Paul Scherrer Institute

Abstract text: X-ray free-electron lasers (FELs) are powerful photon sources offering high-power, femtosecond pulses. Standard X-ray FELs based on the self-amplified spontaneous emission (SASE) mechanism offer excellent transverse but limited longitudinal coherence, with power and spectral profiles consisting of many randomly distributed spikes. In this talk, we present experimental results from SwissFEL of two distinct and complementary regimes to enhance the coherence of the X-ray FEL radiation: 1) the production of isolated sub-femtosecond pulses consisting of a single coherent spike in both the time and the frequency domains [1-3], and 2) the first and so far only demonstration of mode-locked SASE at an X-ray FEL, which produces periodic trains of phase-locked sub-femtosecond pulses, exhibiting a well-defined comb in the frequency domain [4]. We provide evidence in the time [5] and the frequency domains for both approaches. These results will benefit investigations of ultrafast dynamics and coherent spectroscopy and may enable new types of experiments requiring phase-locked X-ray pulses.

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[4] W. Hu et al., Phys. Rev. Lett. **135**, 265001, 2025. https://doi.org/10.1103/wn8d-l7sh
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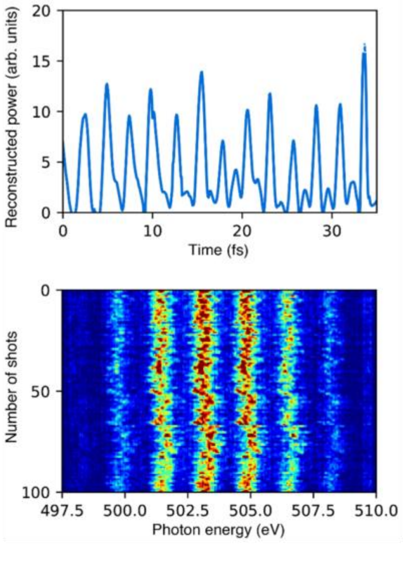

Demonstration of a mode-locked frequency comb in an X-ray free-electron laser. Top: reconstructed temporal profile. Bottom: 100 consecutive single-shot spectra.

When: 2026-06-26, 09:00 - 09:45, Where: Eva von Bahr

O106 - Current Status and Prospects of the SHINE Project

XFEL

Zhentang Zhao[1]
[1] Shanghai Advanced Research Institute, Chinese Academy of Sciences, 201204 Shanghai, China

Abstract text: The SHINE is a high repetition rate X-ray FEL facility under construction and commissioning. This facility comprises an 8 GeV CW superconducting linear accelerator, a 50 PW Super-Intense Ultra-Short laser, 2 undulator lines and 6 experimental stations in Phase-I, with maximum FEL pulse repetition rate up to 1 MHz and radiation photon energy covering the range of 0.2–15 keV. The project implementation started in April 2018, and since then encouraging progress has been achieved. The construction of buildings and the underground tunnels as well as utilities for the main facility was completed in October 2025. Manufactures of equipment and installations of the linear accelerator, the 50 PW super-intense and ultra-short laser, the Phase-I undulator lines, beamlines and experimental stations as well as their commissioning are all in course, and the first lasing of the SHINE is expected in the Autumn of 2026. This talk presents the current status and prospects of this superconducting linac based X-ray FEL project.

When: 2026-06-23, 15:20 - 15:40, Where: Sonja Lyttkens

O107 - Fluorescence imaging of nonlinear x-ray propagation and lasing

XFEL

Svyatoslav Blinov[1], Pavel Krasnov[1], Faris Gelmukhanov[2], Jan-Erik Rubensson[3], Sergey Polyutov[1], **Victor Kimberg**[2, 4]
[1] International Research Center of Spectroscopy and Quantum Chemistry—IRC SQC, Siberian Federal University, Krasnoyarsk, Russia
[2] KTH Royal Institute of Technology, Stockholm, Sweden
[3] Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden
[4] Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Abstract text: We introduce a general approach for probing nonlinear x-ray propagation by imaging secondary fluorescence emitted transverse to the driving field [1]. When a short, intense x-ray pulse excites a deep 1s core orbital, subsequent Kα emission from spin-orbit-split 2p states can undergo stimulated amplification. This nonlinear process reshapes the relative populations of the $2p_{1/2}$ and $2p_{3/2}$ levels along the propagation path, leaving distinct signatures in the delayed L-edge fluorescence (see Fig. 1). By solving the coupled density-matrix and Maxwell equations, we show that these fluorescence signals provide a direct and experimentally accessible probe of x-ray amplification dynamics. We demonstrate the concept for argon atoms and extend it to molecular systems containing third-row elements, where competing effects of lifetimes, transition intensities, and nonresonant absorption determine the efficiency of stimulated emission. Our results establish L-edge fluorescence as a broadly applicable diagnostic of nonlinear x-ray phenomena, opening opportunities for studying light-matter interactions in regimes where direct detection of amplified x-ray signals is technically challenging.

[1] Blinov, S., Krasnov, P., Gelmukhanov, F., Rubensson, J. E., Polyutov, S., & Kimberg, V. (2026). Fluorescence imaging of nonlinear x-ray propagation and lasing. Physical Review Research, 8(1), 013110.

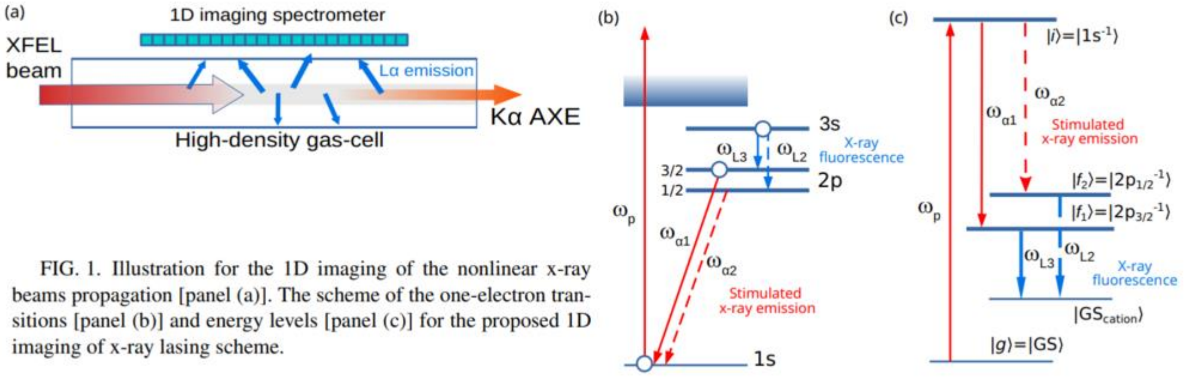

FIG. 1. Illustration for the 1D imaging of the nonlinear x-ray beams propagation [panel (a)]. The scheme of the one-electron transitions [panel (b)] and energy levels [panel (c)] for the proposed 1D imaging of x-ray lasing scheme.

When: 2026-06-24, 09:00 - 09:45, Where: Eva von Bahr

O108 - Following Metalloenzyme Catalysis in Real Time with X-ray Spectroscopy and Diffraction Methods

XFEL

Junko Yano[1]
[1] Lawrence Berkeley National Laboratory

Abstract text: Nature uses remarkably varied systems and mechanisms to perform complex chemical transformations with efficiency, speed, and specificity. At the active site of many enzymes are metal centers, responsible for the rearrangement of electrons, protons, and atoms to carry out electron transfer and catalytic reactions.

Using X-ray crystallography and spectroscopy under physiological temperature, we are investigating light-driven water oxidation in Photosystem II (PS II) (1). PS II carries out this reaction by coupling four-electron oxidation of water at the oxygen-evolving complex (OEC, the Mn_4CaO_5 cluster and surrounding water and amino acid residues) with one-electron photochemistry at the reaction center. In our recent study with a combination of crystallography and X-ray emission spectroscopy at X-ray Free Electron Lasers (XFELs), we obtained data at several key time points with particular emphasis on the $S_3 \rightarrow [S_4] \rightarrow S_0$ step, associated time constants, and and developed mechanistic hypotheses for the chemical changes during the S-state transitions. We also made progress in the data collection method for X-ray absorption spectroscopy (XAS) from dilute biological samples (~ 0.5 mM) like PS II at both Mn K- and L-edges. For K-edge XAS, we built a background-suppressed XAS setup with a drop-on-tape (DOT) sample delivery method that can be applicable to time-resolved spectroscopy (2). Together, these approaches provide a powerful and complementary framework for resolving the electronic and structural dynamics of metalloenzyme catalysis at an unprecedented level of detail.

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2. Bogacz, I. *et al.*, *J. Phys. Chem. Lett.* **2025**, *16*, 3778–3787.

When: 2026-06-22, 16:30 - 16:50, Where: Eva von Bahr

O109 - Investigating the Photodynamics of an Iron Bisporphyrin Photocatalyst with Time-Resolved X-Ray Absorption Spectroscopy and X-Ray Solution Scattering

XFEL

Laura Smith[1]
Brandon Rasmussen[2], Adi Natan[3], Ryan Lamb[4], Jacky Burke[2], Roberto Alonso-Mori[5], Leland Gee[5], Patrick Kramer[5], Taylor McClain[6], Ryan Ribson[5], Sanghoon Song[5], Tim van Driel[5], James Penner-Hahn[4, 6], Roseanne Sension[4, 7], Josh Vura-Weis[2]
[1] Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden
[2] Department of Chemistry, University of Illinois Urbana Champaign, Urbana, IL, USA
[3] Stanford PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, CA, USA
[4] Department of Chemistry, University of Michigan, Ann Arbor, MI, USA
[5] Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA, USA
[6] Department of Biophysics, University of Michigan, Ann Arbor, MI, USA
[7] Department of Physics, University of Michigan, Ann Arbor, MI, USA

Abstract text: Oxygen atom transfer reactions are used to transform simple molecules like alkenes to functionalized molecules such as epoxides and alcohols. Some metal photocatalysts, such as μ-oxo iron bisporphyrin, can catalyze oxygen atom transfer reactions using atmospheric O_2. [1] In the proposed photocatalytic cycle, the bisporphyrin is excited into a ligand-to-metal charge-transfer state that is then proposed to break apart into an $Fe^{II}/Fe^{IV}=O$ porphyrin pair. The $Fe^{IV}=O$ porphyrin then performs the oxygen transfer reaction. However, the quantum yield (reactions per photon absorbed) of a typical bisporphyrin is approximately 10^{-4}. [2] The cause of this low quantum yield has been attributed by some to the $Fe^{II}/Fe^{IV}=O$ porphyrin pair re-forming the ground state too quickly to catalyze a reaction. [3] Others have proposed that most of the excited bisporphyrin forms a non-reactive $Fe^{III+}/Fe^{III}\text{-}O^-$ pair rather than the desired reactive species. [4] To investigate the cause of the low quantum yield, we performed time-resolved X-ray absorption spectroscopy to probe the excited state electronic dynamics and X-ray solution scattering to probe the excited state structural dynamics. These experiments allowed us to identify the excited states formed by the bisporphyrin, and observe the dissociation of the porphyrin halves.

References

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4. Sye, K. M.; et al., *Catal. Sci. Technol.* **2022**, 12 (20), 6092–6097.

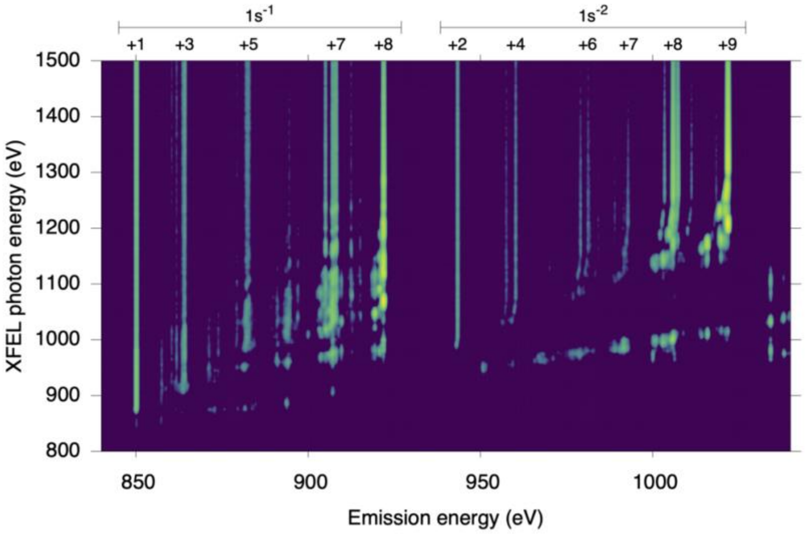
When: 2026-06-22, 14:00 - 14:25, Where: Eva von Bahr

O110 - Non-equilibrium transition from X-ray-heated to collision-driven plasma

XFEL

Sang-Kil Son[1]
[1] Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Abstract text: A transient plasma is formed when intense X-ray pulses interact with matter. Multiphoton ionization produces highly charged ions and hot electrons, and eventually reach a thermal equilibrium. I will present a joint theoretical and experimental study of X-ray multiphoton ionization dynamics and plasma evolution dynamics of near-ambient pressure neon gas interacting with intense X-ray pulses generated by European XFEL. The target density is low enough to model excitation mechanisms in the isolated-atom limit during the pulse, while it is high enough to observe collisional effects afterwards. Multiple resonance excitations are investigated in X-ray emission spectra from all Ne charge states as shown in the figure (theoretical 2D map of X-ray emission spectra). I will also discuss how insights from atomic physics are applied to understand photon-driven plasma formation. Time-resolved X-ray emission measurement enables us to monitor non-equilibrium transition dynamics from a photoionized plasma to collision-dominated regime within nanoseconds, providing insight into thermalization and expansion dynamics of the hundred-eV hot plasma. Our study of quantum-state-resolved X-ray multiphoton ionization dynamics opens up new opportunities for high-resolution X-ray spectroscopy of atoms and plasmas at high intensity.



When: 2026-06-24, 12:05 - 12:30, Where: Eva von Bahr

O111 - Recent advancements in attosecond capabilities at the LCLS-II

XFEL

Agostino Marinelli[1]
[1] SLAC National Accelerator Laboratory

Abstract text: Free-electron lasers are the brightest sources of isolated attosecond x-ray pulses, with a peak brightness that surpasses table-top high-harmonic sources by more than seven orders of magnitude. The recent commissioning of the LCLS-II superconducting particle accelerator has opened a new chapter for attosecond XFELs, increasing the repetition rate by several orders magnitude compared to previous capabilities at LCSL.

In my talk I will present recent advances in attosecond XFELs at the LCLS facility. I will present the demonstration of attosecond pulses with a repetition rate up to 33 kHz using the LCLS-II continuous wave superconducting accelerator, and their application to attosecond pump/attosecond probe spectroscopy experiments.

I will then present recent results attosecond pulse shaping, with the generation of mutually coherent pulse pairs and discuss their possible application to coherent control experiments.

Finally, I will present recent results in attosecond hard x-ray metrology and the first demonstration of hard x-ray attosecond pulses with time-domain measurements.

When: 2026-06-24, 09:55 - 10:20, Where: Eva von Bahr

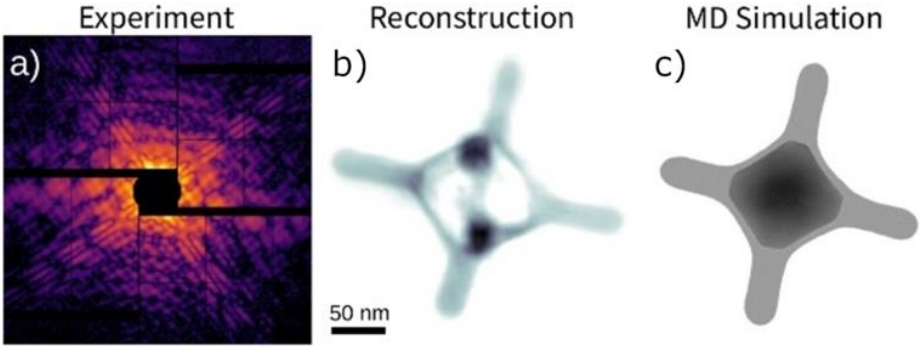
O112 - Single-particle imaging with intense X-ray pulses: probing highly excited matter with extreme precision

XFEL

Daniela Rupp[1]
[1] ETH Zürich

Abstract text: Single-particle Coherent Diffraction Imaging (CDI) allows us to take snapshots of individual nanoscale objects and create movies of their ultrafast dynamics, revealing structures and processes that no other method can access. Intricate diffraction patterns, such as the beautiful example in Figure 1a, are captured by a single illumination of an individual free-flying nanoparticle with an intense short-wavelength light pulse from an X-ray Free Electron Laser (XFEL) or a lab-based high-intensity High-Harmonic Generation (HHG) source. With algorithmic methods [1,2] we then reconstruct femtosecond and nanometer-resolved snapshots of the tiny structures and follow their transformations after laser excitation in real time [3]. Over the last years this class of experiments has advanced from the proof-of-concept stage to a mature methodology that probes highly excited matter with unprecedented precision. An illustration of the level of detail and control we have gained is given by the transient double-cross-like shape shown in Figure 1b. The structure evolves out of a free-flying silver nanocube, 1300 picoseconds after being transformed from solid to overheated liquid by plasmonic excitation with an optical laser pulse. By matching the observed dynamics with large-scale molecular dynamics simulations (Figure 1c), we gain access to previously unknown material parameters such as the speed of sound and viscosity of superheated silver, thus constraining effective transient equations of state for strongly driven matter.

[1] Colombo et al., npj Computational Materials 11, 265 (2025).
[2] Colombo, et al., Science Advances 9, eade5839 (2023).
[3] Dold et al., Physical Review Letters 134, 136101 (2025).



When: 2026-06-24, 11:40 - 12:05, Where: Eva von Bahr

O113 - Single-Pulse Time-Resolved XFEL Imaging of Ultrafast Photoinduced Nonequilibrium Reactions in Single Nanoparticles

XFEL

Changyong Song[1, 2, 3]
Eunyoung Park[1, 2, 3], Sinwoo Kim[1, 2, 3], Jaeyong Shin[4], Sangsoo Kim[4], Daewoong Nam[2, 4]
[1] Department of Physics, POSTECH, Pohang 37673, Korea
[2] Photon Science Center, POSTECH, Pohang 37673, Korea
[3] Center for Ultrafast Science on Quantum Matter (CUQ), Max Planck Korea/POSTECH Initiative, Pohang 37673, Korea
[4] Pohang Accelerator Laboratory, POSTECH, Pohang 37673, Korea

Abstract text: Intense femtosecond laser excitation can drive solids far from equilibrium, initiating ultrafast structural transformations governed by rapid electronic energy redistribution and transient bond depletion. Revealing the underlying reaction pathways remains a major challenge because these processes are irreversible, heterogeneous, and occur on femtosecond–nanometer scales that are inaccessible to conventional stroboscopic measurements. Here we present recent progress in single-pulse, time-resolved single-particle imaging with an X-ray free-electron laser (XFEL), which enables direct visualization of nonequilibrium reactions in individual nanoparticles. By combining femtosecond optical excitation with single-shot coherent X-ray imaging, we capture nanoscale structural evolution during ultrafast transformations and directly visualize transient mass-density redistribution in laser-excited Au nanoparticles. This imaging method now reveals heterogeneous energy-relaxation pathways and photoinduced phase-change behavior that are hidden in ensemble-averaged measurements. The measurements uncover transient structural responses—including directional density redistribution and exotic melting dynamics—that are forbidden under near-equilibrium thermodynamic conditions.

Together with two-temperature molecular-dynamics simulations, these experiments provide a microscopic picture of how electronic excitation drives rapid structural reorganization at the nanoscale. The results establish single-pulse XFEL imaging as a powerful approach for directly probing ultrafast nonequilibrium reaction pathways in nanoscale materials. This approach opens a new route for studying ultrafast reactions in nanoscale systems where structural heterogeneity and irreversibility dominate the dynamics.

When: 2026-06-26, 11:15 - 11:40, Where: Eva von Bahr

O114 - Statistical XUV/x-ray light enhances temporal and spectral resolution of atomic and molecular quantum dynamics

XFEL

Thomas Pfeifer[1]
[1] Max-Planck-Institut für Kernphysik, Heidelberg

Abstract text: To resolve ultrafast events, we need controlled probes that are shorter than the delay between the events. Likewise, to resolve closely-spaced spectral lines, we need to achieve spectrometer resolutions better than their spacing. These statements appear correct, at first.

Here, we shed light on this common knowledge, statistically structured light to be more precise.

Experiments at the extreme-ultraviolet (XUV) FEL FLASH at DESY taught us that correlations in statistically structured SASE FEL pulses can increase temporal resolution. Molecular wavepacket dynamics on time scales shorter than the FEL pulse duration are resolved in the D_2 molecular ion, observed by ion coincidence spectroscopy with a reaction microscope (ReMi) in an XUV-pump–XUV-probe experiment.

Regarding enhanced spectral resolution, we learn from a recent "single-pulse" transmission spectroscopy experiment at EuXFEL. Here, correlations within the physical interaction process itself (X-ray stimulated Raman) can be harnessed (in a manner akin to super-resolution microscopy) to resolve spectral structures (100-meV fine-structure splitting in Ne), beyond the (0.2 eV) x-ray spectrometer resolution.

Finally, we turn to our recent attosecond-pump–attosecond-probe experiment on electron charge migration. Making use of a recently established attosecond double-pulse operating regime at EuXFEL we measure spectral interference structures, encoding the time delay of the stochastically varying SASE pulses. Using post sorting based on shot-to-shot spectral diagnostics, we uncover transient changes of characteristic x-ray absorption below the oxygen K edge, encoding the motion of electrons in the vicinity of the two chemically distinct oxygen atoms in the chemically relevant COOH carboxy group found in organic acids.

When: 2026-06-24, 11:15 - 11:40, Where: Eva von Bahr

O115 - Transient states and ultrafast dynamics in quantum materials from time-resolved RIXS studies at SCS instrument, European XFEL

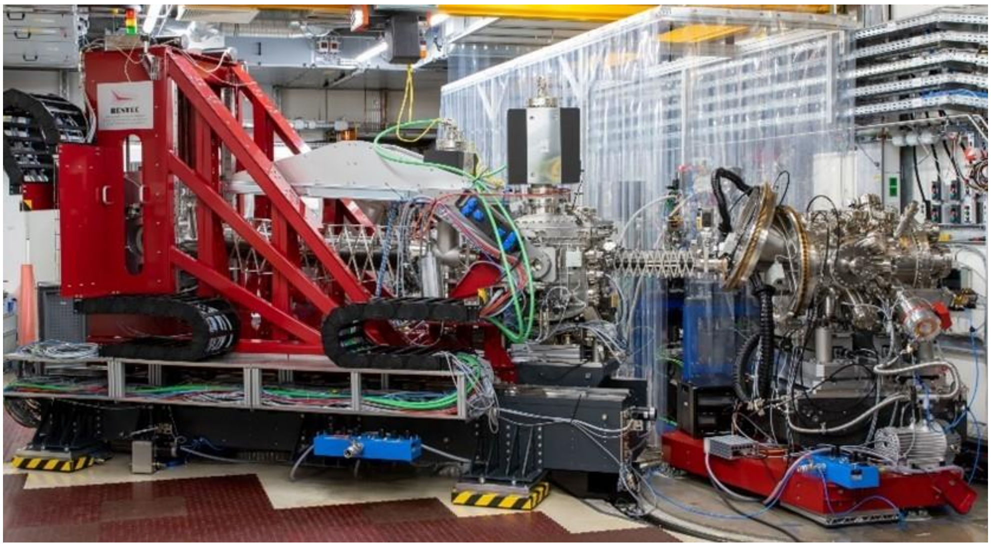
XFEL

Justine Schlappa[1]
[1] European X-Ray Free Electron Laser Facility

Abstract text: Resonant Inelasic X-ray Scattering (RIXS) is a powerfull tool for microscopic studies of condensed matter, because it can access various information about the quantum-state properties. In particular, it is sensitive to low-energy excitations that couple to the electronic valence states, including charge, spin, orbital and also nuclear degrees of freedom. At Free-Electron Laser (FEL) facilities photoexcitation dynamics and novel transient states can be explored. The Heisenberg RIXS (hRIXS) spectrometer was built in order to enable time-resolved RIXS close to the transfer limit of a monochromatic FEL source [1]. The high-repetition rate of the European XFEL, together with the unique properties of the SCS instrument, provide the ideal conditions to host such an instrument [1-3].

I will present examples of time-resolved RIXS studies from quantum materials performed at the SCS instrument. An ultrafast laser excitation allows to instantly modify material's properties in a way that is not accessible through external fields under equilibrium conditions. After variable time delay from 0.1 ps to tens of ps the RIXS probe displays the renormalization of low-energy excitations and reveals details on the photoexcited, non-equilibrium state and its' dynamics. I will discuss the current capabilities of the hRIXS instrument and introduce the ongoing and planned upgrades, concluding with an outlook for future time-resolved RIXS studies at European XFEL.

[1] Schlappa at al., J. Synchrotron Rad. 32, 29 (2025).
[2] Gerasimova at al., J. Synchrotron Radiat. 29, 1299 (2022).
[3] https://www.xfel.eu/facility/instruments/scs/index_eng.html



When: 2026-06-22, 15:45 - 16:10, Where: Eva von Bahr

O116 - Two-color X-ray resonant double core excitation of molecules

XFEL

Eetu Pelimanni[1]
[1] Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, Illinois 60439, USA

Abstract text: X-ray free electron lasers have enabled experimental studies of nonlinear X-ray interactions in molecules, including ultrafast multiphoton absorption schemes that drive multi-core hole electronic state production. These interactions can be monitored via electron, ion and photon - based spectroscopic techniques, obtaining element, state and time-resolved chemical information beyond standard (linear) X-ray interactions. Off-resonant sequential multi-core ionization processes can be realized with single XFEL pulses at photon energies above the core ionization thresholds, and have been observed in several studies. On-resonant interactions on the other hand have received less attention, as to target several core-resonances simultaneously, each with strict photon energy requirements, is generally less straightforward. In this work, recent results obtained from experiments at the European XFEL and SwissFEL are discussed, demonstrating efficient production of double core-excited electronic states via one- and two-pulse XFEL schemes. Such mechanisms enable extensions of common state and site selective resonant X-ray techniques into nonlinear double-resonance spectroscopies, with control in the temporal and 2-dimensional photon energy domains.

When: 2026-06-24, 10:20 - 10:40, Where: Eva von Bahr

O117 - Ultrafast Charge Transfer across Strongly-Correlated Oxide Interfaces

XFEL

Teguh Citra Asmara[1]
Justine Schlappa[1], Robert J. Green[2], Sergii Parchenko[1], Carlos W. Galdino[3], Yuan Wei[3], Zhijia Zhang[3], Yi Tseng[4], Natalia Gerasimova[1], Giacomo Merzoni[1], Benjamin Van Kuiken[1], Martin Teichmann[1], Yi-Ping Chang[1], Laurent Mercadier[1], Devesh Chopra[1], Eugenio Paris[3], Wenliang Zhang[3], Tianlun Yu[3], Giuseppe Mercurio[1], Robert Carley[1], Milan Radovic[3], Thorsten Schmitt[3], Andreas Scherz[1]
[1] European XFEL, Schenefeld, Germany
[2] Department of Physics and Engineering Physics, University of Saskatchewan, Saskatoon, Canada
[3] Center for Photon Science, Paul Scherrer Institute, Villigen PSI, Switzerland
[4] Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Abstract text: Strongly-correlated interfacial phenomena are widely regarded as potential foundations for next-generation functional devices, due to their tunability under diverse external stimuli. Among these stimuli, ultrafast optical excitation is uniquely powerful, as it can drive systems out of equilibrium into transient states that are inaccessible under static conditions. However, most light-driven phenomena have been investigated primarily in bulk-like materials, leaving the dynamics of light-driven interfacial processes largely unexplored. Here we present the first demonstration of light-driven charge transfer across strongly-correlated $LaNiO_3/SrTiO_3$ interfaces, quantifying its dynamics using time-resolved x-ray absorption spectroscopy at free-electron laser. We find that photoexcited electron-hole pairs transfer together across the atomic-scale interface from $SrTiO_3$ to $LaNiO_3$ within ~60–70 fs timescale. This corresponds to an effective frequency of ~15 THz, suggesting its potential for THz-speed information-processing operation similar to photonics while retaining nanometre-scale footprints compatible with modern electronics. We also observe partial charge separation at the interface: some photoelectrons remain in $SrTiO_3$ while most photoholes transfer into $LaNiO_3$, hinting its possible applications in photovoltaics. More broadly, because interfacial charge transfer often underlies other interfacial phenomena, this ability to trigger it dynamically with light opens new pathways for ultrafast control of various other emergent interfacial states.

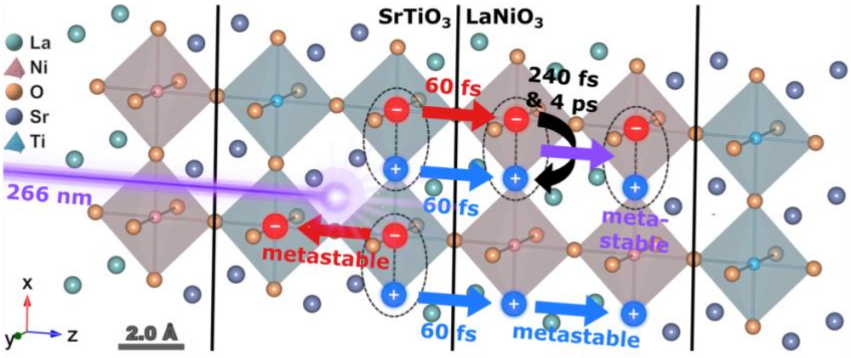


Illustration of the ultrafast charge-transfer processes across $LaNiO_3/SrTiO_3$ interface. Following 266 nm optical laser excitation in $SrTiO_3$, a large fraction of photoexcited electron-hole pairs (EHPs) transfer together across the interface within a common interfacial charge transfer time, τ_{CT}, of ~60–70 fs. Some of these transferred EHPs recombine in $LaNiO_3$ within ~240 fs and ~4 ps timescales, while the rest remain metastable for >100 ps. The fraction of EHPs that do not transfer together undergo charge separation at the interface, with photoholes (⊕) transferring into $LaNiO_3$ within τ_{CT} while photoelectrons (⊖) stay in $SrTiO_3$. Both then persist in their separate layers also for >100 ps.

When: 2026-06-26, 09:55 - 10:20, Where: Eva von Bahr

O118 - Watching Molecules in Action: Ultrafast X-ray probes of Electronic and Structural Dynamics

XFEL

Roseanne Sension[1, 2]
James Penner-Hahn[1, 3]
[1] Department of Chemistry, University of Michigan, Ann Arbor, MI, United States
[2] Department of Physics, University of Michigan, Ann Arbor, MI, United States
[3] Department of Biophysics, University of Michigan, Ann Arbor, MI, United States

Abstract text: The fate of a photoactive molecule is determined by the electronic and structural rearrangements that follow excitation. Femtosecond X-ray free electron lasers (XFELs) have made it possible to use X-ray spectroscopy to probe changes in electronic configuration and atomic structure as a function of time, beginning from the initial excited state. We have applied time resolved X-ray absorption (XAS) at metal K and L edges, combined with time-resolved X-ray emission (XES), ligand K-edge XAS, and optical transient absorption to 3d transition metal complexes including manganese tricarbonyls and cobalt containing cobalamins. Each experimental probe provides an important, but incomplete, and potentially misleading, picture of the dynamics; only by combining a range of probes can we gain a full understanding of the excited state evolution. Polarization anisotropy permits decomposition of the transient optical and XAS difference signal into contributions along the direction parallel to the transition dipole initially pumped and perpendicular to this transition dipole. This decomposition provides additional insight into electronic evolution and allows the analysis of asymmetric sequential structural dynamics of photoexcited molecules in isotropic solution. Comparison with TD-DFT calculations of optical and X-ray spectroscopies at the K-edge, multiplet calculations at the L-edge, and finite difference method near-edge structure calculations of the K-edge XANES region permits interpretation of the sequential excited state dynamics revealed in the X-ray measurements

When: 2026-06-26, 10:20 - 10:40, Where: Eva von Bahr

O119 - X-ray driven argon-hydrogen ion-molecule reactions on ionized nanoparticles at the European XFEL

XFEL

Samuel Sahel-Schackis[1, 2], Adam Summers[1], Ritika Dagar[1], Alexandra Feinberg[1], Martin Grassl[1], Simon Dold[3], Rebecca Boll[3], Yevhenly Ovcharenko[3], Chris Aikens[4], Cesar Costa Vera[5], James Cryan[1], Alberto De Fanis[3], Avijit Duley[6], Felix Gerke[7], Daniel Jost[1], Regina Leiner[8], Ilana Molesky[1], Razib Obaid[1], Jeffrey Powell[9], Bjorn Senftleben[3], Hendrik Tackenberg[10], Paul Tuemmler[10], Sergey Usenko[3], Christian Peltz[10], Thomas Fennel[10], Markus Gallei[8], Eckart Ruehl[7], Artem Rudenko[4], Daniel Rolles[4], Thomas Linker[1], Matthias Kling[1, 2]

[1] SLAC National Acceleratory Laboratory
[2] Stanford University
[3] European XFEL
[4] Kansas State University
[5] Escuela Politecnica Nacional
[6] Indian Institute of Technology Kanpur
[7] Freie Universitat Berlin
[8] Saarland University
[9] Institut national de la recherche scientifique
[10] University of Rostock

Abstract text: Ion-molecule reactions play a fundamental role in interstellar molecular clouds and planetary atmospheres. [1] Charge transfer processes involving argon and hydrogen are particularly important for hydrogen chemistry in the early universe [2] and X-ray emission from comets [3]. However, studying these reactions under astrophysically relevant ionization conditions has remained challenging.

We present a multi-modal experimental approach at the SQS instrument of the European XFEL, combining ion velocity map imaging (VMI), electron time-of-flight (eTOF) spectroscopy, and coherent diffraction imaging (CDI) to investigate ion-molecule reactions on isolated silica (SiO_2) nanoparticles with a surface layer of water (H_2O). X-ray ionization at 1.88 keV generates highly charged nanoparticle surfaces with electric fields on the V/nm scale, creating environments analogous to cosmic-ray irradiated interstellar dust.

Within this framework, we observe argon-hydrogen reactions arising from the argon carrier gas interacting with hydrogen species generated on the nanoparticle surface. The Ar^+ charge states produced by X-ray ionization react with H_2 and its fragments through both charge transfer ($Ar^+ + H_2 \rightarrow Ar + H_2^+$) [4] and proton transfer ($Ar^+ + H_2 \rightarrow ArH^+ + H$) channels [5]. These results establish X-ray irradiated nanoparticles as a novel platform for studying ion-molecule reaction dynamics under controlled, astrophysically relevant ionization conditions.

[1] Waite *et al.*, *Science* **316**, 870 (2007).
[2] Savin *et al.*, *Astrophys. J.* **606**, L167 (2004).
[3] Cravens, *Science* **296**, 1042 (2002).
[4] Michaelsen *et al.*, *J. Chem. Phys.* **147**, 013940 (2017).
[5] Johnsen & Guberman, *Adv. At. Mol. Opt. Phys.* **50** (2010).

When: 2026-06-22, 14:25 - 14:45, Where: Eva von Bahr

O120 - X-ray Stimulated Raman Scattering via Photon-Recoil Imaging in Neon

XFEL

Lukas Germeroth[1]
[1] Universität Kassel

Abstract text: Raman spectroscopy relies on inelastic scattering of photons, typically using narrow-band lasers to address molecules in a spectroscopic fingerprint region. It has become an indispensable tool in chemical and biological analysis [1]. For femtosecond lasers, impulsive stimulated Raman scattering (SRS) is routinely used to excite coherent vibrational and rotational wavepackets [2] and phonons [3].

Ultrabright FELs enable the extension of non-linear physics to the X-ray domain, demonstrated by previous observed SRS using photoemission [4]. The recently established photon-recoil imaging is a sensitive technique to detect X-ray Raman scattering [5], capable to distinguish between spontaneous and stimulated Raman, and to study the interference of different coherent Raman pathways [6].

Here, we use the two-color mode of the European XFEL, extending our previous experiments, thus achieving a stronger SRS signal [7]. We investigate the impact of the detuning of the two pulses on the Raman signal in neon (see Figure 1(a)), and achieve below the spectral bandwidth super-resolution (see Figure 1(b)) by employing partial covariance mapping [8]. Finally, we extend photon-recoil imaging of Raman processes from atoms to molecules.

[1] Singh, Mishra, Materny, Raman Spectroscopy: Advances and Applications (Springer), 2024
[2] Rosca-Pruna and Vrakking, Phys. Rev. Lett. 87, 153902 (2001)
[3] Gerbig et al., New. J. Phys. 27, 053004 (2025)
[4] Weninger et al., PRL 111, 233902 (2013)
[5] Eichmann et al., Science 369, 1630 (2020)
[6] Eichmann et al., under review at Nature Photonics
[7] Germeroth, Master thesis, University of Kassel (2026)
[8] Li et al., Nature 643, 662 (2025)

Figure 1(a)

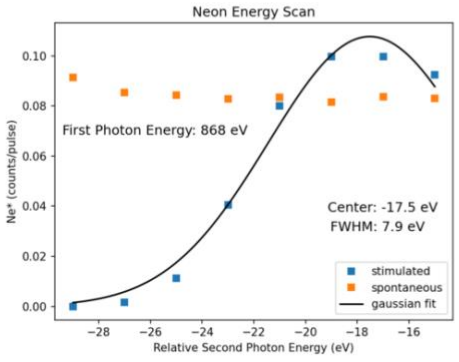
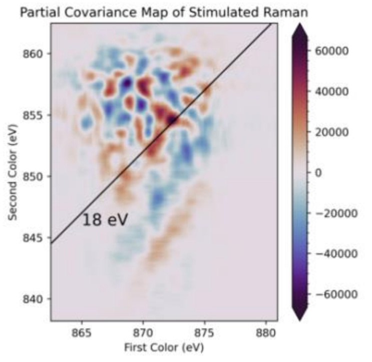


Figure 1(b)



Other

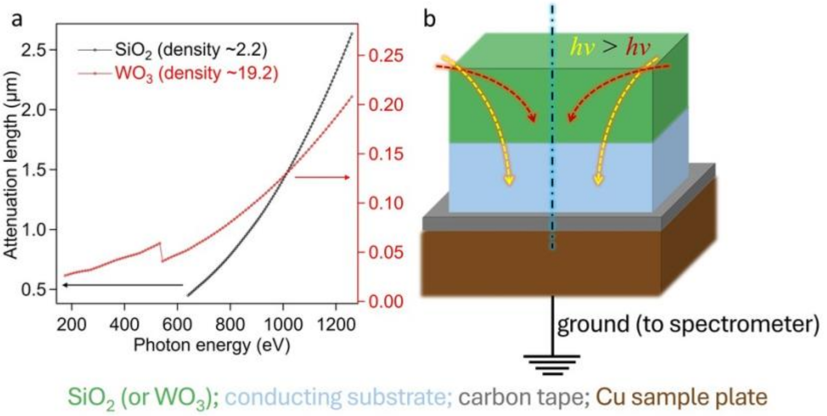
When: 2026-06-26, 11:35 - 11:55, Where: Sonja Lyttkens

O121 - Charging of non-metallic thin films during XPS measurements: the untold story

Other

Archit Dhingra[1]
Grzegorz Greczynski[2]
[1] FinEstBeAMS, MAX IV Laboratory, Fotongatan 2, 22484, Lund, Sweden
[2] Thin Film Physics Division, Department of Physics, Chemistry, and Biology (IFM), Linköping University, 581 83 Linköping, Sweden

Abstract text: Surface science is at the core of a myriad of applications, rendering fundamental understanding of surfaces and interfaces indispensable. Consequently, X-ray photoelectron spectroscopy (XPS) has become one of the most exploited techniques for reliable characterization of surfaces of interest. However, since most of the technological materials are non-metallic, unerring analyses of their core-level spectra cannot be guaranteed unless the inaccuracies in determination of their binding energies are dealt with. Here, fundamental insights into the physics of XPS-induced surface charging of non-metals were gathered by monitoring the changes to the core levels of SiO_2 and WO_3 films as a function of photon-energy and film-thickness. Analyses of the obtained photon-energy and thickness dependent XPS data on these insulators unveil that surface charging of non-metallic samples strongly dependents on both their thickness and the photon energy used during XPS measurements.



Beer–Lambert law applied to charging of insulators. a Photon-energy dependence of attenuation length of X-rays inside SiO_2 (black) and WO_3 (red). **b** Schematic showing photon-energy dependent changes in Beer–Lambert decay profiles. The plots in panel **a** are produced from: https://henke.lbl.gov/optical_constants/atten2.html.

When: 2026-06-25, 15:45 - 16:05, Where: Heinz-Otto Kreis

O122 - Surface chemistry and materials functionalization from time-resolved and time-based coincident electron spectroscopy at the Uppsala-Berlin joint Lab

Other

Alexander Föhlisch[1, 2]
[1] Institute for Methods and Instrumentation in Synchrotron Radiation Research, Photon Science Division, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany
[2] Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

Abstract text: The unparalleled detection efficiency of angle-resolved time-of-flight electron spectroscopy, developed at the Uppsala–Berlin Joint Laboratory for Next-Generation Electron Spectroscopy, provides access to the study of solids and surfaces. This enables the investigation of dynamical photoactivation processes and the probing of electronic structure properties using Auger photoelectron coincidence spectroscopy (APECS).

For MoS_2, we have investigated the inhomogeneity and homogenization of the local n- and p-doping character of bulk MoS_2 alongside relevant intercalation processes. Cleaved surfaces typically display spatially inhomogeneous properties. Exposure to atomic hydrogen reversibly equilibrates the entire surface to a common doping state due to the amphoteric nature of hydrogen atoms, which can act as both donors and acceptors, thereby neutralizing local charge imbalances. Furthermore, transient photoexcitation and lithium intercalation are shown to modify interlayer interactions and charge-transfer pathways. In particular, lithiation strongly accelerates interlayer charge transfer through Coulomb-mediated charge separation within the van der Waals gap.

Using Auger photoelectron coincidence spectroscopy, we have explored the controversial formal oxidation state of partially oxidized copper through the enhanced surface and chemical selectivity of APECS combined with first-principles calculations. We compare metallic Cu(111), with the formal oxidation state Cu(0), Cu_2O (cuprous copper(I) oxide), and CuO (cupric copper(II) oxide) with partially oxidized “29” Cu_xO/Cu(111). The oxidation state of Cu within the top three layers of “29” Cu_xO/Cu(111) is found to be Cu(0.3), close to the formal Cu(0) oxidation state of metallic Cu(111). These findings clarify essential processes in copper-based materials and chemistry.

When: 2026-06-25, 09:00 - 09:45, Where: Eva von Bahr

O123 - Watching Catalysts Work: In situ/Operando Surface Spectroscopy

Other

Hiroshi Kondoh[1]
[1] Department of Chemistry, Keio University, Yokohama, Japan

Abstract text: In the past, surface chemistry dedicated significant effort to characterizing the chemical structures of surfaces [1]. Advances in experimental techniques such as diffraction, scattering, and spectroscopy, have enabled researchers to determine these structures with considerable precision. However, as the field evolved, a new direction emerged: the pursuit of *in situ* and *operando* surface spectroscopy to observe surfaces as they undergo transformation while functioning [2].

Since the 2000s, research in this direction has intensified. Focusing on fundamental catalytic reactions on solid surfaces, we have dedicated ourselves to developing methodologies, primarily centered on synchrotron-based surface spectroscopy, to capture the phenomena occurring on catalytically active surfaces [3]. In this presentation, I will introduce our research conducted at the Photon Factory and discuss the current extent of our understanding regarding surfaces that evolve during catalysis, as well as the key challenges that remain.

Specific examples of catalytic reactions to be discussed include exhaust gas purification, ethylene epoxidation, and photocatalytic water splitting. Finally, I will conclude with a perspective on future challenges and directions.

References

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Poster

AMO

P1 - Coulomb Explosion Imaging of Cryptochrome4b: Distinguishing AlphaFold2 Structure Predictions via Explosion Pattern Analysis

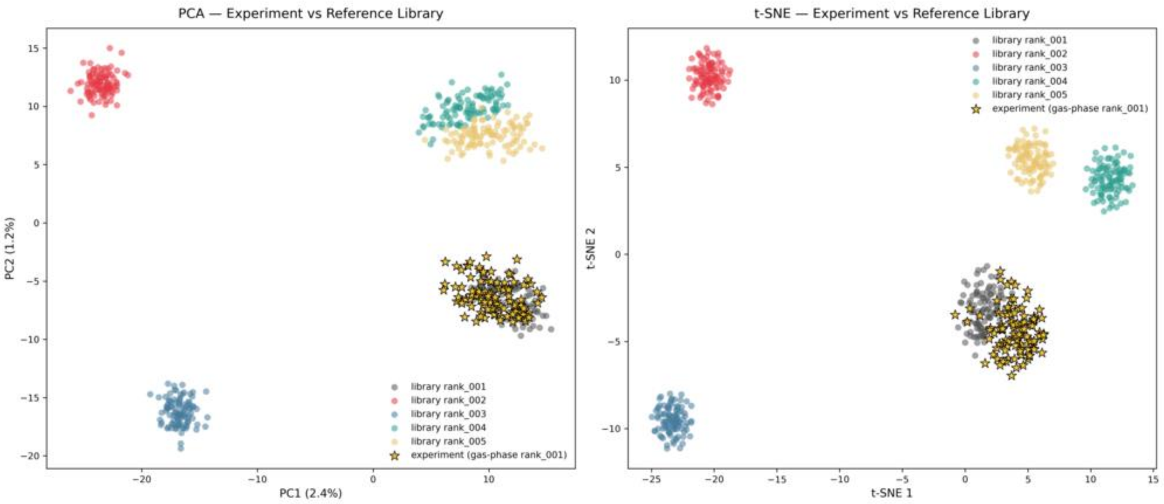
AMO

Friederike Krüger[1]
Tomas Andre[1], Nicusor Timneanu[1], Carl Caleman[1, 2]
[1] Uppsala University
[2] Deutsche Elektronen-Synchrotron DESY

Abstract text: AlphaFold2 has transformed protein structure prediction by generating ranked structural models from sequence alone. For a given protein, each of the predicted models represents a plausible conformation, but there is often no straightforward way to determine which prediction is closest to the true structure.

Coulomb explosion imaging (CEI) could in principle provide such a test. In a CEI experiment, isolated gas-phase proteins are ionised by an intense X-ray pulse and fragment under Coulomb repulsion; the spatial pattern of ion hits on a detector contain structural information about the molecule. Although experiments of this kind on intact proteins have not yet been performed, they are considered feasible. By recording many CEI events from the same protein sample and comparing the resulting explosion patterns against simulated explosions of each AlphaFold2 candidate, dimensionality reduction methods such as PCA and t-SNE could identify which predicted structure clusters most closely with the experimental data.

We demonstrate this concept computationally using Cryptochrome4b, a 99-residue flavoprotein from the European robin (*Erithacus rubecula*), a protein believed to play a role in magnetoreception. The protein was not yet crystallised. Five AlphaFold2 predictions of the same sequence, differing by 2 to 8 Å in Cα RMSD, were each exploded 100 times using a custom ionisation build of GROMACS 4.5.4 at 2000 eV to form a reference library. The gas-phase explosion ensemble of rank 1, treated as a hypothetical experimental measurement, was analysed with the dimensional reduction algorithms PCA and t-SNE to quantify which predicted structure best matches the simulated experiment.



P2 - Gas-phase studies at the MOST beamline of Elettra 2.0

AMO

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Abstract text: Gas-phase photoemission and photoionization spectroscopies provide direct access to the electronic and chemical structure of materials at the atomic and molecular level. At Elettra 2.0, these techniques will be further developed at the Molecular & Optical Science & Technology (MOST) beamline, building on the experience gained at the GasPhase beamline of Elettra.

The research activity focuses on vapor-phase aggregates of increasing complexity, investigated by means of high-resolution synchrotron radiation techniques including XPS, UPS, NEXAFS, ResPES, VEPES, total and dispersed fluorescence spectroscopy, and mass spectrometry. The continuous improvement in energy resolution and experimental sensitivity makes gas-phase studies increasingly relevant for disentangling electronic structure effects that govern material functionality, while the intrinsically high spectral resolution of molecular systems provides stringent reference data for comparison with theory.

MOST introduces significant new opportunities with respect to previous facilities, notably an extended photon energy range and full control of light polarization. In particular, the availability of horizontal and elliptical linear polarization - inherited and expanded from the CiPo beamline by means of the new insertion device - enables advanced dichroic and symmetry-sensitive experiments not previously accessible on GasPhase.

Selected case studies illustrate the potential of gas-phase VUV photoemission at MOST, and perspective developments of the beamline are discussed in view of its role within the Elettra 2.0 source.

P3 - Laboratory astrophysics with photons and ions: Double to tenfold M-shell photoionization of singly charged lanthanum ions

AMO

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Abstract text: In 2017, the LIGO/Virgo collaboration detected the first gravitational-wave signal from the merger of a neutron star binary. Less than two seconds later, a network of telescopes detected a short gamma-ray burst, followed by a longer optical “afterglow” powered by the radioactive decay of the neutron-rich material ejected in the merger, i.e., a kilonova. The kilonova light-curves potentially reveal the abundances of the heavy chemical elements that are produced in the preceding violent neutron-star merger events [1,2]. In order to be able to reliably infer elemental abundances from the astronomical observations, absolute cross sections are required for the basic atomic processes that occur in the afterglow. Generally, these cannot be easily calculated (if at all) to a sufficient precision for the heavy many-electron ions of interest. We used the photon-ion merged-beams setup PIPE, a permanently installed end-station of the PETRA III photon beamline P04 for measuring cross sections for photoabsorption and for multiple photoionizaton of La^+ ions [3], where La^{q+} product ions have been detected with ion charge states $3 \leq q \leq 11$. With these experimental data we have benchmarked new large-scale quantum calculations, in particular, of the dexciation cascades that set in after the initial creation of a *3d* inner-shell hole. Comparisons between the experimental and theoretical results will be presented on the poster.

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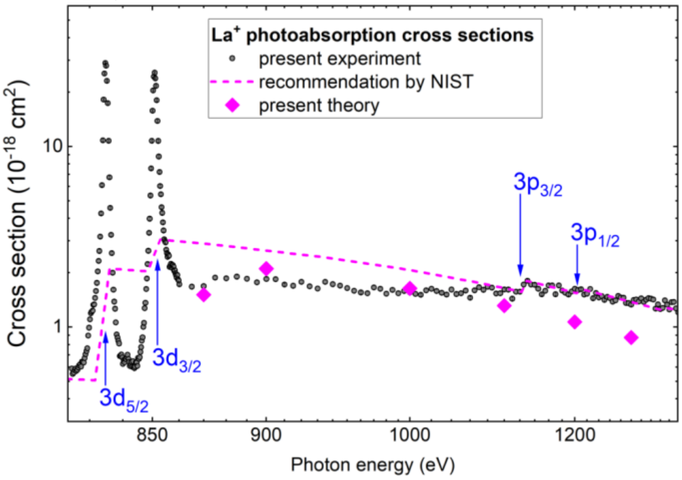

P4 - Latest Results from the FLASH FL26 Beamline for Ultrafast AMO Experiments

AMO

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Abstract text: FLASH is an XUV and soft X-ray free-electron laser delivering femtosecond pulses at high repetition rates. The FL26 beamline is specifically designed for ultrafast atomic, molecular, and optical (AMO) physics experiments. It features a reaction microscope enabling fully differential coincidence measurements, alongside a spectrometer optimized for transient absorption studies in gaseous targets. Unique pump–probe capabilities are provided by a synchronized high-harmonic generation (HHG) source, an optical laser system, and an XUV split-and-delay unit. We present an overview of the experimental setup and highlight recent scientific results demonstrating the capabilities of the beamline.

P5 - Site-dependent core level photoelectron anisotropies in acetone

AMO

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Abstract text: Core-level electron spectroscopy provides a powerful means to probe the local molecular environment. Acetone is an excellent system for such studies due to its two chemically distinct carbon sites, methyl and carbonyl, which give rise to well-separated C 1s photoelectron peaks, enabling site-specific analysis of photoelectron angular distributions (PADs). In this work, we demonstrate how the angular distribution of photoelectrons emitted from acetone after ionization in the vicinity of the carbon K-edge can be a sensitive probe of the local environment.

The experiment was performed using the ICE (Ions in Coincidence with Electrons) endstation at the FlexPES soft X-ray beamline at MAX IV Laboratory, Sweden [1] providing full angular information. The C 1s core levels, with binding energies of 291.01 eV and 293.64 eV [2,3] were measured, allowing us to extract PADs from the photoelectron spectra, enabling determination of β parameter for both the methyl and carbonyl sites.

In Figure 1, we present the measured anisotropy parameter β for the two carbon sites, which reveal pronounced and distinct energy-dependent variations. We believe that these observed features are due to scattering of one photoelectron from neighboring atoms and shape resonance above the ionization threshold. Calculations to quantitatively interpret the observed trends are currently in progress.

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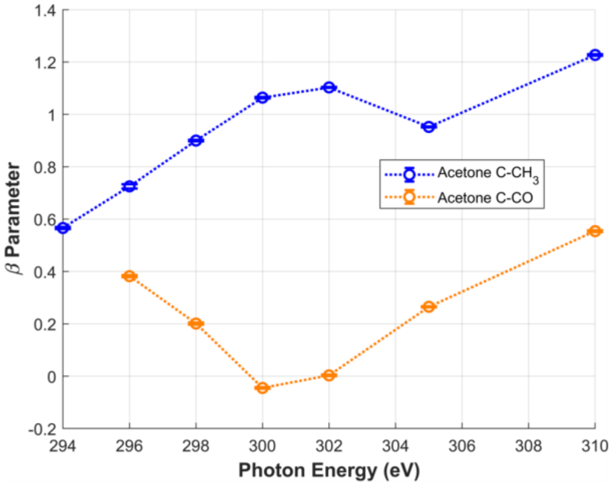

Figure 1: Photon energy dependence of the anisotropy parameter β for C 1s photoelectrons from the methyl (CH3) and carbonyl (CO) sites in acetone.

Correlated Materials

P6 - Probing the Yb 4f crystal-field ground state by polarization-dependent resonant X-ray emission spectroscopy

Correlated Materials

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Abstract text: X-ray spectroscopy is a powerful tool for investigating the electronic and magnetic states of functional materials. BL39XU at SPring-8 is a hard X-ray spectroscopy beamline that enables X-ray absorption, emission, and nano-probe spectroscopy using variable X-ray polarization under extreme conditions. Recently, BL39XU has been upgraded toward SPring-8-II with an ultra-low emittance storage ring. As part of this upgrade, a double X-ray phase retarder system has been installed to control the linear polarization with a variable plane, providing new opportunities to investigate electronic orbitals based on optical selection rules.

Recently, changes in the line shape and/or intensity originating from electronic orbital symmetry have been observed in the polarization dependence of resonant X-ray emission spectra, reflecting both optical selection rules and crystal symmetry. Electric quadrupole (E2) transitions in 4*f*-electron systems, such as at the $L_{3,2}$-edges, involve a change in the orbital quantum number of ±2 and strongly reflect 4*f*-orbital symmetry. While this symmetry is primarily determined by the X-ray absorption process, the signal can be clarified using X-ray emission spectroscopy due to the separation of electric dipole (E1) transitions. This method has been applied to Yb compounds, and the Yb 4*f* crystal-field ground states in the heavy-fermion compound $YbCo_2Zn_{20}$ has been determined. This approach provides an effective tool for investigating 4*f*-orbital symmetry in strongly correlated electron systems.

P7 - Soft X-ray Spectroscopic Study on the Mechanism of Enhanced Ferromagnetism in a La2/3Sr1/3MnO3 Membrane

Correlated Materials

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Abstract text: $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) is a promising material for spintronic applications due to its half-metallicity and high Curie temperature (T_C) exceeding 300 K. However, the performance of LSMO-based devices is hindered by “dead layers” that degrade ferromagnetism and conductivity within LSMO near the interface with other oxides. Recently, epitaxial lift-off using a water-soluble buffer layer, such as $Sr_4Al_2O_7$ (SAO), has emerged as an effective technique to mitigate these issues, enhancing both magnetization and T_C [1]. Nevertheless, the underlying physical mechanisms remain unclear. In this study, we grew an LSMO/SAO heterostructure on an $SrTiO_3$ substrate via molecular beam epitaxy and transferred the LSMO membrane onto a p-type Si substrate by dissolving the SAO layer. The LSMO membrane exhibited significantly enhanced ferromagnetism, with a magnetic moment of 3.2 μ_B/Mn and T_C of 323 K, compared to 2.0 μ_B/Mn and 312 K in the as-grown film. X-ray magnetic circular dichroism (XMCD) revealed that the orbital magnetic moment m_{orb} of Mn in the membrane is approximately three times larger than that in the as-grown film (Fig.1). The enhancement in T_C and m_{orb} is attributed to the increased itinerancy of the Mn 3*d* electrons revealed by resonant photoemission spectroscopy [2]. These findings provide an explanation for the improved ferromagnetixsm in LSMO membranes. This work was partly supported by Grants-in-Aid for Scientific Research, ERATO and FOREST of JST, and the Spintronics Research Network of Japan (Spin-RNJ). [1] T. Arai *et al*., Appl. Phys. Lett. **124**, 062403 (2024). [2] T. Takeda *et al*., Phys. Rev. Mater. **8**, 054415 (2024).

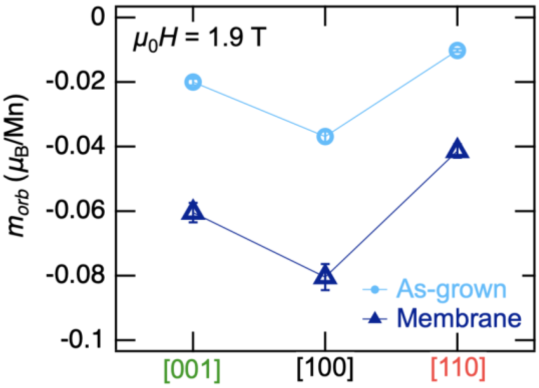

Fig. 1: Orbital magnetic moment of Mn in the membrane and as-grown film estimated by XMCD sum rules.

P8 - Two-dimensional heavy fermion in Ce-Cu/Cu(111)-(2×2) surface alloy by surface segregation

Correlated Materials

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Abstract text: Heavy fermion (HF) systems, arising from hybridization between localized magnetic moments and itinerant conduction electrons, are a prototypical class of strongly correlated electron systems. In parallel, the dimensionality of a system plays a decisive role in determining its fundamental physical properties. The coexistence of strong correlations and reduced dimensionality is therefore expected to host novel quantum phenomena. Recently, we reported a ytterbium (Yb)-based two-dimensional heavy fermion (2DHF) system, $YbCu_2$ on Cu(111), demonstrating that rare-earth surface alloys on metallic substrates provide a promising platform for realizing 2DHF states. Cerium (Ce), which is electron–hole symmetric to Yb, is another strong candidate for engineering such systems. However, the fabrication of Ce-based surface alloys remains a challenging topic, because even under ultrahigh vacuum conditions, deposited Ce atoms are readily oxidized by trace residual oxygen before alloying with the substrate. In this study, we successfully fabricated an ordered Ce-containing surface alloy on Cu(111) exhibiting a (2×2) reconstruction using a surface segregation technique. The surface electronic structure was investigated by synchrotron-based angle-resolved photoemission spectroscopy (ARPES).

From the Ce 4d–4f resonant ARPES measurement, two metallic bands and a flat Ce 4f state just below the Fermi level are observed. Photon-energy-dependent measurements confirm that these electronic bands have a 2D nature. Furthermore, at low temperatures, these metallic bands hybridize with the Ce 4f state, suggesting the emergence of 2DHF states in Ce-Cu/Cu(111)-(2×2) surface.

P9 – Demonstration of Multimodal Tool Combining HREELS and ARPES/XPS

Correlated Materials

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Abstract text: Electrons in quantum materials couple to bosonic excitations, such as phonons and plasmons, making it essential to characterize both these excitations and the electronic band dispersion. Multimodal characterization, where a single sample is analyzed using multiple complementary techniques, offers a powerful approach to uncovering the interplay between various excitations and electronic structure. High-resolution electron energy loss spectroscopy (HREELS) is a technique for observing surface excitations including phonons, magnons, plasmons, excitons, and vibrational modes. Multimodal characterization has been difficult with a traditional single channel HREELS instrument because it requires its own detector, the measurements are time consuming, and angular resolution is limited.

To improve the efficiency of HREELS measurements and to realize multimodal measurement with photoemission spectroscopy, we developed a solution by combining a monochromatic collimated electron source and a hemispherical electron analyser, commonly used for ARPES and XPS [1]. The multichannel 2D detector of the analyser simultaneously measures hundreds of channels in both the energy and angular directions, and the measurements are orders of magnitude faster than the single channel setups. By mounting light sources for photoemission spectroscopy, this setup becomes a multimodal characterization tool that combines state-of-the-art HREELS and ARPES/XPS using the same electron analyser. It allows to study the interplay between various surface excitations and electronic properties. Using graphene and Cu(111) as examples, phonon dispersion, high energy/angular resolution, and high throughput are demonstrated with a recently developed HREELS/ARPES multimodal system.

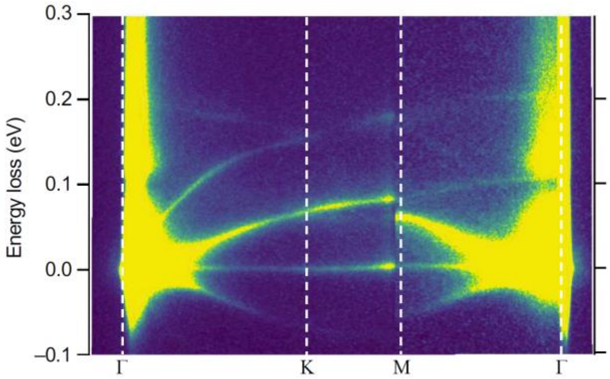

Fig. 1: Phonon dispersion of graphene measured using multichannel HREELS [2]

References

[1] H. Ibach *et al.*, Rev. Sci. Instrum., **88**, 033903 (2017).
[2] Data courtesy: Prof. Choongyu Hwang at Pusan National University

Energy materials

P10 - Mapping Frontier Orbital Alignment in Non-Fullerene Acceptor Organic Solar Cells by XPS and Element-Resolved NEXAFS

Energy materials

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Abstract text: The transition from fullerene to non-fullerene acceptors has drastically increased the power conversion efficiency of organic photovoltaics, now exceeding 20%, with the PM6:Y7 blend system emerging as a promising active layer. In bulk heterojunction device architectures, it can be sandwiched between charge transport layers of transition metal oxides to ensure efficient energy level alignment and charge extraction, which directly impact device efficiency. However, accurately determining the frontier orbital alignment remains experimentally challenging and subject to ongoing debate.

We present a spectroscopic methodology combining X-ray Photoelectron Spectroscopy (XPS) and Near-Edge X-ray Absorption Fine Structure (NEXAFS) to map the frontier orbital energetics between PM6:Y7 with different donor-to-acceptor ratio and oxide transport layers (ZnO and MoO_3) on a common energy scale relative to the Fermi level, allowing access to the transport gap, which is found to be modulated by both blend composition and substrate. In addition, by selectively probing absorption K-edges of elements unique to each blend component and aligning the corresponding NEXAFS spectra to the core-level ionization potentials, we decouple the individual contributions of PM6 and Y7 to the NEXAFS onset shifts across blend compositions. A non-linear dependence of the onset on composition is also observed, indicating the presence of an optimal PM6:Y7 donor-to-acceptor ratio for favourable energy level alignment, which is found to lie between 1:1 and 1:2. Finally, chlorine - unique to Y7 - emerges as a key element in modulating the NEXAFS onset of the blend and its alignment with ZnO relevant for electron transfer.

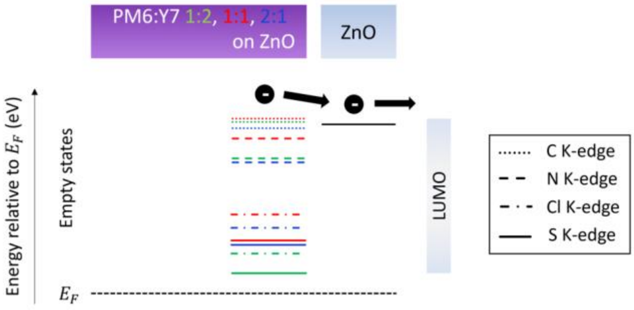

Figure 1. Energetic alignment between NEXAFS onsets at the C, N, Cl, and S K-edges of PM6:Y7 blends with different donor-to-acceptor mass ratios and the conduction band minimum of ZnO.

P11 - Overlooked! The Role of Octahedral Fe Carbides in Fischer-Tropsch Synthesis

Energy materials

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Abstract text: Fischer-Tropsch synthesis (FTS) is the conversion of syngas (CO and H_2) to hydrocarbons for synthetic fuels or petrochemicals. As one of the few commercially viable options, iron (Fe) catalyzes FTS via intermediate formation of carbides as active phase. The range of reportedly active carbide phases is structurally classified into trigonal prismatic (*tp*) and octahedral (O_h) carbides. However, the co-existence of different carbides has so far obscured a distinct picture of the catalytic activity and role of each species in FTS. Based on previous work of our group, we hypothesized the presence of *tp* and O_h carbides to be more entangled than anticipated in literature.

Here we used *in-situ* ambient pressure X-ray photoelectron spectroscopy to study adsorbate distribution and the reaction progression on Fe(110) at near-industrial pressure. Since the structurally different carbides exhibit a clear chemical shift, we could investigate each species separately, employing a gas pulsing scheme at 600 K. Cycles consisted of a pulse of reaction mixture (500 mbar, 3:1 H_2:CO) followed by a hydrogenation period (120 mbar, H_2). Our preliminary results suggest that O_h carbides precede the build-up of other species in reaction mixture but are also active in the hydrogenation step of FTS (see Figure 1). In contrast, *tp* carbides only evolve after multiple cycles and appear static in pure H_2. Thus, contrary to reports of *tp* carbides being of central importance for Fe-based FTS, we could infer O_h carbides to play a significant role, both in the carbide formation and hydrogenation steps.

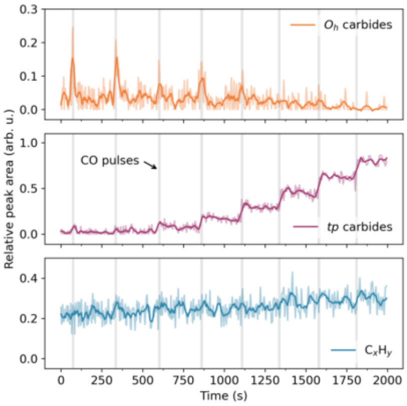

Figure 1. Fitted peak areas of X-ray photoelectron spectra of the C 1s core level in FTS reaction mixture (3 H_2: 1 CO, 500 mbar), indicated by grey bars, and in pure H_2 (120 mbar), at 600 K. Each pulse leads to an immediate increase of O_h carbides, followed by rapid hydrogenation, whereas *tp* carbides build up only after multiple cycles and remain static after each pulse.

P12 - Probing Interfacial Chemistry and Energy Band Alignment in FAPbI3-based Perovskite Solar Cells using Synchrotron Based Photoemission Spectroscopy

Energy materials

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Abstract text: Interfacial processes critically influence the performance and long-term stability of perovskite solar cells (PSCs). Photoemission spectroscopy (PES) is a powerful, non-destructive technique that provides direct insight into the chemical and electronic structure of PSC interfaces. In particular, synchrotron-based PES enables probing of buried interfaces that are inaccessible to conventional laboratory methods. In this work, we demonstrate how synchrotron PES can be employed to investigate interfacial chemical reactions, energy band alignment, and ion migration in a complete perovskite device stacks. The use of tunable photon energies allows control over probing depth and enhances sensitivity to subtle interfacial changes. We focus on device architectures ITO/SnO2/FAPbI3/spiro-OMeTAD. Our measurements reveal clear evidence of ion migration and interfacial chemical modification at the FAPbI3/spiro-OMeTAD junction. Both Pb 4f and I 3d core level spectra indicating that deposition of the spiro-OMeTAD hole transport material induces ion migration into the organic matrix and the chemical interactions with functional groups within spiro-OMeTAD. The N 1s spectra, shows the emergence of a new peak and a systematic shift toward lower binding energy, indicate chemical modification and downward band bending at the interface. To further elucidate these effects, we systematically varied the thickness of the spiro-OMeTAD layer on FAPbI3, with and without phenethylammonium iodide (PEAI) passivation. The PEAI layer forms a thin two-dimensional perovskite layer that suppresses interfacial reactions and stabilizes the surface. These results provide detailed insight into interfacial degradation pathways and offer guidance for improving PSC stability and by extension device efficiency.

P13 - Reactively Sputtered NbO_x/NbS_2 Memristive Heterostructures Probed by HAXPES

Energy materials

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Abstract text: Oxide-based memristive devices rely on electric-field-driven ion migration and redox processes, which are governed by the chemical and electronic structure of buried interfaces. These interfacial properties critically influence switching behavior, device stability, and charge transport.In this work, we investigate a memristive heterostructure consisting of a NbS_2 bottom electrode and a NbO_x active switching layer. The NbS_2 layer is grown via reactive magnetron sputtering in an Ar/H_2S atmosphere, followed by Nb deposition and subsequent oxidation to form NbO_x, providing a scalable route for integrating transition metal sulfides into oxide-based memristive systems.

The electronic and chemical properties of the heterostructure are studied using hard X-ray photoelectron spectroscopy (HAXPES), enabling access to buried interfaces. Depth-resolved measurements are performed to track variations in oxidation states across the NbO_x/NbS_2 interface as well as within the NbO_x layer. These results provide insight into oxidation state evolution in the memristive heterostructure, relevant for device design and optimization.

P14 - Revealing Oxide, Self-assembled monolayer interfaces in Perovskite photovoltaic systems with X-ray photoelectron spectroscopy

Energy materials

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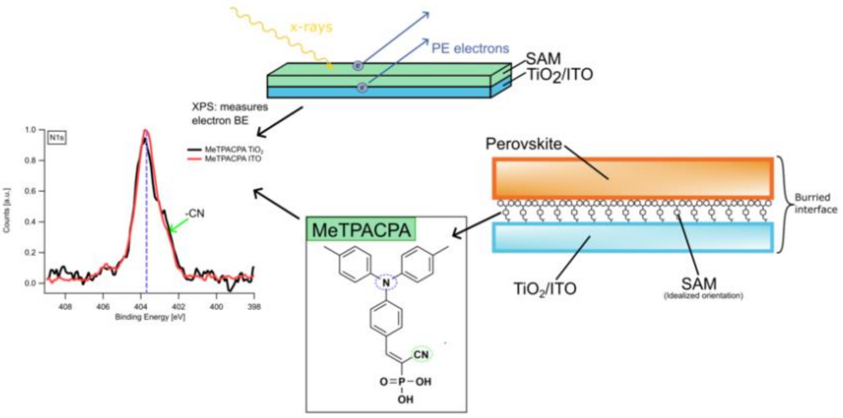
Abstract text: Inverted (p-i-n) lead halide perovskite solar cells (PSCs) have appeared as a promising alternative to conventional (n-i-p) architectures, given their advantage of lower processing temperatures, reduced hysteresis and compatibility with integration of tandem solar cells. In order for these cells to achieve competitive efficiencies, minimizing non-radiative combination losses at buried interfaces, especially between the perovskite absorber and the hole-transport layer, is required. Self Assembled Monolayers (SAMs), particularly Carbazole-based phosphonic ones, have been implemented in some of the highest-efficiency (PSCs).

The interpretations behind the success of this material have largely been inferred from device metrics and macroscopic electrical measurements. Spectroscopic analysis of the interfaces of SAMs within interfaces and particularly buried interfaces (which would be the case in practical applications) are severely lacking. The goal of this project has thus been to characterize the interfaces between oxide substrates (such as indium-doped tin oxide (ITO)) and SAM, eventually as a part of the buried SAM/Perovskite interfaces in inverted PSCs.

Through x-ray photoelectron spectroscopy (XPS) analysis, where the probing depth is adjusted by using photon energies ranging from hard to soft x-rays, SAM adsorption on the surface, ITO surface energetics and molecular orientation can be revealed. A fundamental understanding of these molecules in PSCs will help explain the details of their success and help make the best choice of SAMs for high efficiency.



P15 - Soft x-ray spectroscopic study on redox flow battery electrolytes

Energy materials

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Abstract text: Redox flow batteries (RFBs) are promising candidates for large-scale stationary energy storage to accommodate renewable energy fluctuations. Among various RFB systems, titanium-manganese (Ti-Mn) RFBs have attracted attention as a cost-effective alternative to vanadium-based systems. However, the formation of precipitates in the catholyte during charging remains a critical challenge, leading to degradation of cyclability and efficiency, as well as clogging in the flow path and carbon electrodes. In this study, we performed element-selective electronic structure analyses of Ti-Mn aqueous electrolyte solutions using soft X-ray absorption spectroscopy (XAS) and scanning transmission X-ray microscopy (STXM) to clarify the redox reactions and elucidate the mechanism of precipitate formation. Ex situ soft XAS measurements at the Ti and Mn $L_{2,3}$-edges were conducted at BL-2B of KEK-PF in fluorescence mode. The electrolyte composition was Mn (1 M), Ti (1.33 M), and H_2SO_4 (3 M). Spectra were analyzed using charge-transfer multiplet calculations (CTM4XAS). Ti L-edge XAS confirmed that Ti remains in the Ti^{4+} state in the catholyte, while reduction to Ti^{3+} occurs in the anolyte upon charging. Mn L-edge XAS revealed that Mn in the charged catholyte solution maintains the Mn^{2+} state rather than being oxidized to Mn^{3+}. Analysis of dried carbon felt electrodes showed coexistence of M^{n3+} and Mn^{4+} near the outlet, confirming charge disproportionation ($2Mn^{3+} \rightarrow Mn^{2+} + Mn^{4+}$). Furthermore, STXM measurements at BL4U of UVSOR demonstrated that precipitates are mainly composed of Mn^{4+} and also contain Ti^{4+}, indicating they are not simple MnO_2 but rather complex mixed precipitates.

P16 - Surface-to-Bulk Evolution of Cationic and Anionic Redox in a P2-Layered Oxide Sodium-Ion Cathode

Energy materials

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Abstract text: P2-type $Na_{0.67}Mn_{0.5}Fe_{0.45}Mg_{0.05}O_2$ (NMF-Mg) is a promising sodium-ion battery cathode, yet its practical use is limited by structural instabilities such as irreversible P2–O2 phase transitions and Mn^{3+}-driven Jahn–Teller distortion [1,2]. Understanding how these structural effects couple to charge compensation across surface and bulk is therefore essential for rational material design. In this work, we investigate the charge storage dynamics in NMF-Mg electrodes cycled to defined states of charge (SOC).

X-ray photoelectron spectroscopy (XPS) at 1000 eV and 7150 eV was used to probe surface and near-surface chemistry (Figure 1). O 1s spectra show a reversible shift from ~534 eV in the charged state, associated with oxidized transition-metal coordination and cathode–electrolyte interphase (CEI) species, to ~532 eV in the discharged state, linked to oxygen bound to reduced metal centers. F 1s spectra reveal a strong increase in NaF (~685 eV) upon sodiation, which is more pronounced in bulk-sensitive measurements, indicating PF_6^- decomposition and NaF formation throughout the CEI. Na 2s spectra exhibit clear state-of-charge-dependent shifts, reflecting changes in the sodium coordination environment during cycling.

To access bulk redox processes not fully resolved by XPS, Fe and Mn K-edge X-Ray Absorption Spectroscopy (XAS) will be presented to resolve transition-metal redox activity and local structural evolution. In addition, oxygen K-edge resonant inelastic X-ray scattering (RIXS) maps will be shown, revealing oxygen participation in charge compensation beyond transition-metal redox chemistry.

1 Eom, S. et al. Mater. Today Energy 38, 101449 (2023)
2 Zhang, L. et al. Energy Reviews 4, 100166 (2025)

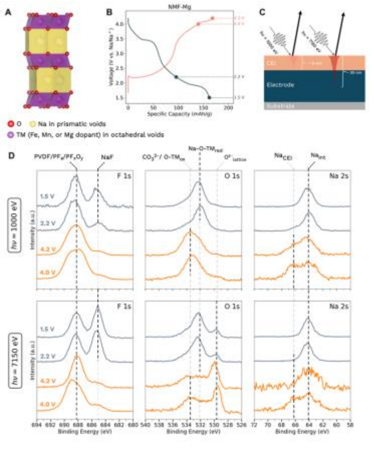

Figure 1. (A) Crystal structure of a P2-type layered oxide sodium-ion cathodes. (B) Voltage profile of NMF-Mg during the second electrochemical cycle, with the selected cutoff voltages marked. (C) Schematic illustration of the probing depths for XPS measurements at 1000 eV (soft X-ray) and 7150 eV (hard X-ray). (D) F 1s, O 1s, and Na 2s spectra of NMF-Mg electrodes cycled to the respective cutoff voltage during cycle 2, measured at 1000 eV (top) and 7150 eV (bottom).

P17 - Temperature Dependent Structural Evolution in Low-dimensional Perovskite Nanoplatelets

Energy materials

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Abstract text: Low-dimensional metal halide perovskite nanoplatelets are widely studied and have emerged as promising materials for next-generation optoelectronic devices owing to their tunable optical properties, narrow emission linewidths, and high photoluminescence quantum yields. However, a comprehensive understanding of their structural evolution across different dimensionalities and under varying temperatures remains underexplored. These insights are vital for understanding the carrier-phonon interactions and thermal transport mechanisms in perovskite nanoplatelets.

In this work, we systematically investigate the crystal structure and ordering in perovskite nanoplatelet thin films, across quantum confined nanoplatelets to bulk-like nanocrystals, over a wide temperature range using grazing-incidence wide-angle X-ray scattering (GIWAXS). Using Temperature-dependent in situ GIWAXS measurements we examine the change in crystallographic orientation with respect to dimensionality. We observe that low-dimensional nanoplatelets maintain structural ordering over a broad temperature range, whereas larger nanocrystals show more pronounced temperature-induced changes in ordering, exhibiting bulk-like behavior. Structures with intermediate dimensions exhibit gradual changes, highlighting the role of surface energy and lattice stability.

We also gain insight into how slow evaporation thin film influences the preferential in-plane and out-of-plane orientation of perovskite nanoplatelets, both of which are critical for charge and energy transport within the films.

HHG/VUV

P18 - Attosecond quantum beat interferometry: Impacts of light field spectral amplitude

HHG/VUV

Samuel Eriksson[1]
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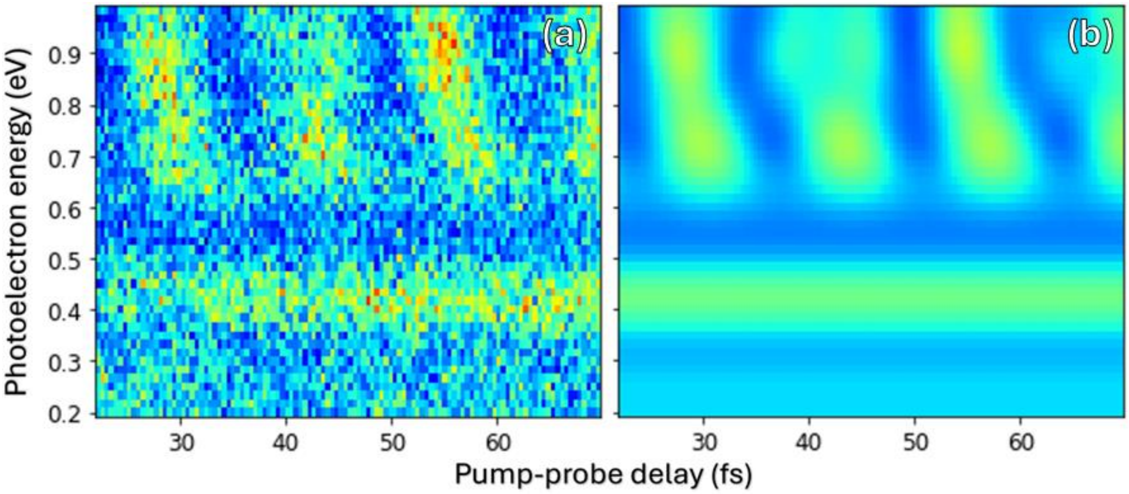
Abstract text: The development of broadband extreme ultraviolet sources has made it possible to study complex superpositions of bound and continuum electron states via pump-probe schemes. In our case, a short extreme-ultraviolet (XUV) attosecond pulse train excites several bound states of the Rydberg p-series in helium near the ionization threshold. A coherent, delay-controlled, few-cycle near-infrared (NIR) broad bandwidth (1.2–2 eV) probe pulse subsequently ionizes into the continuum. Due to the energy differences between states, contributions from different ionization pathways acquire different phases and can interfere, producing quantum beats in the signal as the delay between the XUV pump and NIR probe is scanned.

Spectrograms, obtained by scanning the pump-probe delay while detecting photoelectrons with a home-made 3D momentum spectrometer, have been recorded and are being analyzed. We have developed a numerical method to extract the reduced density matrix of the state prepared by the pump and the ionization amplitude due to the probe without prior knowledge of the XUV and NIR fields. The method uses a Monte Carlo approach to retrieve the ionization amplitude and has been benchmarked against simulated data over a range of photoelectron resolutions, showing good performance and robustness under experimental conditions.

The figure shows an experimental dataset (a) compared with the retrieved fit (b). The method reproduces modulations along the photoelectron energy axis, due to the spectral amplitude, as well as along the pump–probe delay axis, due to the coherences in the XUV-prepared superposition and the spectral phase of the NIR probe.



P19 - Attosecond Rotational Doppler Effect in Solid-state High Harmonic Generation

HHG/VUV

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Abstract text: The traditional Doppler effect was first proposed by C. Doppler in 1842 to describe the frequency shift of a sound wave moving towards or away from an observer. Its counterpart, the rotational Doppler effect, is associated with the angular momentum of waves. The rotational Doppler effect has been extended from rotating macroscopic media to rotating microscopic molecules, with rotational frequencies ranging from Hz to THz.

We highlight that the ultrafast motion of electrons on the attosecond time scale can be excited and steered by a waveform-shaped femtosecond laser pulse, offering an ideal platform to investigate the rotational Doppler effect. High harmonic generation (HHG), in particular, provides an exceptionally sensitive probe for observing subcycle electron dynamics. We demonstrate an attosecond rotational Doppler effect in HHG from a non-rotating crystal, driven by a waveform-shaped femtosecond laser pulse, whose rotational frequency is on the PHz scale. By controlling the waveform of the driving laser pulse, the frequency shifts exhibit red or blue shifts. Our work demonstrates a novel attosecond rotational Doppler effect in high-order nonlinear processes, providing insight into the fundamental mechanisms of the rotational dynamics in HHG, and inspires potential applications for precision measurements.

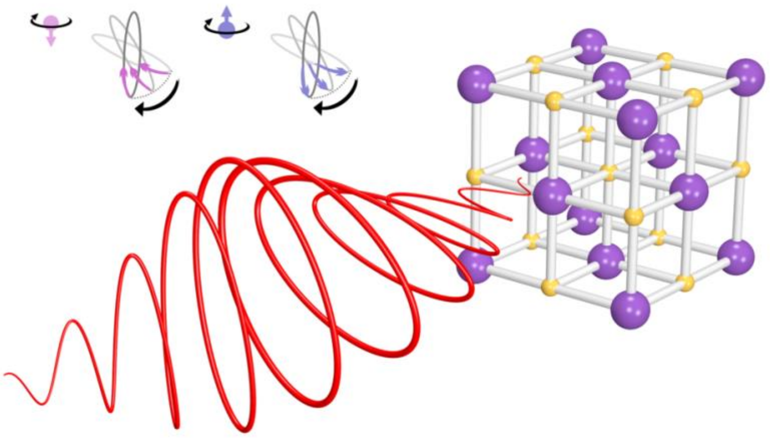

Fig. 1. Attosecond rotational Doppler effects explored using HHG spectroscopy in MgO crystal.

P20 - Present status and future perspectives of the micro-ARPES system at NanoTerasu BL06U

HHG/VUV

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Abstract text: Angle-resolved photoemission spectroscopy (ARPES) is a powerful technique that enables direct observation of the electronic structure of materials. It has been widely used for exploring novel physical phenomena in materials such as topological insulators and low-dimensional materials, as well as for elucidating microscopic mechanisms of electronic device materials.

A soft X-ray ARPES beamline, BL06U, has been constructed at the 3 GeV high-brilliance synchrotron radiation facility NanoTerasu (Sendai, Japan) [1]. BL06U provides high-brilliance soft X-rays in the energy range of 50–1000 eV with switchable polarization (horizontal and vertical linear polarization, left- and right-circular polarization). The beamline consists of two branches; in one of them, the B-branch, a micro-ARPES system has been installed, with a focused beam of less than 10 μm achieved. The user operation has began in March 2025.

In this poster, we mainly report on the specifications and future development plans of the micro-ARPES system. The DA30-L analyzer (Scienta-Omicron) was installed this year, and ARPES measurements using the deflector mode have been available to users since April 2026. A preparation chamber in which sample surface preperation can be performed will be opened to users from September 2026. Furthermore, to realize soft X-ray spin-resolved ARPES with a micro-focused beam, we are developing the double very-low-energy-electron-diffraction (VLEED) spin detectors which offers approximately two orders of magnitude higher efficiency than conventional Mott-type detectors[2] and enables three-dimensional spin vector analysis.

[1] K. Horiba *et al.*, J. Phys.: Conf. Ser. **2380**, 012034 (2022). [2] T. Okuda *et al.*, Rev. Sci. Instrum. **79**, 123117 (2008).

Instrumentation

P21 - A user-friendly materials science end station at the FinEstBeAMS beamline of MAX IV

Instrumentation

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Abstract text: The Solid State End Station (SSES) is a key component of the FinEstBeAMS beamline at the MAX IV Laboratory, developed through international collaboration between Finland and Estonia with infrastructural support from Sweden. Integrated within the ultraviolet and soft X-ray branch of FinEstBeAMS, SSES enables high-precision investigations of surfaces, interfaces, and solid materials under ultra-high-vacuum conditions. Utilizing radiation from an elliptically polarizing undulator (EPU), the end station offers tunable photon energies from 4.5 eV to 1300 eV and selectable polarization states from linear to circular. The beamline achieves a resolving power of 11 000 at 400 eV photon energy with a 10 µm monochromator slit, while the focused beam spot size at SSES can reach approximately 15 µm × 20 µm by closing the silt at beamline. These parameters make SSES ideally suited for micro scale characterization, electronic structure analysis, and interface studies using ultraviolet and soft X-ray spectroscopies. As part of the MAX IV user portfolio, SSES is openly accessible to the scientific community, providing a versatile platform for solid-state and surface research.

P22 - Current status of nano-ARPES beamline BL06U at NanoTerasu

Instrumentation

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Fumi Nishino[1], Hideaki Iwasawa[1], Nobuhito Inami[1], Tomoyuki Takeuchi[1], Takashi Imazono[1], Yoshiyuki Ohtsubo[1], Jun Miyawaki[1], Kohei Yamamoto[1], Kento Inaba[1], Akane Agui[1], Takeshi Nakatani[1], Kentaro Fujii[1], Hiroaki Kimura[1], **Koji Koriba**[1]
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Abstract text: The beamline BL06U at NanoTerasu is designed for angle-resolved photoemission spectroscopy (ARPES) using micro- and nano-focused beams, including spin-resolved measurements. A 4 m-long APPLE-II type undulator provides brilliant soft X-rays with various polarizations (horizontal and vertical linear, and left- and right-circular) in the 50–1,000 eV energy range. A collimated plane grating monochromator (cPGM) is employed as a monochromator [1].

BL06U can be operated by switching between two branches. In the B-branch, a focused beam of less than 10 μm has been achieved using a Wolter-I mirror, and user operation as a micro-ARPES station began in March 2025. Meanwhile, the nano-ARPES station is under construction in the A-branch. Unlike many other nano-ARPES stations that use Fresnel zone plates for nanoscale beam focusing, this nano-ARPES station adopts an ultra-high-precision mirror optical system. This approach aims to generate a high-flux nano-focused beam and achieve highly efficient ARPES measurements.

As a first step, a 1 μm focused beam using a Wolter-I mirror will be realized and made available for user operation. In the next step, the goal is to achieve soft X-ray ARPES measurements using about a 100 nm focused beam with a developed tube-shaped mirror. In this presentation, we report on the current commissioning status of the BL06U beamline, with a primary focus on the progress of the A-branch nano-ARPES station.

[1] K. Horiba *et al.*, J. Phys.: Conf. Ser., **2380**, 012034 (2022).

P23 - Development of a full-field imaging X-ray transmission microscope for X-ray absorption spectroscopy

Instrumentation

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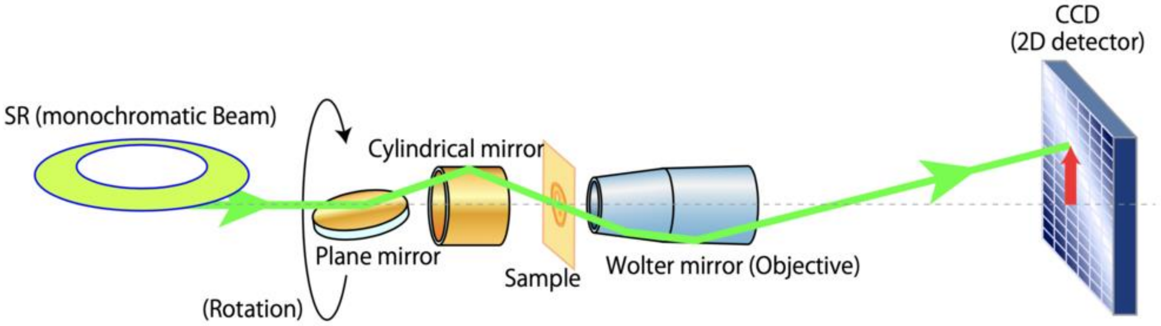
Abstract text: In Photon Factory (Tsukuba, Japan, 2.5 GeV, 450 mA), an upgrade plan is under discussion, featuring a proposed energy-switchable storage ring to cover a wide wavelength range of X-rays [1]. As a demonstration of this upgrade, a new versatile beamline, BL-12A, has been designed to utilize this wide spectral range. BL-12A features two optical paths equipped with a plane grating monochromator and a double-crystal monochromator, respectively. These paths share a common focal point, providing a continuous energy range of 50 ~ 5,000 eV [2].

To use the wide energy range of BL-12A, we have developed a full-field imaging transmission X-ray microscope (FFTXM) to perform 2D X-ray absorption spectroscopy (XAS) with high spatial resolution. The optical system, illustrated in Fig. 1, employs a condenser system consisting of rotating plane mirrors and a Wolter mirror as the objective to image the transmitted X-rays onto a 2D detector (e.g. CCD camera). Since the system relies exclusively on total reflection, it offers high efficiency and is free from chromatic aberration, enabling rapid image acquisition. These advantages are expected to facilitate time-lapse imaging and high-speed 2D XAS. In this presentation, we report the image acquisition results and characterize the condenser optics of the FFTXM.

[1] T. Sato, et al., *J. Synchrotron Rad.*, **32** (2025) 1143-1151.
[2] T. Ohigashi, in preparation.



P24 - Dichroism measurements of soft and tender X-ray absorption spectroscopy with high-speed polarization switching by segmented undulator

Instrumentation

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Abstract text: Polarization of photon provides quite a wide range of physical information. Among them, x-ray circular and linear dichroism (XMCD and XMLD, respectively) are one of the standard element-specific tools to unveil the spin and orbital texture of materials. At NanoTerasu, a new 3 GeV high-brilliance synchrotron radiation facility which started its operation in April 2024 [1], we are constructing a beamline BL13U dedicated for high performance XMCD/XMLD measurements with versatile photon polarization and photon energy range from soft (180 eV) to tender (3000 eV) X-ray region [2]. Furthermore, the unique photon source, the series of four undulator segments combined with electromagnetic phase shifters is adopted to achieve accurate and high-speed polarization switching [3].

In this presentation, we're going to show the latest XMCD and XMLD dataset obtained by using the segmented undulator. Thanks to the high-speed polarization switching, errors and noises from external environments are drastically reduced and thus small XMCD signal down to 0.3 % could be measured with sufficient signal/noise ratio. Further updates of the dichroism measurements leveraging the segmented undulator will also be discussed.

References

[1] S. Obara *et al.*, Phys. Rev. Accel. Beams 28, 020701 (2025).
[2] Y. Ohtsubo *et al.*, J. Phys.: Conf. Ser. 3010, 012079 (2025).
[3] K. Inaba *et al.*, J. Synchrotron Rad. 33, 73 (2026).

P25 - Multi-mode electron optics for k-imaging ARPES, X-ray photoelectron microscopy (XPEEM) and RIXS

Instrumentation

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Gerd Schönhense[1]
[1] Institute of Physics, Johannes Gutenberg University, Mainz, Germany

Abstract text: A multi-mode lens system has been developed, based on a novel objective lens enabling several modes of photoelectron recording [1,2]; examples in Fig.1. We demonstrate its performance by results from prototype instruments at different photon sources. *Reduced electric field strength* at the sample in comparison with classical cathode-lens optics has proven important for the study of cleaved samples with sharp edges, particularly in time-resolved ARPES at fs sources using pump-probe techniques [3]. *Enlarged k-range* is advantageous for photoelectron diffraction. *Space-charge effects are suppressed* by operating the front lens in a retarding mode, as demonstrated in experiments at the free-electron laser FLASH [4,5]; example Fig.1c. Real-space imaging on selected core levels (*X-PEEM*) yields element-specific images for characterizing structured samples [2]. *Very large fields of view* (example Fig.1a,b) in X-PEEM mode are crucial for implementing the concept of PAXRIXS; a first prototype instrument is installed at beamline P04 of PETRA III [6]. The RIXS photon spectrum is 'translated' into a photoelectron spectrum using an ultrathin converter foil, with the position on the converter being a measure for the momentum transfer. The new electron optics enables switching between ARPES, XPEEM and PAXRIXS just by varying lens voltages.

[1] Tkach et al., *Ultramicr*.**276,**114167(2025)
[2] Tkach et al., *Rev.Sci.Instrum*.**97,**033703(2026)
[3] Fragkos et al., *Nat.Commun*.**16**,5799(2025)
[4] Schönhense et al., *Rev.Sci.Instrum*.**92**,053703(2021)
[5] Pressacco et al., *Nat.Commun*.**12**,5088(2021)
[6] Fawaz et al., this conference

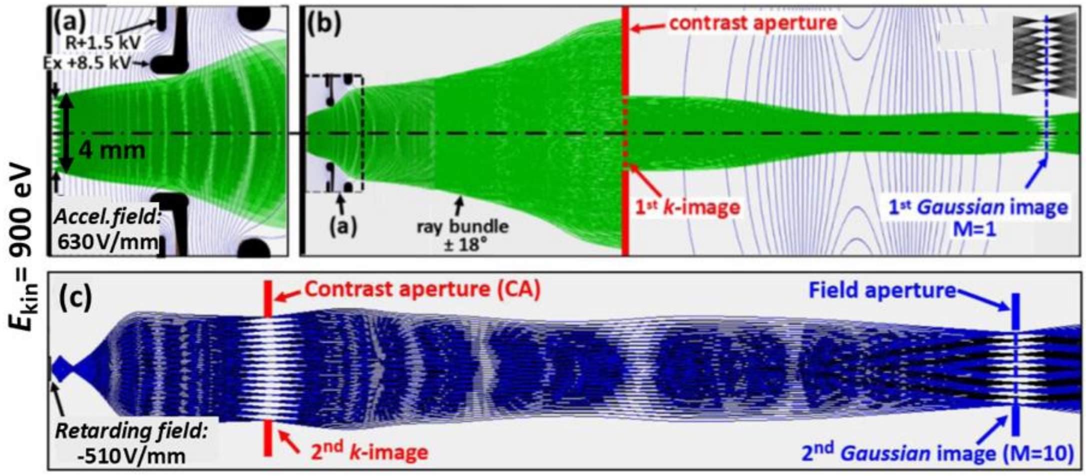

Fig.1. XPEEM with 4mm field-of-view (a,b) and with retarding field at the sample (c). (from [1])

P26 - NanoTerasu Facility Report: Key Achievements and Impact of QST

Instrumentation

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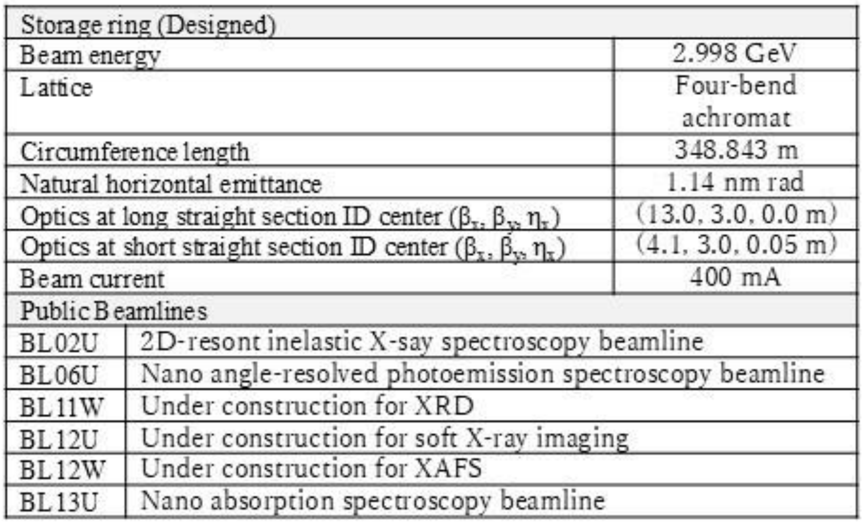
Abstract text: The National Institutes for Quantum Science and Technology (QST) is responsible for the construction, operation, and maintenance of the accelerator and public beamlines, as well as for facility network and radiation safety at NanoTerasu, a new 3 GeV synchrotron radiation facility in Japan. User operation of the accelerator began in April 2024 with a stored beam current of 160 mA. Following the installation of a bunch-by-bunch feedback (BBF) system, the storage ring has successfully achieved stable operation at the designed stored current of 400 mA.

The facility has fourteen 5.44 m straight sections and fourteen 1.64 m straight sections, each of which can accommodate an insertion device. Public beamlines were initially constructed to comprise three instruments: a two-dimensional resonant inelastic X-ray scattering beamline, a nano angle-resolved photoemission spectroscopy beamline, and a nano X-ray absorption spectroscopy beamline. These beamlines have been open to users since March 2025. In addition, several other beamlines are currently under construction including an X-ray diffraction beamline scheduled to begin user operation in 2027, soft X-ray imaging (user operation start: 2029), and X-ray absorption fine structure (user operation start: 2028).

In this presentation, we report on the current operational status of the NanoTerasu storage ring, the available and upcoming beamlines (Table), and recent progress in facility commissioning and user operation.



Storage ring (Designed)	
Beam energy	2.998 GeV
Lattice	Four-bend achromat
Circumference length	348.843 m
Natural horizontal emittance	1.14 nm rad
Optics at long straight section ID center (β_x, β_y, η_x)	(13.0, 3.0, 0.0 m)
Optics at short straight section ID center (β_x, β_y, η_x)	(4.1, 3.0, 0.05 m)
Beam current	400 mA
Public Beamlines	
BL02U	2D-resont inelastic X-say spectroscopy beamline
BL06U	Nano angle-resolved photoemission spectroscopy beamline
BL11W	Under construction for XRD
BL12U	Under construction for soft X-ray imaging
BL12W	Under construction for XAFS
BL13U	Nano absorption spectroscopy beamline

P27 - Soft X-ray Absorption Spectroscopy at TPS 35A1: Achieving a Wide Energy Range, High Flux, and Versatile Sample Environment Capabilities

Instrumentation

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Chueh-Cheng Yang[1], Hok-Sum Fung[1], Shu-Chih Haw[1]
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Abstract text: Soft X-ray absorption spectroscopy (sXAS) is a key analytical technique across materials science, chemistry, physics, and biology, as it provides local electronic-structure information with both orbital and element specificity. Within the soft X-ray regime (100–2500 eV), sXAS enables detailed investigations of essential elements, including light elements such as C, N, and O, as well as first-row transition metals that play pivotal roles in catalysis, magnetism, and energy-storage materials.

To support advanced sXAS studies, the TPS 35A1 beamline is under construction, designed to deliver a broad energy range, high photon flux, and highly adaptable sample environments. The beamline covers 200–2500 eV and incorporates an active mirror–plane grating monochromator (AM-PGM) system, which provides high flux, excellent energy resolution, and wide tunability. The TPS 35A1 endstation is equipped with multiple detection modes—including TEY, PEY, TFY, iPFY, and PFY—enabling measurements with different probing depths in both step-scan and high-speed fly-scan modes (up to one spectrum per minute). Moreover, the sample environment is engineered to support in situ and operando experiments, allowing measurements under controlled temperature, applied potentials, and reactive liquid or gas atmospheres for catalysis-related research.

According to the current project timeline, hardware construction of TPS 35A will be completed by the end of this year. Beamline commissioning is scheduled for Q1–Q3 of this year, with user operations expected to begin in Q4.

Reference

(1). H. S. Fung et al. AIP Conf. Proc. 2007, 879 (1), 563-566.

P28 - TRISS: An ion trap mass spectrometer endstation for X-ray Spectroscopy

Instrumentation

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Carl Caleman[1], Olle Björneholm[1], Noelle Walsh[2], Stacey Ristinmaa Sörensen[3]
[1] Uppsala University
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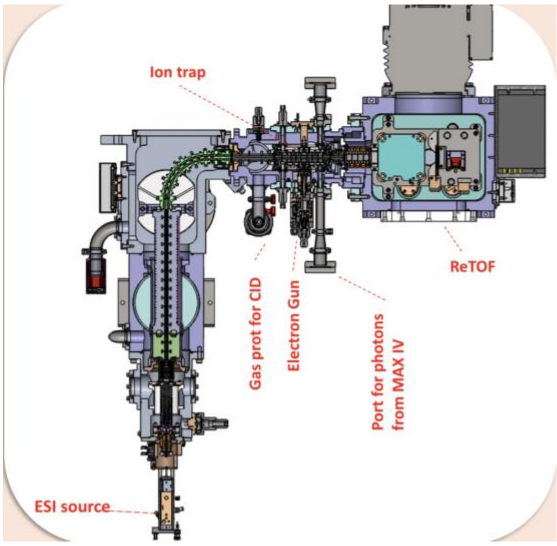
Abstract text: Ionic matter plays a crucial role in diverse processes, from atmospheric and interstellar chemistry to biological systems. However, traditional X-ray studies on free ions are hampered by the challenge of achieving sufficient target density. The Trapped Ion Spectrometer Setup (TRISS) offers a solution by accumulating ions in a trapping field prior to X-ray interaction , enabling the investigation of systems like molecular ions, biomolecules, and nanoscale clusters.

TRISS combines an Electrospray Ionization (ESI) source, a segmented linear ion trap (Omnitrap), and a Reflectron Time-of-Flight (ReToF) mass spectrometer. The Omnitrap facilitates ion accumulation, specific mass-to-charge isolation via resonant excitation, and Collision-Induced Dissociation (CID). A dedicated trapping segment enables photoexcitation and photodissociation studies.

Offline commissioning has successfully validated core functionalities, including ion trapping, selective isolation, and fragmentation. CID experiments demonstrated the isolation of protonated nitroimidazole (114 m/z). Colliding nitrogen gas with the trapped isolated molecules generated fragments; analysis showed that increased gas pulse duration decreased the parent molecule's intensity while increasing fragment ion intensity. Initial online commissioning provided essential diagnostic data to guide the current optimization of beamline integration. Future online commissioning is planned to achieve full endstation functionality, ensuring complete operational readiness for X-ray induced photodissociation studies.



Liquids

P29 - Insight into the hydration of dimethyl sulfoxide studied by ATR-VUV/UV spectroscopy coupled with chemometrics

Liguids

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Abstract text: Dimethyl sulfoxide (DMSO) is an amphiphilic, aprotic solvent consisting of a hydrophilic sulfoxide group and two hydrophobic methyl groups. There remains an active discussion about the behavior of DMSO in water. Some researchers conclude that DMSO strengthens the interaction among water molecules [1], while others the opposite [2]. A key to resolving the conflicting results lies in finding the hydration structure of DMSO. This study is intended for that from concentration-dependent absorption spectra of the aqueous solution measured on a VUV/UV beamline with a newly installed ATR assembly.

The experiments were performed on BL-12 of HiSOR, Japan. We made a prism holder box with two rod wings sticking out to suppress stray light. It held a fused silica prism in an inverted triangular way. It was placed along the light axis so as to satisfy the total reflection conditions. The sample solutions were prepared with the molar fraction of DMSO between 0.01 and 0.10.

The measured spectra strongly depend on the concentration, as shown in Fig. 1. Chemometric analysis is employed for the spectra to extract information on the microstructure. The principal component analysis concludes that the spectra are well explained by three components. The MCR-ALS analysis shows that the major microstructure changes at the molar fraction of 0.04 and 0.06. The result is in accord with that reported by a mass spectrometric study.

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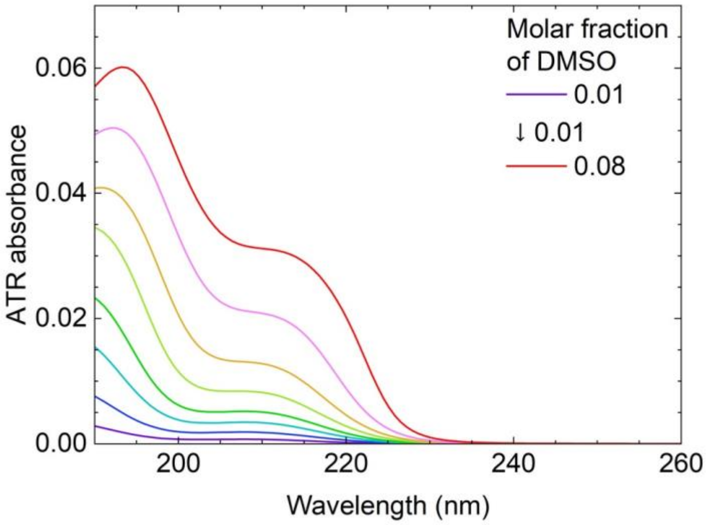
[2] Z. Lu et al., *J. Phys. Chem. A* **113,** 12207 (2009).



P30 - IR-drop effects in dip-and-pull electrochemical X-ray photoelectron spectroscopy

Liquids

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Abstract text: Operando studies of batteries promise valuable insights into the chemical reactions and physical processes that occur during charging and discharging cycles. X-ray photoelectron spectroscopy (XPS) was developed to identify the chemical composition of a sample, making it useful for tracking electrochemical reactions, such as the intercalation of lithium ions into electrode materials and various side reactions. However, XPS can probe only the top few nanometers of a sample, whereas electrochemical reactions predominantly occur at the solid-liquid interfaces within the sample. To access the information at the interface, the dip-and-pull method is often used, where a very thin film of liquid is created on the sample surface. Studies without any redox-active species show that the film can be electrochemically connected to the bulk electrolyte, but limitations arise when a faradaic reaction is investigated. The small volume of liquid composing the thin film makes ion transport significantly slower than in the bulk electrolyte, resulting in a large IR drop in the system. This study shows that the faradaic reaction occurs only to a very limited extent in the thin liquid film and exhibits behavior different from that of the bulk reaction. Therefore, care should be taken when interpreting operando spectroscopy results from dip-and-pull experiments.

P31 - Structure of hydration water revealed by soft X-ray absorption spectra of aqueous DMSO solutions

Liquids

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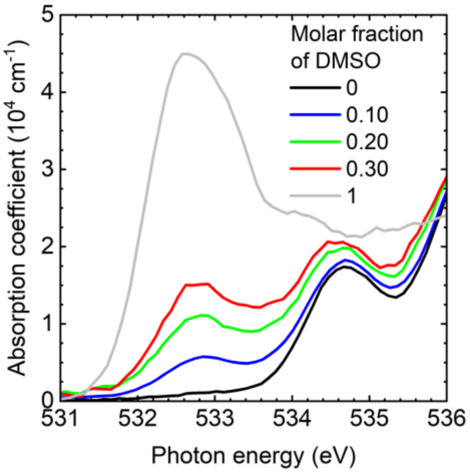
Abstract text: Soft X-ray absorption spectroscopy is a sensitive technique that possibly distinguishes hydration water from bulk water. This study focuses on hydration structure of a typical aprotic–protic system, aqueous dimethyl sulfoxide (DMSO) solution by the measurement of the O 1s absorption spectra. The solution is a suitable system for study due to its non-ideal features: for example, having a large negative value of the excess enthalpy [1].

The experiments have been carried out on BL3U, UVSOR, Japan. The measured spectra are shown in Figure 1. The intensity of both water and DMSO absorption bands increases with the concentration, and also the peak positions of the bands shift. Overlapping the bands makes it difficult to obtain information on hydration without appropriate analysis methods. Here we propose new two quantities to deduce the hydration components of the bands. The first quantity, the excess absorption coefficient μ^{E}, extracts hydration components as a deviation from the ideal mixture. The second quantity, μ^{S}, shows the concentration dependence of the hydration complex. The plot of against the molar concentration shows sudden changes at two concentrations, corresponding to the change of hydration structures. This result is consistent with that by a mass spectrometric study [2].

[1] T. Kimura and S. Takagi, *Netsu Sokutei* **13**, 2 (1986). [2] D. N. Shin *et al.*, *J. Phys. Chem. B* **105**, 6759 (2001).



RIXS

P32 - Combining ARPES and RIXS in a Novel Photoelectron Microscope

RIXS

Chafic Fawaz[1], Olena Tkach[2], Yaryna Lytvynenko[2], Tom Lacmann[3], Sergii Chernov[4], Olena Fedchenko[2, 5], Harshit Agarwal[2], Moritz Hoesch[4], J. K. Dey[4], Jakob Dilling[4, 6], Lukas Bruckmeier[4, 6], Markus Scholz[4], Jan Schunck[4, 7], Siegmar Roth[1], Kai Rossnagel[4, 7], Martin Beye[8], Mathieu Le Tacon[1], Hans-Joachim Elmers[2], **Gerd Schönhense**[2]
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[2] Institute of Physics, Johannes Gutenberg University, Mainz, Germany
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Abstract text: ARPES and Resonant Inelastic X-ray Spectroscopy (RIXS) usually employ hemispherical electron spectrometers and high-resolution X-ray spectrometers with long optical paths, respectively. We combined photoelectron momentum microscopy, a powerful ARPES approach [1], with the concept of PAXRIXS [2,3] in a special time-of-flight photoelectron microscope. The RIXS photon spectrum is ‘translated’ into a photoelectron spectrum using an ultrathin converter foil. In this configuration, the microscope operates in XPEEM mode, capturing a real-space image of the converter foil. The momentum transfer is determined by the position at which a RIXS photon hits the converter. The first *ToF-PAXRIXS instrument* is installed at beamline P04 of PETRA III. Its key feature is an easy switch between the two operating modes by changing just the lens settings and moving the converter in or out of the optical axis. Ideally this should be possible without moving the sample, to keep the probing spot fixed. In ARPES mode (converter moved out), the distance between sample and extractor electrode can be large (typically 8-12 mm). In RIXS mode (converter moved in), the XPEEM field-of-view is very large (≥4 mm). This is facilitated by a novel type of front lens which enables various operating modes [4]. The figure shows results for $YBa_2Cu_3O_{7-x}$.

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[3] Schunck et al., *New J.Phys*.**26**(2024)053008
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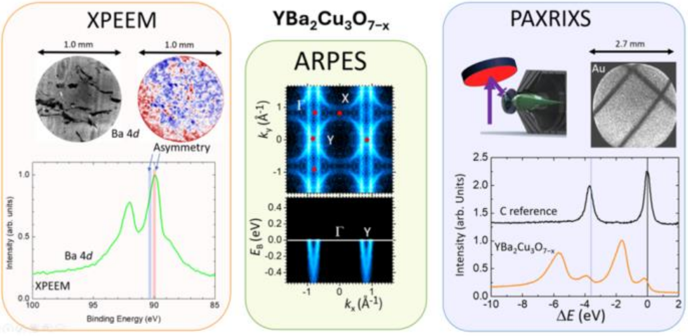

Fig.1. In this example XPEEM reveals different surface terminations, ARPES shows the valence bands in k_x-k_y and E_B-k_x sections, and PAXRIXS shows the energy-loss spectrum. Top right: Scheme of PAXRIXS and PEEM image of the converter with auxiliary wires for adjustment.

P33 - Multimode effects in resonant inelastic X-ray scattering from ammonia

RIXS

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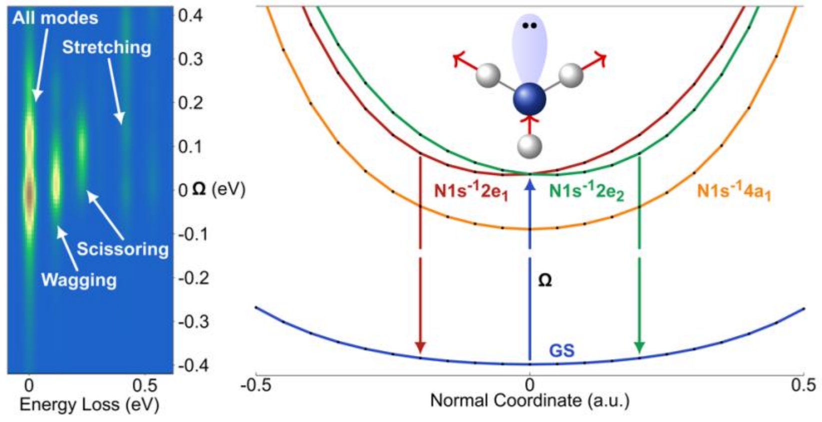
Abstract text: Resonant inelastic X-ray scattering (RIXS) provides an element-specific probe of local electronic structure in gas-phase and condensed-phase, but is also sensitive to ultrafast nuclear motion yielding low-energy excitations. Here, we investigate vibrational dynamics in gas-phase ammonia following excitation of the nitrogen 1s core electron into the unoccupied $4a_1$ and 2e orbitals. Vibrationally resolved RIXS measurements at the *Veritas* beamline at *MAX IV* (Lund) are interpreted on the basis of the Kramers-Heisenberg dispersion formula with quantum dynamics simulations based on ab initio potential energy surfaces (PES) of the electronic ground state and the lowest A_1 and E core-excited states.

The N1s → $4a_1$ excitation induced ultrafast N-H elongation and dissociation. Core-excitation into the 2e orbitals lifts the degeneracy through vibrational excitations of asymmetric N-H stretching modes. PES along the vibrational normal modes are calculated at the level of algebraic diagrammatic construction (ADC(2)-x) and restricted active space second-order perturbation theory (RASPT2). The accompanying figure highlights how our RIXS simulations reproduce the spectroscopic features and clarify how mode-specific nuclear motion controls the detuning dependence of the RIXS signal. By connecting vibrationally resolved RIXS features to the potential energy landscapes, this work establishes a gas-phase reference for understanding hydrogen bonding interactions in aqueous ammonia.



Multimode nuclear dynamics in electronically elastic RIXS of gas-phase ammonia.
Left: Simulated RASPT2 RIXS map depicting the energy-loss window of ammonia's normal modes.
Right: Ground- and core-excited potential energy curves along the **e**-type asymmetric N-H stretch.

P34 - Network-Structural Analysis in the crystallization process of zeolite by Resonant X-ray Emission Spectroscopy

RIXS

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Abstract text: Zeolite crystallization involves the development of three-dimensional silicate networks from initially disordered precursors, but the local ordering process remains difficult to access experimentally. Here, we investigate the crystallization of an MWW-type zeolite using O 1s X-ray emission spectroscopy (XES), supported by ab initio spectral simulations. The O 1s XES line shape is sensitive to local Si–O–Si network geometry, allowing changes in bond distances, bond angles, and O–Si–O–Si torsion angles to be followed during hydrothermal treatment. The results indicate that torsional ordering toward staggered conformations develops at an early stage, before clear long-range crystallinity is observed by conventional structural probes. These findings suggest that local topological ordering of the silicate network can precede framework crystallization. This study highlights O 1s XES as a useful probe of local network geometry in zeolitic and related oxide materials.

P35 - Plan for Developing the Sample Environment for NanoTerasu BL02U

RIXS

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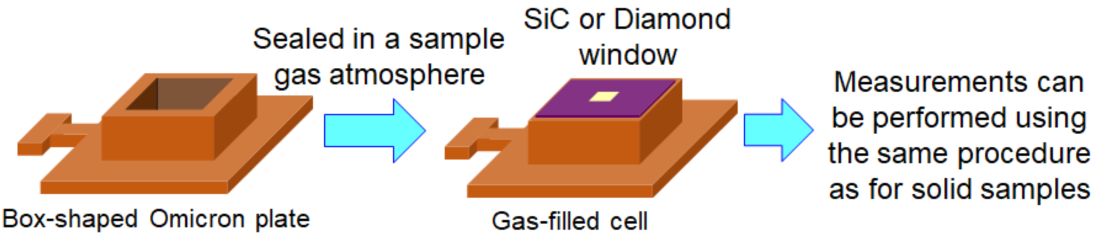
Abstract text: At NanoTerasu BL02U, which has achieved the world’s highest energy resolution in resonant inelastic soft X-ray scattering (RIXS), active research is underway to evaluate material properties based on spin and magnon excitations in strongly correlated systems. On the other hand, very few studies have been published on ultra-high-resolution experiments on gas-phase samples using soft X-ray RIXS and soft X-ray emission spectroscopy (XES). This is believed to be due to the fact that soft X-ray spectroscopy requires ultra-high vacuum, and that the usefulness of soft X-ray RIXS/XES in the field of atoms and molecules is not yet fully understood. We have recently developed a high-density gas-phase sample introduction method that enables soft X-ray RIXS/XES measurements while maintaining the vacuum level inside the measurement chamber. Preliminary experiments at SPring-8 have yielded interesting results for oxygen and noble gases.
Therefore, we plan to utilize this technique at NanoTerasu BL02U to conduct ultra-high-resolution RIXS/XES experiments on gaseous samples, isolated samples, and functional materials.



P36 - Proton-Coupled Electron Transfer (PCET) at ZnO-Water Interface

RIXS

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Abstract text: The process of proton-coupled electron transfer (PCET) refers to the coupled transfer of electrons and protons during chemical and biochemical reactions. [1] Often occurring via ultrafast multi-step pathways, PCET plays a central role in energy-related processes such as the oxygen and hydrogen evolution reactions (OER/HER) at semiconductor–water interfaces. [2] Zinc oxide (ZnO), a wide-bandgap semiconductor, is widely studied due to its excellent optical properties and tunability via transition metal doping, making it a promising material for photocatalytic and photovoltaic applications and a model system for PCET investigations. [3,4] The ZnO–water interface is crucial in applications such as biosensing and catalysis. Theoretical studies indicate that water molecules interacting with ZnO surfaces can undergo dissociation and recombination via proton transfer involving surface-H_2O and OH^- species. [5,6] Resonant inelastic x-ray scattering (RIXS) spectroscopy is an element-specific technique that probes electronic and vibronic excitations, sensitive to local structure, hydrogen bonding, and charge transfer. [7] We present a high-resolution RIXS study at the oxygen K-edge of ZnO aqueous colloids with sizes of 8 nm and 25 nm. XAS measurements reveal distinctive absorption features, particularly below the water pre-edge. RIXS spectra collected in this region are highly sensitive to the electronic structure of ZnO colloids, while XES spectra above 550 eV show only minor variations in the liquid water lone-pair $1b_1$ orbital. These results are discussed in the context of PCET mechanisms.

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Acknowledgment: Funding by the Deutsche Forschungsgemeinschaft (DFG) via the CRC 1633 “Pushing Electrons with Protons” (project #510228793), projects C04 and C05 is gratefully acknowledged.

P37 - RIXS study on Prussian White Cathodes: understanding the role of spin state in elevating battery capacity

RIXS

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Abstract text: Prussian white, $Na_2Fe[Fe(CN)_6]$, is a promising cathode material for sodium-ion batteries owing to its low-cost Fe-based composition, high sodium content, open framework for rapid Na^+ transport, reversible Fe redox chemistry, long cycle life, and good rate capability.[1] In this work, the evolution of the electronic structure during reversible Na-ion insertion/extraction was investigated, with particular focus on the two crystallographically and electronically distinct Fe redox centers arising from the different coordination environments of the cyanide ligand. To clarify the role of these Fe sites during electrochemical cycling, valence-excited states of $Na_2Fe[Fe(CN)_6]$ at different states of charge were probed using X-ray absorption spectroscopy and resonant inelastic X-ray scattering at the Fe $L_{2,3}$ and N K edges. Simultaneous interrogation of the central Fe sites and ligand N atoms enabled identification of metal-centered, ligand-centered, ligand-to-metal charge-transfer, and metal-to-ligand charge-transfer excited states. The combined Fe L_3-edge and N K-edge analysis corroborated reversible Fe^{3+}/Fe^{2+} redox behavior and distinguished the sequential participation of the two Fe sites with different spin states during Na-ion extraction/insertion.[2] Detailed RIXS mapping further showed that both metal-to-ligand and ligand-to-metal charge-transfer processes evolve systematically with state of charge. The resulting Fe–CN charge delocalization is proposed to contribute to the high reversibility of Na-ion storage in Prussian white. This study highlights the effectiveness of combined spectroscopy in elucidating the charge-storage mechanism of Prussian white, providing insights for designing improved and commercially viable sodium-ion cathodes.

Reference (1) L. Wang et.al J. Am. Chem. Soc., 2015, 137, 2548–2554.

Theory

P38 - Exploring Protein Structures Using X-ray Laser-Driven Explosions

Theory

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Abstract text: Studying the conformational states of isolated molecules has been one of the driving scientific goals in structural biology, motivating the development of ultra-short X-ray free-electron laser (XFEL) pulses.
Single-particle experiments at XFELs rely on diffraction to retrieve the electron density. However, the spatial positions of ions following molecular fragmentation - caused by the Coulomb explosion - have been shown to be reproducible, capturing structural fingerprints of proteins. Here, we demonstrate that the ellipsoidal envelope of a protein can be determined in three dimensions by resolving the principal axes of the explosion map, with an error of only few Ångströms. These results show that structural information can be extracted directly from ion data obtained during laser-induced explosions.

P39 - Role of local structural variation in X-ray photoelectron spectrum of oxide interfaces

Theory

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Abstract text: In this poster contribution, we will present our ongoing computational and experimental work on X-ray photoelectron spectra of oxided surfaces.

XFEL

P40 - Orientation Reconstruction of Proteins using Coulomb Explosions

XFEL
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Abstract text: We solve the orientation recovery of a tumbling protein in the gas phase from single-event measurements of the spatial positions of its ions after an X-ray laser induced explosion. We simulate diffracted X-ray signal and ion dynamics under experimental conditions and compare our method to conventional orientation recovery in single-particle imaging with X-ray free-electron lasers using only diffraction data. We reconstruct 3D diffraction intensities using orientations recovered from the ion signatures and retrieve the electron density with established phase-retrieval algorithms. We test our orientation recovery procedure on 56 proteins ranging from 14 to 52 kDa (1800 to 6500 atoms), achieving roughly an angular error of around 5°. The resulting 3D electron-density reconstructions are compared to ground-truth volumes simulated at the same nominal resolution, and achieve the resolution at the edge of the detector in conditions similar to current single-particle imaging setups. We investigate the reconstruction quality and demonstrate that ion data can be used for reliable orientation recovery of particles in single-particle imaging, achieving orientation on par or better than currently used recovery techniques. This work shows the potential of ion detection for retrieving additional information from the sample fragmentation, and boost single particle imaging with X-ray lasers in the cases where the diffraction signal is a limiting factor.

P41 - Synchronized Droplet Delivery for XFEL Experiments

XFEL

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Abstract text: We investigate the synchronization of microscopic water droplets with X-ray free-electron laser (XFEL) pulses by correlating optical image analysis with diffraction data. We show that imperfections in the spatial and temporal overlap between the droplet train and incoming XFEL pulses lead to variations in the recorded diffraction intensity, highlighting the importance of stable synchronization for reducing shot-to-shot variability during data collection.

The performance of the droplet delivery system was evaluated from optical images by quantifying droplet velocity, droplet spacing, droplet diameter, and the stability of droplet formation. In addition, we combine classical image analysis, dimensionality reduction, and Monte Carlo modelling to interpret variations in the optical and diffraction signals. This analysis links changes in X-ray/droplet overlap to both the measured diffraction intensity and the observed droplet explosion dynamics after XFEL interaction.

Our results demonstrate that optical imaging provides a practical diagnostic for identifying synchronization errors and sample-delivery instabilities in droplet-based XFEL experiments. During nominal operation, the droplet train was synchronized with the first peak of the XFEL pulse train with a hit rate of approximately 97%. Nominal operation, characterized by uniformly spaced droplets with low size variability, was observed in approximately 85% of the recorded shots.

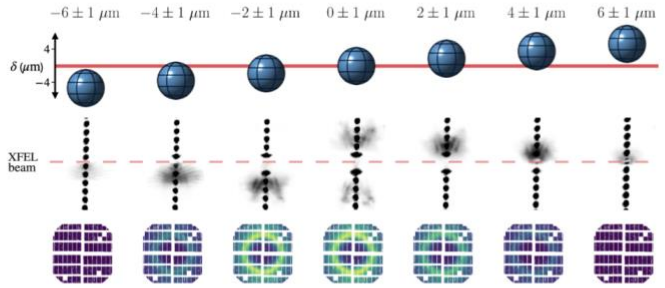

Figure 4.19. Correlation between X-ray/droplet overlap, optical response, and diffraction intensity. Residual delivery jitter produces shot-to-shot variations in the transverse offset δ between the droplet center and the XFEL beam. **Upper:** Schematic of the droplet position for different offset ranges, where $\delta = 0$ corresponds to central X-ray/droplet overlap. **Middle:** Average segmented optical images of the interaction region. The dashed red line marks the XFEL beam position, black regions indicate the droplet train, and diffuse grey regions show the pressure-wave response after X-ray exposure. **Lower:** Mean diffraction intensity for the same offset ranges. Central overlap gives the strongest diffraction signal, showing that synchronization jitter directly contributes to variations in recorded intensity.

Other

P42 - Reinvestigation of the temperature dependent electronic structure of Sn/Ge(111)- √3×√3 surface

Other

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Abstract text: Surface reconstruction of Sn on Ge(111) has attracted sustained interest due to unusual temperature dependent phase transitions. 1/3 monolayer coverage of Sn atoms on Ge(111) result in a √3×√3 reconstruction at room temperature which transforms into a 3×3 phase below ~210 K. Interestingly, a new √3×√3 phase transition was reported below 30 K. The results of low energy electron diffraction (LEED), scanning tunnelling microscopy (STM) and photoemission studies suggested this second transition as a Mott insulator phase. However, this Mott transition has been rejected by other STM and scanning tunnelling spectroscopy (STS) studies. In this work, the electronic structure of Sn/Ge(111) surface was reinvestigated to evaluate the significant features of the low temperature second phase transition. The photoemission studies were performed at Bloch beamline at the MAX IV synchrotron facility, Lund, Sweden. The electronic structure was studied by ARPES using a photon energy of 26 eV at 18 K. 'Kinks' are observed in two surface state band (S1 and S2). In particular, two distinct kinks are observed in the S2 band. The kink near Fermi is due to electron-phonon coupling and an unusually band splitting is observed at the second kink at higher binding energy. Energy distribution curve analysis reveals a relative intensity reduction of the S2 band at 18 K, which might be caused by a band splitting of S2. This observation casts doubt in the existing models explaining the insulating phase at low temperature and suggests the need for developing new theoretical models.

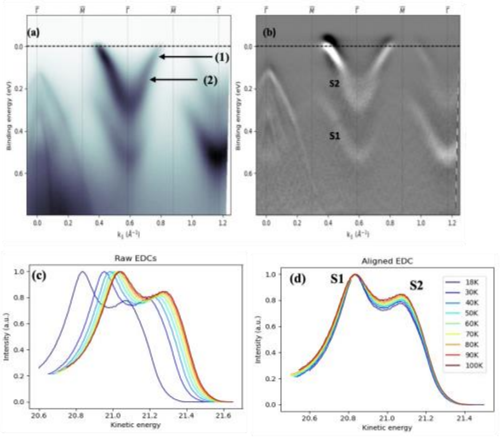

FIG. 1: (a) Raw ARPES data along the $\bar{\Gamma}$- $\bar{M}$ - $\bar{\Gamma}$ symmetry of 3×3 SBZ at 18 K, hν= 26 eV, (b) A second derivative image of fig.(a). Temperature dependent EDCs at hν=26 eV (c) Raw EDCs (d) EDCs aligned to the S1 peak position at 18 K.

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