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Monday 9th

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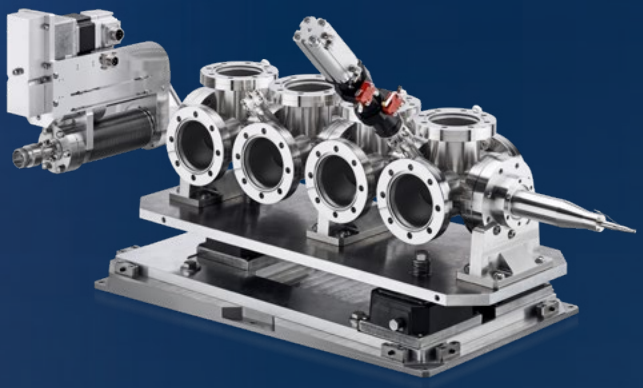

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Liquid-Jet Photoelectron Spectroscopy of Aqueous Solutions: Recent Breakthroughs and Current Challenges

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ABSTRACT

Liquid-jet photoemission spectroscopy (LJ-PES) has a long track record as a direct probe of both the electronic- and molecular/solute structure as well as interfacial characteristics of aqueous solutions. Energies of both directly emitted photoelectrons and electrons generated through second-order processes can be accurately determined with respect to the vacuum level as well as the Fermi level. The latter capability enables detailed characterization of explicit solution surface properties, including structure and charge distributions, thereby establishing a direct link between surface science and electrochemical descriptors. In addition, non-local ionization/relaxation processes and ultrafast electron delocalization upon core-hole excitation provide access to rich bulk-solution dynamical information. This includes proton, electron, and charge transfer, and enables explicit insight into the first-solvation shell energetics and composition. LJ-PES has been applied to a broad range of systems, spanning from simple atomic solutes to complex biomolecules in aqueous environments, such as adenosine triphosphate in interaction with metal cations.

Despite these breakthroughs, several key aspects of solutions, such as chiral solute-solvent interaction or low-yield reaction intermediates and products, remain experimentally challenging to access via LJ-PES. Many of these challenges arise from strong electron scattering in solution at low kinetic energies and from the still insufficiently understood electron scattering lengths in liquids. I illustrate these limitations with few examples: (1) the difficulty of accurately determining solute concentration profiles from the solution surface into the bulk on an absolute length scale, unless independent length calibration is available; and (2) the challenge of achieving an efficient electron detection, simultaneously covering a wide electron angular emission range aiming at extraction of the associated structure information, e.g., chirality in aqueous solution. I highlight the continued development of liquid-jet technologies to address these challenges.

A Flow-Focused Droplet Train for Investigating Solution Phase Processes with Ambient Pressure X-ray Photoelectron Spectroscopy

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We present a newly commissioned droplet train that enables micro- to millisecond time-resolved ambient-pressure X-ray photoelectron spectroscopy (AP-XPS) studies of solution-phase processes. The droplet train is based on gas flow focusing, which uses a pressure drop across an orifice to shape a liquid into a jet flowing through it. This approach provides enhanced positional stability and, because the liquid does not contact the orifice, improved resistance to clogging. The liquid jet is broken into uniformly sized and regularly spaced droplets by vibration using a piezoelectric element, producing droplet repetition rates of several thousand droplets per second.

Micro- to millisecond time resolution is achieved by varying the height of the droplet generation point above the analysis position (defined by the intersection of the X-ray beam and the analyzer axis) and by introducing an appropriate time-zero trigger. When combined with tender X-ray AP-XPS, which generates high kinetic energy photoelectrons, routine measurements of liquids at pressures up to 25 mbar (i.e., above the vapor pressure of water at room temperature) can be performed with reasonable data acquisition times. The higher kinetic energy of the photoelectrons also increases bulk sensitivity compared to conventional soft X-ray AP-XPS measurements.

This capability opens new possibilities for time-resolved XPS studies of reactions and processes in bulk liquids. The droplet train is one of the experimental modules available at the Spectroscopic Analysis with Tender X-rays (SpAnTeX) end-station of the Berlin Joint Lab for Electrochemical Interfaces (BElChem) at the BESSY II synchrotron in Berlin, Germany. After introducing the technical aspects of the droplet train, we will present example measurements, including studies of nanoparticles in solution and aqueous CO_2 capture solutions, and conclude with an outlook on future developments of the instrument.

Probing Supramolecular Structures in Solution by Resonant Energy Transfer in the X-Ray Range

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ABSTRACT

Resonant energy transfer between donor and acceptor atoms in the X-ray range can span several nanometres, and lies at the heart of far-zone resonant energy transfer (FZRET) spectroscopy.[1] Sensitive to the donor–acceptor distance, this advanced spectroscopic technique enables structural studies with atomic spatial resolution. For its first application to a liquid microjet,[2] a concentrated aqueous solution of potassium acetate was selected. The investigation of multiple donor–acceptor pairs allowed the characterisation of cation–anion, cation–water, and cation–cation distance distributions, thereby probing the supramolecular organisation of the solution. These experiments revealed an inhomogeneous ion distribution in water, consistent with the presence of nanometre-sized ionic aggregates in solution.

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Ultrafast Relaxation in Isolated and Aqueous Nucleobases: Substituent and Solvent Effects

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ABSTRACT

Nucleobases display remarkable photostability due to ultrafast internal conversion (IC) from the optically bright 1ππ∗ excited state to the electronic ground state (S0), enabling rapid dissipation of excess electronic energy and limiting photochemical damage.[1] In pyrimidine nucleobases, an additional relaxation pathway involves an optically dark 1nπ∗ state with a longer lifetime, which can mediate intersystem crossing to the triplet 3ππ∗ state.[1-5] The quantum yield of the 1nπ∗ state is therefore a key parameter for understanding nucleobase photolesion mechanisms.

Here, we performed ultrafast extreme ultraviolet time-resolved photoelectron spectroscopy (EUV-TRPES) measurements of 6-methyluracil (6mUra) and 5-fluorouracil (5FUra) in the gas phase, as well as 6mUra and 5-fluorouridine (5FUrd) in aqueous solution to investigate the substituent and solvent effects on the ultrafast relaxation dynamics. In the gas phase, IC from the 1ππ∗ to the 1nπ∗ state occurs within tens of femtoseconds, followed by ISC to the 3ππ∗ state on a picosecond timescale. In contrast, in aqueous solution 6mUra relaxes almost exclusively to S0 within ~100 fs, closely resembling the dynamics of unsubstituted uracil and proceeding significantly faster than in thymine (5-methyluracil).[6] The distinct relaxation dynamic for C5 and C6-substituted molecules indicates that IC from the 1ππ∗ state to S0 is facilitated by out-of-plane motion of the C5 substituent.[7]

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Real-Time Tracking of the intramolecular vibrational dynamics of liquid water

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ABSTRACT

Water's polarity and hydrogen-bond network give rise to its unique chemical and biochemical behaviour. Its vibrational motions, occurring on a few-femtosecond timescale, govern ultrafast energy transfer within the hydrogen-bond network. However, direct real-time observation of these motions has remained elusive due to the extreme temporal resolution required.

In this contribution, we present the ground-state vibrational dynamics of liquid water initiated by a sub-5 fs near-infrared (NIR) pump pulse via Impulsive Stimulated Raman Scattering (ISRS). Using few-fs ultraviolet (UV) probe pulses transmitted through a 5 µm-thick liquid jet, we monitor the coherent vibrational wave packet dominated by the OH stretch mode, exhibiting a 10 fs oscillation period and a 25 fs damping time. These results reveal the rapid dephasing of the OH stretch mode preceding its relaxation through coupling to the bending vibrations, highlighting the importance of intermolecular couplings of liquid water in the high frequency vibrational dynamics.

Femtosecond Fieldoscopy

Hanieh Fattahi, MPI for the Science of Light

Femtosecond Fieldoscopy provides direct access to the electric field of light in ambient air, offering near-petahertz detection bandwidth together with exceptional sensitivity and a broad dynamic range. When applied to spectro-microscopy, the technique achieves attosecond temporal resolution and spatial resolution beyond the diffraction limit.

In this approach, ultrashort excitation pulses impulsively drive resonant molecular modes in a sample, initiating vibrational coherences that decay on a timescale determined by molecular dephasing. As a result, the transmitted electric field contains contributions from the excitation pulse itself, the sample's delayed molecular response lasting several picoseconds, and a long-lived response from atmospheric gases that persists for up to hundreds of nanoseconds. By isolating and analyzing the decaying molecular field in the time domain, Femtosecond Fieldoscopy enables highly sensitive spectroscopic measurements with an exceptional dynamic range. The method has successfully resolved overtone, Raman, and combination bands in liquid samples, and recent developments have enabled super-resolution imaging well below the diffraction limit of the excitation pulses, paving the way toward non-perturbative, label-free imaging. In this talk, I will present an overview of these advances demonstrated by my group.

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Hydrophobic solvation at electrochemical interfaces

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Hydrophobicity locally arises in exotic ways at electrified metal-water interfaces. There, the ordering templated by strongly interacting metal surfaces on the physisorbed water adlayer induces formation of a soft water-water interface that shows "air-water-like" behaviors.[1,2]
In this presentation, I will discuss their molecular origin, and the similarities and differences to canonical hydrophobic interfaces.

Such a local hydrophobicity gives rise to interesting structural and solvation properties, which are strongly space-dependent: even a small variation of a few angstroms on the distance of the reactive species to the surface can dramatically change their solvation envoronment and chemistry, and subtle positional effects, such as the shape of the cavity formed by a solute and its orientation with respect to the surface or another reactant, which are usually negligible, can determine the energetics of chemical processes at these interface.

These emerging factors have been recently proposed to regulate a growing number of electrochemical processes at metal electrodes, as well as at some oxide-water interfaces. I will briefly show a few examples, including renewable energies,[3] acid-base chemistry,[4] electric double layer formation,[5] and heterogeneous catalysis.[6]

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Practical User Guide of Liquid Sample Delivery Systems for User Facilities and Table-top X-ray Spectroscopy Applications

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ABSTRACT

Liquid sample environments are essential for preserving native structure and function in biological systems. However, their use in X-ray spectroscopy includes specific challenges, such as radiation damage, sample oxidation, and limited available sample volumes. In the contribution we will report a systematic experimental test of several liquid sample delivery systems (LSDS) based on X-ray spectroscopy experiments performed under laboratory and synchrotron conditions. The tested approaches include geometries originally developed for in-vacuum operation, such as colliding liquid jet systems [1]. While the measurements presented here were conducted under ambient conditions, the results provide a comparative assessment for the practical selection and optimization of LSDS across different experimental modes.

In our study, a stirrer-cell-based LSDS was identified as particularly suitable for biological applications. The design enables continuous sample refreshment during X-ray exposure while operating with liquid volumes as low as 60 µL. Based on the original concept [2], the system has been further developed to allow online control of key parameters, such as temperature and pH, during high energy spectroscopic measurements.

The contribution will present current results obtained within an ongoing international collaboration as well as introduce the capabilities of a highly automated X-ray spectroscopy end station at the ELI Beamlines Facility. By sharing technical solutions, performance benchmarks, and transferable experimental strategies, this contribution aims to engage with the community working with liquid samples across synchrotron, laser-based, XFEL, and table-top instruments.

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Liquid sample delivery at EuXFEL

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ABSTRACT

One of the most distinctive characteristics of the European XFEL is the high repetition rate of the X-ray pulses. The intra-train repetition rate of up to 4.5 MHz represents a significant challenge for the sample injection systems[1]. The Sample Environment & Characterisation (SEC) group of the EuXFEL is developing sample delivery systems for all scientific instruments, in addition to providing user support in sample preparation, characterization, and delivery.
A notable sample delivery method employed by the group is the injection of liquid samples, particularly through the utilization of nozzles that have been fabricated with sub-micrometer precision using 3D printers[2]. Additionally, the group employs a variety of Drop-on-Demand (DoD) systems[3].

Cylindrical microjet injection systems remain the most prevalent type of sample injection system employed in the fields of soft and hard X-ray science. Nevertheless, this methodology is subject to several intrinsic constraints. For example, the curved surface of the nozzle presents a challenge in determining the path length of the X-rays within the sample. The sample must have a well-defined and controllable thickness of just a few tens of microns or less, and the efficiency of sample usage requires the use of micron-sized liquid sheet jets. In light of these limitations, various 3D-printed nozzle designs have been developed to produce micron-thick and highly stable microscopic flat sheet jets. These designs are based on colliding and impingement[4] nozzle designs, to make this technology more widely available to users, especially for spectroscopy.

Furthermore, this talk will summarise the high-throughput 3D-printed liquid sample environments, including GDVNs, mixed GDVNs and DFFNs, which have highly reproducible geometric properties suitable for time-resolved serial femtosecond crystallography (SFX)[5] and single particle imaging (SPI)[6] experiments at the XFEL.
In addition, an overview is given of the liquid injection setups and injection platforms available at the facility, which can be used by user groups for testing and training purposes.

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Characterization of non-aqueous solvents using liquid jet photo-electron spectroscopy

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ABSTRACT

Since the early 2000 years liquid-jet (LJ) photo-electron spectroscopy (PES) has become a standard method to investigate the electronic structure of solvents and solutes in liquid condensed matter systems. Naturally, liquid water has been the solvent to study (first) due to its importance for humans in general and because of the many applications in particular in physics, chemistry, biology and other sciences. Moreover, these studies have also triggered advances on the experimental side to further miniaturize and to standardize micro-fluidic delivery systems as well as on the theoretical side to develop detailed concepts and computational protocols to model solution phase phenomena.

In this talk, an extension is given how LJ-PES can be used to investigate non-aqueous solvents. The aim is to broaden the perspective onto non-polar (organic) solvents which are abundantly used in synthesis or petrol chemistry. Naturally, for example toluene or octane dissolve many non-polar solutes which are otherwise difficult to dissolve in water.

Furthermore, as a second solvent class, liquid metal alloys will be presented and their electronic structure characterization using LJ-PES methods. In particular, Gallium based liquid metal alloys are used in different applications such as thermometers replacing Mercury, stretchable electronics and robotics, or as a drug delivery agent in medicine. Here, a fundamental study of Gallium as a solvent for tin or indium is given with a perspective to their potential catalytic applications.

Ultrafast Dynamics in Acetone Probed by Time-Resolved Photoelectron Spectroscopy Using Few-Femtosecond Pulses

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Few-femtosecond ultraviolet (UV) light pulses are required for the real-time monitoring of electron dynamics in electronically excited neutral molecules[1]. UV light plays a crucial role in driving a wide range of photochemical and photobiological processes. With the development of our extremely short UV pulses, we are now able to capture these ultrafast dynamics with unprecedented precision. In this study, we present a time-resolved photoelectron spectroscopy (TRPES) investigation of acetone, utilising UV pump pulses with a transform-limited duration of 2.1 fs and near-infrared (NIR) probe pulses. This combination achieves an overall time resolution of 5.6 fs. Acetone, the simplest ketone and a commonly used solvent, exhibits complex Rydberg–valence interactions that strongly influence its excited-state dynamics. Although previous time-resolved experiments have been conducted, they were limited by their temporal resolution, which hindered the study of ultrafast dynamics occurring on the few–tens-of-femtoseconds timescale[2,3]. Our results reveal pronounced electronic and vibrational coherences, as well as clear signatures of ultrafast relaxation to the $\pi\pi^*$ state. A slow 24 ± 1 fs oscillation is observed for approximately 100 fs in the photoelectron spectrum, and an additional fast beating at 3.2 ± 0.2 fs, corresponding to an energy of 1.3 eV, is also detected. The latter may indicate the presence of an electronic coherence. These findings provide new insight into the ultrafast dynamics of acetone.

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Tuesday 10th

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Electronic structure and photochemical dynamics of photoactive protein chromophores in aqueous solution

Helen H. Fielding

Department of Chemistry, University College London, UK

Knowledge of the electronic structure of an aqueous solution is a prerequisite to understanding its chemical and biological reactivity and its response to light. One of the most powerful experimental techniques for studying the electronic structure of molecules in aqueous solution is liquid-microjet photoelectron spectroscopy (LJ-PES) as it provides a direct measure of electron binding energies (eBEs). X-ray LJ-PES is an excellent method for the determination of accurate eBEs of solute molecules in their ground electronic states, although high solute concentrations ($\gtrsim$ 10 mM) are required to ensure a sufficient signal-to-noise ratio of the photoelectron spectrum of interest since the photoelectron spectrum of water (55.5 M) dominates. Ultraviolet (UV) LJ-PES has the advantage that multiphoton ionisation/detachment can be employed for µM concentrations of sparingly soluble organic chromophores with UV photons that do not have enough energy to ionise water, and resonance-enhanced multiphoton PES also provides information about electronically excited states.[1,2] A challenge with UV LJ-PES has been that inelastic electron scattering of low electron kinetic energy electrons distorts the spectra. Our group has developed LJScatter[3] for retrieving true photoelectron spectra from distorted spectra. Here, we present the idea behind LJScatter, and new studies of the electronic structure and photochemical dynamics of the photoactive yellow protein chromophore in aqueous solution.

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Investigations of heterogeneous processes at liquid-vapor interfaces

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ABSTRACT

Heterogeneous reactions at liquid-vapor interfaces play a major role in the environment and atmosphere. The investigation of chemical reactions and transport processes, in particular at aqueous solution-vapor interfaces, at realistic partial pressures, temperatures and time scales, is thus of great importance for a better understanding and theoretical modeling of some of the most important processes in the environment and atmosphere. This talk discusses the challenges and obstacles for measuring heterogeneous chemical reactions at liquid-vapor interfaces using X-ray photoelectron spectroscopy and suggests experimental strategies to overcome these challenges.

Quantifying Electronic Energetics And Surface Properties Of Aqueous Solutions

Stephan Thürmer

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ABSTRACT

Liquid-jet photoelectron spectroscopy (LJ-PES) gives direct access to the electronic structure of aqueous solutions, information on bonding interactions, solute charge states and charge transfers via measurement of binding energies (BEs) of both solvent and solute. Yet, obtaining accurate BEs has been notoriously difficult due to the presence of undesired extrinsic liquid-jet potentials, such as the streaming potential, Φ_{str},[1] which lead to arbitrary energy shifts in PES. Interfacial properties are, in principle, inferable from work-function, WF, measurements. However, WF values from solution can only be obtained indirectly via energetic reference to a metal; such referencing is also compromised by arbitrary energy shifts of the liquid spectra.

We developed robust vacuum referencing as well as equilibrated Fermi-level referencing methods for BEs, which enable us to discern changes as a function of concentration in the solvents electronic structure as well as in WF, due to surface-dipole effects.[2-4] A breakthrough for applicability of Fermi-referencing to arbitrary solutions is the quantification of all potentials in a LJ-PES experiment, most prominently Φ_{str}. We succeeded in quantifying Φ_{str} as a function of solute type and concentration, which enabled us to determine BE and WF values from model electrolyte solutions over a wide range of concentrations for the first time.[5]

These techniques mark a major advance in our ability to quantify electronic-structure interactions and chemical reactivity, which now extends to the measurement of absolute-scale bulk and interfacial solution energetics, including those of relevance to aqueous electro-chemical processes. Furthermore, quantification of the streaming potential promises to reveal insights about the solution-nozzle interfacial structure. I will discuss details of this technique, present results of exemplary solutions, and give an outlook on future developments.

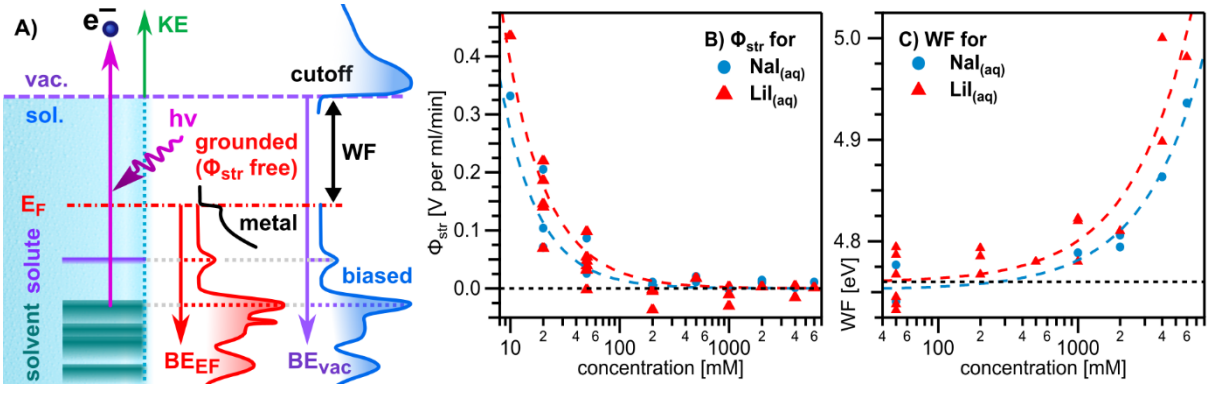

Figure: A) Overview of relevant energetics. B) Φ_{str} and C) WF values from solution.

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From Gas-phase to Liquid Phase: Probing the Electronic Structure of Amino Acids with X-ray Spectroscopy.

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ABSTRACT

The isolation of biomolecules in the gas phase eliminates all interactions with the solvent, allowing for stepwise control of these interactions by progressively increasing the number of bound water molecules, thereby bridging the gap between isolated molecules and aqueous conditions. A single water molecule can already induce significant structural changes in the molecule, such as the location of the protonation site or geometry[1,2].

Over the past thirty years, efforts have been made to develop experimental techniques for studying hydrated species in the gas phase. Comparing the gas-phase structure with the singly hydrated gas-phase structure provides insight into the influence of molecular water on its properties. In contrast, performing a liquid-phase study allows us to gain insights into the influence of water as a solvent and approach the conditions relevant to biology. Moreover, the addition of a solvent allows charge redistribution between the molecule and the solvent, thereby altering the local charge distribution and 3D structure.

Soft X-ray radiation provides a local probe into the atomic environment based on the electronic excitations of core electrons to unoccupied molecular orbitals, thereby capturing both the electronic and geometric structures of the system under investigation. In this study, we first combined X-ray absorption spectroscopy with tandem mass spectrometry to obtain information about the electronic structure of singly hydrated, protonated phosphotyrosine. We further explore the influence of the solvent on phosphotyrosine and address ultrafast charge-transfer dynamics using Auger–Meitner spectroscopy (AMS) in aqueous solution in the soft X-ray range and extend it to the tender X-ray domain.

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Beating Complex Solution Chemistry With The Selectivity Of Soft X-Rays

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ABSTRACT

Liquid water at ambient conditions is ubiquitous in chemistry and biology as well as in technology, energy, and atmospheric processes. Since parts of the phase diagram of water are unsettled - most notably the supercooled liquid homogeneous nucleation region - repercussions thereof on our molecular-level under-standing for even the common ambient conditions remain. Breathtaking advances in X-ray–based approaches over the last decade give us now the tools to derive molecular potential energy surfaces as a quantitative view on the molecular manifold within the fluctuating hydrogen bonding network. With selective cuts along the local asymmetric OH bond coordinate and the symmetric normal mode excitations an experimental foundation to benchmark competing molecular-level models of water has been achieved (1).

This talk will show how x-ray spectroscopy can be instrumentalized to obtain information on water structure and the water potentials in the hydrogen bond network (2). Aqueous solutions reach an equilibrium that could either facilitate or hamper solvation, an effect that can be mitigated by the water molecules (3) and detected by x-ray spectroscopy. In a further step, the dynamics of ligand exchange in aqueous solution and the role water molecules play in it will be presented (4).

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Real-time theoretical description of coherent electronic dynamics probed by high-harmonic generation and chiral spectroscopies

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ABSTRACT

The interaction of molecules with ultrafast electromagnetic fields induces coherent electronic dynamics that can be probed through a variety of nonlinear and chiral spectroscopies. High-harmonic generation (HHG) and electronic circular dichroism (ECD), despite probing different observables, both originate from the time-dependent coherent response of the electronic wavefunction to an external field. In particular, these spectroscopies provide complementary access to electronic populations, coherences, and orbital contributions, through the time-dependent electric and magnetic dipole moments.

In this contribution, I will present a real-time theoretical framework based on the propagation of the electronic wavefunction under external electromagnetic fields. This approach enables the simulation of both high-harmonic generation (HHG) spectra and electronic circular dichroism (ECD) signals from first principles, providing direct insight into the role of electronic structure, coherence, and transition dipole dynamics.

For HHG, I will show how the emitted harmonic spectra encode detailed information on orbital-resolved contributions, electronic coherence, and symmetry properties of the molecular system. In particular, the analysis reveals the role of multiple ionization channels, interference between electronic states, and the influence of molecular symmetry and chirality on the harmonic emission. This provides a microscopic interpretation of strong-field electron dynamics and the origin of characteristic spectral features.

For ECD, I will demonstrate how chiral optical signals arise from the coherent electronic response and how they are modified by environment-induced interactions, such as coupling with plasmonic nanostructures. Applications to molecular systems and plasmon–molecule coupled systems show how electronic coherence and environment effects influence the chiral optical response.

These results highlight the potential of real-time theoretical approaches to interpret advanced nonlinear and chiral spectroscopies and provide a unified microscopic description of ultrafast electronic and chiral dynamics in molecular systems.

X-ray natural circular dichroism of chiral molecules in liquids

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Molecular chirality is central to biology and chemistry. Identification of enantiomers of chiral molecules is based on optical circular dichroism (CD), which was developed starting from the XIXth century on and it measures the absorption difference of left and right circularly polarised light by the sample. CD signals are intrinsically weak, usually 0.1% of the linear absorption, which makes them challenging to measure. Pushing CD spectroscopy into the X-ray domain promises several advantages: a) an enhanced signal (since the terms of light-matter Hamiltonian for CD are inversely proportional to the wavelength), b) element-selectivity, and c) an ability to identify identical but inequivalent atoms in a molecule, not only by their chemical shifts but also their different chiral response, which depends on their position with respect to the chiral centre. Although several theoretical studies have underlined the advantages of soft X-ray natural CD (XNCD), [1–5] its measurement on disordered media (powders) has remained a challenge, and the few studies performed on amino-acid residues and organic molecules do not show clear signatures of chirality, [6–8] probably due to radiation damage, linear dichroism and other effects.

With the advent of the liquid microjet technique, [9,10] it has become possible to inject liquid samples into vacuum and investigate their soft X-ray absorption both in steady-state and time-resolved studies. We have extended the use of the flat liquid microjets to perform XNCD studies of chiral molecules in solution.

We will present for the first-time evidence of XNCD spectra of such systems in the case of fenchone in ethanol. The measurements were carried out at the O K-edge of the molecule, which is not a chiral centre. The results show a good agreement with our theoretical results which are also presented, both in terms of spectral shape as order of magnitude of the intensity.

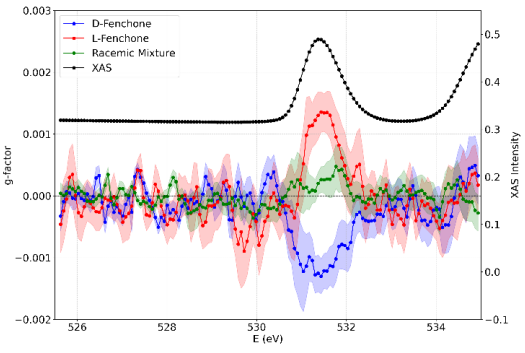

Figure 1: Fenchone O K-edge XNCD spectrum.

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Relativistic-intensity laser-plasma interaction at kHz repetition rate on a liquid sheet target

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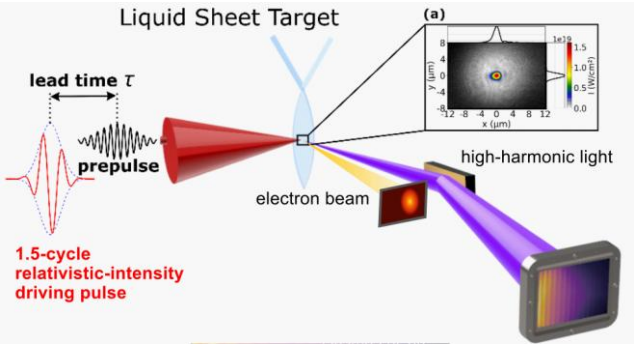
Plasma mirrors—reflective, overdense plasmas formed on condensed-phase targets—serve as versatile active optical devices for ultra-high intensity lasers and as model systems for studying (relativistic) plasma dynamics. Relativistic high-harmonic generation (RHHG) from plasma mirrors offers a promising route to generate intense attosecond pulses, efficiently converting laser light into XUV and soft X-ray pulses [1].

Traditionally, plasma mirrors have relied on bulk solid targets, which limit shot numbers due to surface refresh requirements. The advent of liquid-leaf targets with their continuous replenishment at multi-kHz rates marks a breakthrough in laser-plasma interactions, e.g. for particle acceleration [2]. The first demonstration of RHHG in a single-shot application [3] has proven that their surface quality is also suitable for plasma mirrors.



By employing flat ethylene glycol sheet targets with controlled plasma density gradients and relativistic-intensity, waveform-controlled near-single-cycle laser pulses, we have achieved reproducible high-flux RHHG with unprecedented stability [4]. Tuning of the driving laser waveform enables the generation of continuous XUV spectra, indicative of the isolated attosecond pulses [4].

The combination of laser waveform stability and liquid sheet targets yields a reliable, high-flux XUV beam, corresponding to a kHz-train of attosecond pulses with record-high intensity potential. This scalability paves the way for next-generation high-energy attosecond lasers.

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High-harmonic generation in liquid crystals using a temperature-controlled flat jet device: Probing mesophase transitions and local order

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ABSTRACT

In this work, we report high harmonic generation spectroscopy experiments on thermotropic liquid crystals (LCs) using a custom-built recirculating flat jet device, specifically engineered for these complex soft-matter systems.[1] LCs are distinguished from conventional liquids by their anisotropic molecular organization, which manifests in multiple mesophases characterized by a different extent of orientational and positional order. In the nematic phase, molecules are oriented along a common director but remain positionally disordered, while smectic phases exhibit the same orientational alignment together with positional order in the form of molecular layering. Despite this defined molecular arrangement, LCs flow like liquids, enabling their use in flat jet geometries. The intrinsic hierarchy of order necessitates dedicated temperature control beyond that of standard liquid jet systems, which we explicitly implement to ensure mesophase stability under experimental conditions.

Using high harmonic generation (HHG) as a optical probe, we observe distinct signatures for different mesophases, with the harmonic response reflecting subtle changes in local orientational and positional order. Remarkably, these HHG signatures are highly sensitive to sub-degree variations in temperature and exhibit harmonic-order-dependent contrasts, highlighting the ability of HHG to resolve emergent local order within the condensed phase. Furthermore, intermolecular interactions, including the formation of transient anti parallel dimers, imprint characteristic angular emission patterns, providing insights into collective electronic correlations.

Our results demonstrate that HHG in liquid crystals can serve as a sensitive probe of mesoscopic order and emergent structural dynamics, while the recirculating flat-jet platform establishes a versatile foundation for future experiments in XUV and attosecond spectroscopy. Ongoing technical developments aim to adapt the system for vacuum-compatible operation and thinner sample layers, broadening its applicability to a wide range of soft-matter and liquid-phase techniques.

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Shaping Light with Liquids: Attosecond Physics for Tunable EUV Sources

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ABSTRACT

High-harmonic generation (HHG) in bulk liquids is now understood through the scattering-limited three-step model [1]. In liquids, the harmonic cut-off stays nearly constant across laser parameters, a consequence of strong scattering and on-site recombination [1-2]. This raises a fundamental question: if liquids enforce a fixed cut-off, how is the excess energy redistributed as the driving intensity increases?

We report here the emergence of a second plateau in liquid-phase HHG spectra, indicating a new regime of electron dynamics driven by hole delocalization and recombination with neighboring molecules [3]. This plateau exhibits weak cut-off scaling and a characteristic ellipticity dependence, supported consistently by experiments, ab-initio simulations, and semi-classical modeling. Further, we use attosecond interferometry to reveal a strong linear atto-chirp and chemically tunable spectral minima [4-6], providing sub-femtosecond access to recollision pathways and the interplay of electrons, structure, and local fields. These findings deepen our understanding of ultrafast dynamics in condensed, disordered media. In addition, they point to a materials-driven strategy for designing tailored attosecond light sources, where solvation structure, chemical composition, and confinement can be engineered to enhance recollision channels and shape emission properties.

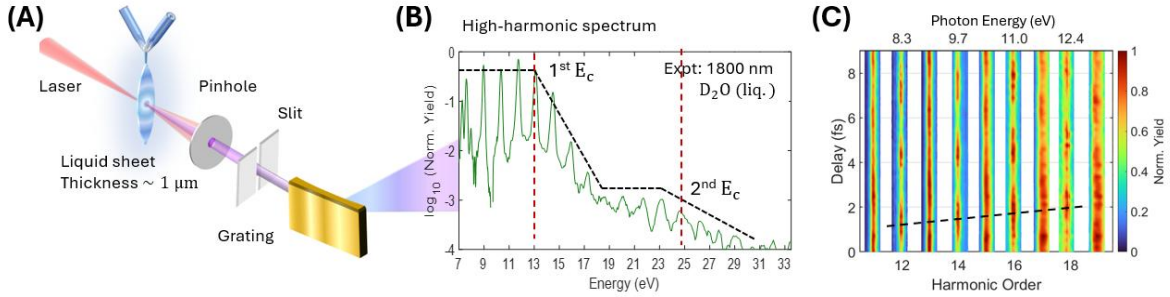

Figure 1. (A) Schematic of experimental set-up for generating HHG from bulk liquids (B) HHG spectrum from D_2O liquid at ~ 4.8 $\times 10^{13}$ W/cm^2 for 1800 nm wavelength. (C) Harmonic yield modulation in liquid ethanol with 1800/900-nm two-color laser pulses focused to a peak intensity of ~ 4 $\times 10^{13}$ W/cm^2

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X-Ray Induced Intermolecular Decay Of Solvated Ions Investigated By Multi-Electron Coincidence Spectroscopy

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ABSTRACT

X-ray induced electron spectroscopy on liquid samples has made tremendous progress throughout the last decades through the development of the liquid microjet technique.

The investigation of secondary non-local ionization mechanisms such as intermolecular Coulombic decay (ICD) and electron-transfer-mediated decay (ETMD) remain challenging, however, due to the low energy of the emitted electrons. Their signal is often buried below an enormous background of slow electrons produced by scattering effects. Utilizing a magnetic bottle electron spectrometer for coincident multi-electron detection, this challenge can partially be overcome by significant suppression of the background. We 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 of the 2p shell 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.

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Attosecond spectroscopy of decoherence in liquid phase water

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ABSTRACT

The dynamics of electron scattering in liquid water is central to a variety of fields, both in fundamental and applied science, including ultrafast chemistry and radiolysis [1]. At present, the comparison between the Photoelectron Angular Distribution (PAD) recorded in gas and liquid phase represents the experimental method of choice to characterize elastic and inelastic mean free paths in water [2]. Their values reported in the literature are consistently below 10 nm for photoelectrons with energies under 100 eV. These distances correspond to mean scattering times below few femtoseconds and thus attosecond spectroscopy should offer a complementary approach to the characterization of electron scattering in liquid water.

In this work, we performed Reconstruction of Attosecond Beating By Interference of two-photon Transitions (RABBIT) [3] on gas and liquid phase water over a broad kinetic energy range between 30 and 60 eV, exploiting the FAB1 laser of the ATTOLab platform [4]. RABBIT consists of an atomic scale electron interferometer realized through two-photon transitions induced by an IR dressing field overlapped with an XUV Attosecond Pulse Train (APT). It results in a photoelectron spectrum that exhibits a cosine modulation as a function of the delay between the APT and the IR. The phase of these oscillations usually encodes photoemission scattering dynamics while their contrast assumedly encodes the coherence of the Electron WavePacket (EWP). In the experiment, we measured a reduction in the oscillations contrast for liquid water compared to the gas phase. Various sources of decoherence were evaluated via control experiments and simulations. As a result, we were able to recognize elastic scattering of photoelectrons in the liquid environment as the dominant process leading to the observed contrast reduction. Moreover, we developed a stochastic model of RABBIT spectroscopy in liquids to interpret our findings and relate them to electron mean free paths and scattering phases.

This work represents, to the best of our knowledge, the first application of RABBIT spectroscopy to the study of electron scattering dynamics in liquids. Our results show that the EWP decoherence can be used as a novel observable to benchmark mean free paths reported in the literature and to measure the scattering phases of photoelectrons.

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Computational Modelling for Liquid-Jet Photoemission Spectroscopy: Electronic Structure and Electron Transport

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ABSTRACT

Compared to solids and gases, our understanding of the electronic structure and ultrafast dynamics of liquids remains far less mature. This situation has changed rapidly with the advent of the liquid microjet and related approaches, which enable photoelectron and Auger spectroscopies, along with emerging modalities such as PECD, to be applied directly to liquid samples. Liquid-jet photoemission spectroscopy (LJ-PES) is increasingly becoming a quantitative structural tool [1–3], with new types of spectroscopies to emerge [4,5]. However, interpreting these measurements relies critically on *ab initio* modelling.

In the first part of this talk, I will discuss computational strategies for electronic structure of liquids and solutions, emphasizing that the appropriate model depends on the role of the environment: from a weak perturbation (capturable by continuum descriptions), to a structure-defining solvent, to an active chemical participant. I will focus on water and highly concentrated aqueous solutions [6,7], where solute/solvent interactions span distinct regimes and challenge standard approximations. I will highlight progress enabled by correlated one-electron approaches and fragmentation/embedding methods [9], and I will address when and how nuclear quantum effects become essential for reliable predictions [10].

In the second part, I will turn to the formation and transport of low-energy electrons in liquids, a prerequisite for interpreting LJ-PES intensities, lineshapes, and energy shifts. I will summarize insights from cluster benchmarks [11], from condensed-phase decay pathways such as intermolecular Coulombic decay in water [12], and from detailed analysis of the full photoemission spectrum as a sensitive probe of electron/liquid interactions [13]. Finally, I will discuss current computational pictures of how electrons are born and evolve in water, and the implications for spectroscopy and radiation chemistry [14,15].

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Liquid-Jet Velocity-Map Photoelectron Imaging

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ABSTRACT

Volatile liquid-jet photoelectron spectroscopy (LJ-PES) enables direct studies of the electronic structure of solutes and common solvents and has greatly enhanced our understanding of electron energetics and scattering phenomena in both bulk and interfacial liquid-phase environments.[1,2] To date, such measurements have been performed with hemispherical or time-of-flight-based electron analysers, respectively suffering from low-electron-collection efficiencies or insensitivity to electron angular distributions. As commonly demonstrated with gas-phase samples, the velocity-map imaging technique offers ultimate electron collection efficiency, simultaneous spectral and angular distribution measurements, and down to few-percent energy resolutions for tens-to-hundreds of eV electron kinetic energies. However, thus far, velocity-map photoelectron imaging conditions have generally been deemed or found to be incompatible with volatile-liquid sample environments.

Here, we present pioneering soft X-ray liquid-jet velocity-map photoelectron imaging results, as generated from liquid-microjet targets and allowing simultaneous and optimal measurements of liquid-interface electron energetics, state symmetries, and electron-scattering distributions. Exemplary results will be presented for organic solvents, liquid water, and select aqueous solutions. Associated data-processing challenges, further instrument developments, and some of the unique applications of the newly developed instrument will also be described.

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X-Ray-Induced Charge-Transfer-Processes In Solution

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ABSTRACT

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? In this presentation, 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 stagesof 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. Some examples will be:

- The first steps towards a solvated electron, showing how the electron delocalization occurs on the sub-femtosecond timescale.
- The formation of a radiation-damage hotspot on a hundred-femtosecond timescale following Auger-Meitner decay in a solvated ion.
- How to get an insider's view of the solvation shell around to selectively probe how it differs from the bulk solution.

I will also give an outlook on how these types of studies could be developed towards other research questions.

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Theoretical Description Of High Order Harmonic Generation In Liquids

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ABSTRACT

High-order harmonic generation (HHG) is a non-linear strong-field process that produces coherent extreme ultraviolet (XUV) radiation and enables attosecond spectroscopy of ultrafast electronic dynamics [1]. While HHG has been extensively investigated in gases [2] and solids [3], its study in liquids has remained limited due to significant experimental challenges, despite the central role of liquid environments in chemical and biological processes. The first experimental observation of HHG in liquids in 2018 [4], followed by the first theoretical study only in 2022 [5], marked the beginning of a rapidly developing field in which many fundamental aspects remain to be elucidated.

In this work, we contribute to closing the gap between theory and experiments by developing an efficient fully quantum one-dimensional model tailored to capture HHG in disordered liquid phases. In parallel, we are using ab initio Ehrenfest molecular dynamics [6] simulations using the deMon2k software package [7] to incorporate the coupled electron–nuclear motion and the fluctuating local environments characteristic of liquids. These simulations will employ optimized Gaussian basis sets specifically adapted to describe continuum electronic states in HHG [8], which are essential for accurately modeling strong-field ionization and high-harmonic generation in condensed-phase systems.

These complementary approaches aim to provide a robust foundation for understanding strong-field interactions in liquid-phase systems. The methods currently under development are intended to clarify the key mechanisms underlying HHG in liquids and to guide upcoming theoretical and experimental developments in attosecond science applied to complex media.

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Angle-Resolved Photoemission from Liquid Jets

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ABSTRACT

Due to the short mean free path of electrons in condensed media, photoelectron spectroscopy is a powerful tool to investigate surface properties, including the composition of liquid surfaces. The prospect of depth profiling liquid samples, by either changing the kinetic energy of the photoelectrons or, in the case of liquid flat jets, changing the emission angle, offers possibilities to gain insight in the surface structure that can be highly valuable for many applications.

However, one major difficulty in making quantitative estimates from intensities in photoelectron spectra lies in the poorly constrained values for inelastic and elastic scattering cross sections (total and differential). An avenue to obtaining more information on these parameters is to investigate the angular distribution of the photoelectrons. Here I will show some recent results from experiments of angle-resolved photoemission from liquid surfaces, using cylindrical and flat jets [1-3], as well as from Monte Carlo simulations of electron transport, where samples ranging from strong surfactants to bulk-solvated species have been investigated.

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Water dipole orientation, Proton Transfer and Auger electron acceleration in Liquid water probed with Core-Level Spectroscopies

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The study of liquids using core-level spectroscopies is at the forefront of modern research, providing unique insight into electronic structure, solvation, and chemical interactions. In this work, we illustrate the power of these approaches through three representative examples. First, we will investigate aqueous Cu^{2+}, revealing [1] how X-ray photoelectron spectroscopy combined with simulations allows determination of the orientation of water dipoles in the first solvation shell of copper. Second, copper–glycine complexes are studied, showing proton transfer within the amino acid during complexation, and how this governs metal–ligand coordination, as evidenced by N 1s and Cu 2p spectra [2]. Finally, Auger electron acceleration effect in aqueous Ca^{2+} are highlighted through analysis and simulation of the Ca K-LL Auger spectrum [3]. Together, these examples demonstrate how core-level spectroscopy, combined with advanced modeling, provides detailed molecular-level understanding of solvation, coordination, and exotic electronic processes in liquids.

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Probing Protonation State Dependent Charge Transfer-to-Solvent in *L*-cysteine via Sulfur *Kβ* Valence-to-Core Resonant Inelastic X-ray Scattering

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ABSTRACT

L-cysteine is a highly versatile amino acid capable of undertaking several diverse functional roles within proteins, owing largely to the ability of its thiol group to deprotonate and engage in bonding giving rise to unique structural feature like disulfide bonds and strong coordination with metal centres. [1] The electronic structure of aqua-solvated *L*-cysteine has been a subject of long-standing interest due to its fundamental biological relevance. [2] While previous studies have successfully established a foundational understanding of static properties like speciation and hydrogen-bonding networks surrounding the thiol moiety, the dynamic ultrafast electronic phenomena remain largely unexplored. [3-5]

L-cysteine in aqueous solution exists predominantly in its zwitterionic thiol form, whereas increasingly alkalinity shifts the equilibrium towards a deprotonated thiolate species, becoming dominant at higher pH values. This study examines the influence of these protonation states on charge delocalisation at the sulfur site following *X*-ray induced core-shell excitation. Sulfur *Kβ* valence-to-core Resonant Inelastic *X*-ray Scattering (RIXS) provides a valence sensitive probe to explore the nature of charge delocalisation processes occurring on the timescale of core-hole lifetimes but due to the relatively weak signal strength at the sulfur *Kβ* emission line, it has been difficult thus far to access it with sufficient photon flux to obtain meaningful electronic structure information.

The multi-crystal *X*-ray spectrometer – MOSARIX, developed recently by our group provides us unprecedented access, making it possible to perform highly photon efficient high-resolution measurements in this tender *X*-ray region. [6] With this capability, we resolve distinct spectral signatures corresponding to the thiol and thiolate forms of *L*-cysteine. While the thiol species remains largely inert to the solvent environment, the thiolate engages with the solvent and exhibits pronounced charge transfer-to-solvent features below the ionization threshold. Using Molecular Dynamics and Ab initio Quantum Chemistry calculations, we showcase the existence of diffused molecular orbitals in the thiolate form that extend into the solvent continuum in contrast to the thiol form where the orbitals are largely localized on the sulfur site.

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Posters

Probing the Water Structure Around Dissolved Argon via Extended X-Ray Absorption Fine Structure (EXAFS) Spectroscopy

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ABSTRACT

Are there hidden, structural heterogeneities in ambient water and does nature manipulate these localized structures to optimize its functions(1)? Years of research across many fields have yielded compelling evidence to support a picture of water with short lived structures that may help explain how water uniquely supports life on earth(2). While these structures are still unknown, by using an inert gas such as argon, we can examine the hydrogen bond network around the dissolved gas to gain insight into what these localized structures may look like. Initial EXAFS (Extended X-Ray Absorption Fine Structure) experiments in conjunction with theoretical modeling, show a potential cavity or cage-like structure around the dissolved gas. As argon gas only weakly interacts with water, it must be accommodating the existing hydrogen bond network, this makes it an excellent spectroscopically available placeholder for the biologically important gas, O2. If inert gases such as argon or O_2 are preferentially located in low density cages, it raises the question of how such gases are so efficiently extracted by fish and other aquatic life forms. The atomic-level information of the molecular structure of water around dissolved gas atoms should advance our understanding of liquid water and how gases are dissolved and possibly extracted from it for aquatic respiration.

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Attosecond spectroscopy of iodomethane

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ABSTRACT

Attosecond spectroscopy techniques such as Reconstruction of Attosecond Beating By Interference of two-photon Transitions (RABBIT) [1] have paved the way for investigating electron dynamics on their natural time scale in atoms and molecules. The RABBIT technique is based on a time domain interferometric scheme in which the oscillation contrast provides insight into the coherence of the ionization process, while the phase encodes photoemission delay.

To the best of our knowledge, only one study has applied the RABBIT technique to CH_3I [2], focusing on spin-orbit delays in the valence states and not addressing core-level dynamics. In contrast, processes such as Auger decay in CH_3I have been extensively studied using static measurements [3].

In this work, we apply the RABBIT technique to iodomethane over a broad photon energy range between 20 and 70 eV, allowing us to investigate both resonant Auger decay and valence electrons dynamics. Phase analysis reveals a phase jump close to π/2 between resonances, consistent with the presence of a resonant Auger contribution. Regarding the contrast analysis, we observe an unexpected feature at higher energies, far from resonance, where a pronounced dip in the contrast appears and requires further investigation. At lower photon energies, preliminary valence measurements exhibit spin-orbit features, suggesting that extracting spin-orbit-dependent contrast and phase information could be possible.

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High repetition rate attosecond beamline for photoemission spectroscopy

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Synopsis We present a new experimental setup dedicated to attosecond photoemission spectroscopy. A post-compressed high-power Ytterbium laser source enables the experiment to run at a high repetition rate while a 3 beam architecture allows a pre-excitation of the medium and its photoemission by an XUV attosecond pulse train in presence of an IR dressing beam.

The beamline is driven by a new 80-W Ytterbium laser source providing 340 fs pulses, each carrying 2 mJ of energy at a reprate of 40 kHz. A post compression stage based on a multi-pass cell filled with Argon shortens the pulses down to 25 fs with 1.6 mJ energy per pulse.

The optical setup primarily consists of a 3 arm Mach Zehnder interferometer. An amplitude division of the beam on a beamsplitter precedes a wavefront division on a drilled mirror (DM). The most energetic of the three beams generates high-order harmonics in the form of an attosecond pulse train. The intermediate power beam has an annular shape from its reflection onto the DM and will be used to pre-excite the medium, e.g., to induce molecular alignment. Finally, the weakest beam -that went through the DM- will be the dressing beam. The recombination of the beams is realised in two steps, each with a DM. The delays between all the pulses are controlled and actively stabilized using parts of the beams that are collected at the last DM.

The size and intensity of each beam at the key locations of HHG and photoemission foci were computed using propagation simulations and show satisfactory results with respect to the experimental conditions required to perform photoemission spectroscopy using RABBIT [1] and Mixed-FROG [2] techniques.

As for the end-stations, the inline two foci geometry [3,4] enables simultaneous measurements in two magnetic bottle electron spectrometers or replacing one of them by a velocity map imaging spectrometer to access the electron/ion angular distribution. RABBIT measurements can then be performed with a reference gas spatially separated from the studied gaseous molecule or liquid target.

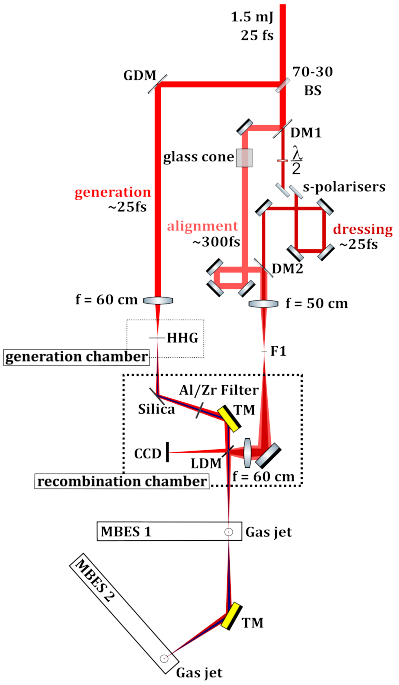

Figure 1. Experimental setup. DM : Drilled Mirror, GDM : Generation DM, LDM : Last DM, TM : Toroidal Mirror, MBES : Magnetic Bottle Electron Spectrometer.

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Tender X-ray Emission Spectroscopies in Liquid Systems: New Capabilities with MOSARIX Spectrometer

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ABSTRACT

Resonant inelastic X-ray scattering (RIXS) is a powerful technique for probing electronic structure, charge-transfer processes, and ultrafast dynamics with elemental specificity. While RIXS is well established in the soft- and hard-X-ray regimes, its extension to the tender X-ray range (2–5 keV) has remained experimentally challenging. This energy range is of particular interest because it provides access to the K edges of light elements (e.g., P, S, Cl, K, Ca) and the L edges of heavier elements (e.g., iodine). Moreover, tender X-rays offer increased bulk sensitivity compared to soft X-rays, which is advantageous for studies of liquids and complex environments.

We demonstrate that tender X-ray RIXS and X-ray emission spectroscopy are now experimentally feasible using the MOSARIX, our multi-crystal spectrometer installed at the GALAXIES beamline of the SOLEIL synchrotron. MOSARIX employs nine HAPG crystals arranged in a von Hamos geometry, combining large solid angle, high reflectivity, and high energy resolution[1]. This configuration provides unprecedented efficiency, enabling the detection of weak signals and operando measurements. Operation under ambient or helium atmosphere allows windowless detection and compatibility with liquid jets and in situ sample environments.

As a first application, we investigate radiative intermolecular decay (IRD) in aqueous solutions. In IRD, a core hole created on a selectively excited ion is filled by an electron from the surrounding solvent or ligands, resulting in X-ray emission. For aqueous Ca ions, we show that the IRD signal is sensitive to changes in the local chemical environment, including solvation structure, ion pairing, and chemical speciation. RIXS measurements across the Ca K edge provide resonant enhancement of the IRD signal, yielding additional sensitivity to ion–ligand hybridization and ultrafast electron delocalization.

We further present tender X-ray RIXS measurements of aqueous NaI at the iodine L_2 edge as a model system for ultrafast charge-transfer dynamics. The resulting RIXS maps, supported by theoretical calculations, reveal excitation into both localized and delocalized electronic states on timescales shorter than approximately 200 attoseconds.

These results demonstrate that recent instrumental advances establish tender X-ray RIXS as a robust and versatile tool, opening new opportunities for investigating electronic structure and dynamics in liquids and complex systems.

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3D Printed nozzle for a flat liquid jet for THz spectroscopy

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ABSTRACT

Field-resolved terahertz (THz) spectroscopy in the liquid phase is often fundamentally limited by the parasitic effects of sample containers. Standard windows introduce significant absorption, dispersion, and birefringence, while potentially triggering nonlinear responses that obscure the intrinsic dynamics of the analyte. To overcome these constraints, we present a method for field-resolved THz spectroscopy using windowless liquid sheets generated by a custom-designed, 3D-printed nozzle illustrated in Figure 1a.

The use of 3D printed nozzle designs gives the advantage of a fixed geometry, which significantly reduces the mechanical degrees of freedom and therefore simplifies the alignment. Furthermore, 3D printing provides a versatile and rapid prototyping platform to optimize fluidic geometries for various solvents. Our nozzle was specifically engineered to produce stable liquid sheets with a target thickness of 100µm; experimental characterization demonstrates the production of sheets in the range of 89.9µm for saturated sugar solutions, measured by Fabry Perot oscillations displayed in Figure 1b. By directly measuring the electric field, this windowless approach enables a precise normalization of the THz signal, depicted in Figure 1c, relative to the sheet thickness and solution concentration. This development provides a robust framework for high-sensitivity THz measurements of liquids, free from the artifacts typically associated with solid-state interfaces A photograph of the flat liquid sheet is captured in Figure 1d.
While flat liquid sheets have been used for water to do THz Spectroscopy [1], we are aming to use it for different bio samples like saturated sugar solutions.

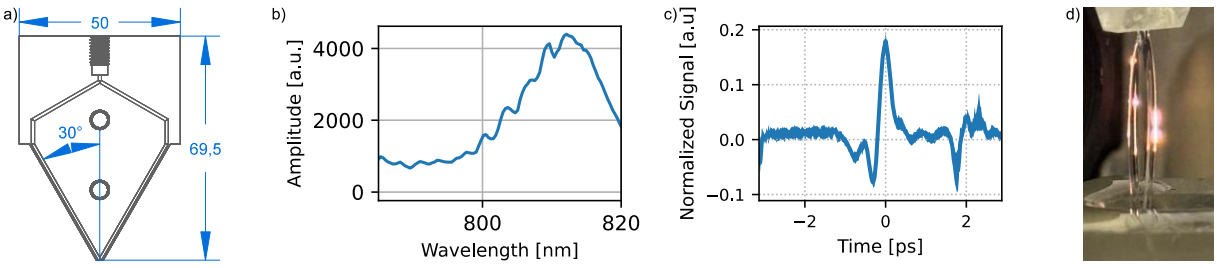

Figure 1 a) Shows the design for the printed nozzle. b) Spectrum of the Fabry-Pérot Oscillations for the Thickness measurements. c) Time Domain THz Measurement of a Saturarted Sugar solution. d) Picture of the Flat liquid sheet formed by the nozzle.

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Towards simulating X-ray induced ultrafast electron delocalization dynamics of hydrated ions

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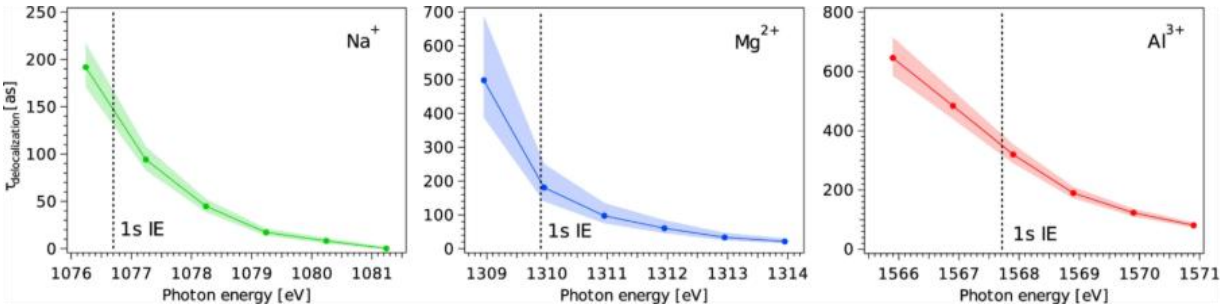
ABSTRACT

Recent experiments on the electron dynamics that take place during the X-ray excitation process of alkali ions solvated in water clearly show that spectral features below the core-electron ionization threshold differ little from the ones above it. This peculiarity has been attributed to the formation of a charge-transfer-to-solvent (CTTS) state, where the electron is delocalized from the parent ion, and the delocalization time was estimated to be on the order of tens to hundreds of attoseconds.[1]

In this work, we propose a way to simulate such electron dynamics that take place on the same timescale as the excitation by the time-dependent X-ray field. Toward this goal, we intend to employ the floating spherical Gaussian orbital (FSGO) framework,[2] pioneering work in electronic structure theory, in conjunction with the time-dependent variational principle.[3] We will show preliminary results, validating the numerical implementation of the FSGO part. Additionally, we present high-level benchmark electron dynamics calculations on sodium cation water clusters using RhoDyn.[4]



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Ultrashort and tunable UV source for attosecond transient absorption spectroscopy in liquid sample

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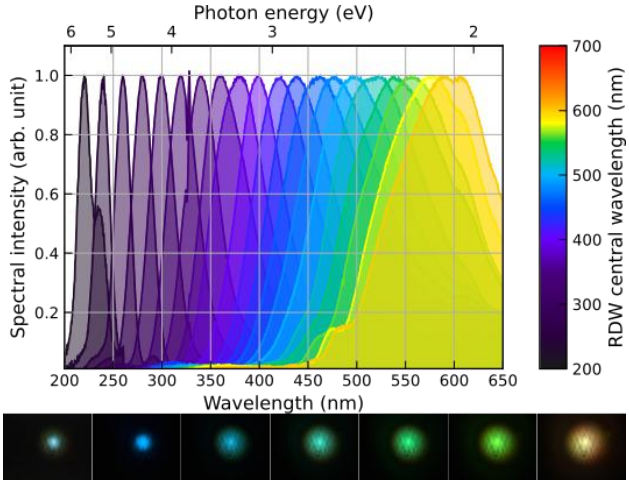
ABSTRACT

The improvement of laser's stability and repetition rate using ytterbium-based systems constitutes a significant opportunity for ultrafast science. However, this development is limited by the long pulse duration provided by these systems, which are not well suited to observing rapid dynamics occurring on the femtosecond to attosecond timescales. Fortunately, the maturity of post-compression techniques [1-2] based on self-phase modulation, combined with recent developments in nonlinear optics [3] extending to millijoule level soliton dynamics and resonant dispersive waves (RDW), makes it possible to generate a combination of attosecond and ultrashort pulses in the UV. This technological breakthrough paves the way for the study of ultrafast photo-induced dynamics of solvated species.

In this study, we employ a two-stage hybrid system [4] to post-compress laser pulses at the millijoule level, reducing the pulse duration close to the single optical cycle regime, with an overall transmission efficiency exceeding 45%. These short IR pulses are then split into two arms, one dedicated to HHG with photon energy up to 100 eV, and the other sent to a second stretched hollow-core fiber for deep ultraviolet generation. We demonstrate the generation of ultrashort UV light over a wide range of 4 eV and with a pulse energy in the microjoule range, ideally suited for attosecond transient absorption spectroscopy.



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Unveiling the Water/Solid Interface in Low-Carbon Cements through Cryo-XPS

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ABSTRACT

Concrete is the second most used substance by humanity, after water. Its production relies on Portland cement (PC), which contributes about 8% of global anthropogenic CO_2 emissions.[1] Most of these emissions come from clinker, formed by the thermal decomposition of limestone: $CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$ ($T \approx 1450\,°C$), releasing 0.8 tons of CO_2 per ton of clinker. A promising approach to reduce cement's carbon footprint is partially replacing clinker with supplementary cementitious materials (SCMs). Among these, calcined clays are particularly attractive, and cements containing them are already produced and used in some countries.[2]

Considering that concrete hardening is driven by the hydration reactions of clinker in the presence of aggregates, studying the interactions at the water/calcined clay interface is essential to understand the hardening process of this type of low-carbon concrete. One particularly relevant interaction is the electrostatic interaction between clay particles and the ions present in water. Indeed, the hydration water in concrete has a high pH, meaning that the silanol (Si–OH) and aluminol (Al–OH) groups on the surface of calcined clay particles can become deprotonated. As a result, the particles carry a negative surface charge, which is balanced by cations present in the water.

In this contribution, a XPS study of the water/calcined clay interface is presented. To preserve the water/solid interface under ultrahigh vacuum conditions, we performed cryo-XPS experiments, in which the interface was rapidly frozen to prevent water crystallization and maintained in this state throughout the measurement process. We show that the results cannot be interpreted using simple methods based on the relative sensitivity factors (RSFs) of the analyzed core levels. Instead, we simulated the peak areas using SESSA software[3] with relatively simple models, given the complexity of the interface. Model optimization allowed us to calculate the surface charge density of the particles at different pH values, which agreed well with alternative measurements of the same parameter obtained by potentiometric titration. We thus demonstrate that the methodology developed—combining cryo-XPS experiments with SESSA simulations—is a more powerful approach than previous studies of inorganic water/solid interfaces using RSF-based cryo-XPS analysis.[4]

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Energy as a Control Knob: Steering Ultrafast Non-Adiabatic Dynamics in Manganese(III) Acetylacetonate

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The Jahn-Teller (JT) distortion in octahedral Mn(III) complexes typically manifests as an axial elongation, giving rise to pronounced uniaxial magnetic anisotropy and underpinning the central role of Mn(III) ions[1-3] in the development of single-molecule magnets (SMMs). Actively manipulating this distortion on ultrafast timescales offers a promising route toward optical control of magnetisation. Recent work[2-4] has demonstrated that femtosecond photoexcitation of $Mn(acac)_3$ (acacH = acetylacetone) can induce a transient switch from the axially elongated to a compressed JT geometry, occurring within a vibrational period while preserving wave-packet coherence. Here, we use ultrafast transient absorption spectroscopy to investigate how excitation energy functions as a control knob for this photoinduced JT switch in solution. By selectively accessing different excited electronic states, we reveal a pronounced excitation-energy dependence in the yield of the compressed geometry, with higher excitation energies favouring its formation. This behaviour is attributed to an increased initial velocity of the nuclear wave packet along reactive JT vibrational modes, enabling more efficient traversal of non-adiabatic pathways. Furthermore, we find that the reaction coordinate itself is strongly influenced by the initially populated electronic state, underscoring the decisive role of coherent nuclear motion in steering non-adiabatic dynamics. These results demonstrate how excitation energy can be used to direct ultrafast structural and electronic dynamics in Mn(III) complexes, providing key mechanistic insight for the rational design of optically controlled single-molecule magnets.

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Photoelectron Circular Dichroism Of Liquid Samples

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ABSTRACT

Photoelectron Circular Dichroism (PECD) is an intense chiroptical effect defined as the forward/backward asymmetry along the light propagation axis upon photoionization of a chiral molecule by circularly polarized light. PECD is particularly sensitive to molecular and electronic structure, and benefits from the intrinsic strengths of photoelectron spectroscopy (PES), which for core-level ionization include surface, atomic-site, and chemical-state sensitivity. Despite these strengths, PECD has until recently been applied almost exclusively to molecules in the gas phase. Using our custom liquid-jet photoelectron spectroscopy apparatus,[1] we previously performed PECD experiments for neat liquid fenchone.[2] This work confirmed the feasibility of applying PECD to liquid samples, but also laid bare a number of experimental challenges inherent to this method. PECD is most intense for low kinetic energy (< 20 eV) photoelectrons, which for condensed-phase systems means that the primary photoelectrons of interest will be subject to scattering events and will become unavoidably convoluted with the high-intensity background signal comprised of scattered and secondary electrons.[3,4] The former effect will result in a loss in measured angular anisotropy, while the latter complicates data analysis. Here, we report on our experimental efforts to circumvent these effects by focusing on the surface-active molecule α-methylbenzylamine (MBA), and we compare our results for this molecule with our recent work on the bulk-soluble amino acid alanine,[5] thereby exploring PECD's sensitivity to protonation state and solvation conditions.

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Study Of Biomimetic Membranes Composed of Glycosylated Lipids

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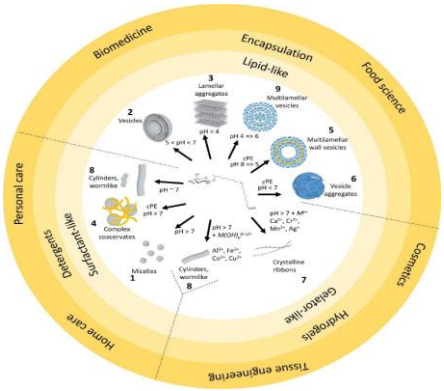

Figure 1: Phase behaviour of G-C18:1 (C<5 wt% in water) with pH and salt addition

Introduction: Bio-based surfactants, derived from biomass via fermentation of glucose and vegetable oils[1, 2], have gained popularity due to their eco-friendly advantage over petroleum-derived surfactants, rely on the pollutive chemical processes. Microbial glycolipids (MGs) are the bio-based surfactants, and their amphiphilic nature allows them to interact with lipid bilayer membranes-key structure in all living organisms[3] -while also exhibiting antibacterial, anticancer, and antiviral properties[4, 5]. Modification to lipid membranes can significantly impact cell function, highlighting the potential of MGs in diverse application as shown in Figure 1. The self-assembly of microbial (MGs) into bilayers and their impact on biological membranes remains underexplored. Some key biophysical properties are not well understood. This study focused on exploring the biophysical properties of membrane-forming MGs and their interaction with phospholipid-based biomimetic membranes.

Materials and method: Biosurfactants known to form membrane-like structures such as Acetylated G-C18:1, Acetylated Lactonic SL-C18:1, mono-rhamnolipid, trehalolipids were prepared. Lamellar structures were prepared using Milli-Q water (18.2 MΩ). The pH is adjusted using NaOH and HCl solution (0.5M, 1M, and 5M). Fibrillation was induced with calcium chloride ($CaCl_2$) as a source of Ca^{2+} ions. The glycolipids studied included Glucolipids (G-C18:1, G-C18:0) and Sophorolipids (SL-C18:1, SL-C 18:0). Phospholipids vesicles, including DOPC (1,2-Dioleoyl-*sn*-glycero-3-phosphocholine) and DPPC (1,2 Dipalmitoylphosphatidylcholine), were synthesized in uni-lamellar vesicles (ULVs) and multi-lamellar vesicles (MLVs) forms to study the amphiphilic interactions.

Results: Biophysical properties of membrane-forming biosurfactants were analyzed using small-angle X-ray scattering (SAXS), small-angle neutron scattering (SANS), neutron spin-echo (NSE), differential scanning calorimetry (DSC), and Langmuir-Blodgett Trough, revealing bilayer thickness, bending rigidity, melting temperature, and area/molecule. Similar techniques are aimed to use further to elaborate MGs and PLs interaction.

Discussion and Conclusion: The results align with the project objectives. Further refinement of SAXS and SANS data is ongoing. Confocal microscopy is needed to confirm Giant uni-lamellar Vesicle (GUV) formation and glycolipid effects, with GUV protocols requiring optimization through several trails.

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Ultrafast charge transfer dynamics in phosphorylated amino acids in aqueous solution

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ABSTRACT

Charge transfer (CT) plays a fundamental role in chemistry and biology, particularly in aqueous environments where most reactions occur. Post-translational modifications such as phosphorylation strongly alter local charge distributions and intermolecular interactions in proteins. In this study, we employ Auger–Meitner spectroscopy (AMS) to address ultrafast CT dynamics of the phosphorylated amino acid phosphotyrosine (pTyr) in aqueous solution, focusing on the role of the phosphate group at the biomolecule–water interface. AMS is a powerful technique for investigating electron dynamics in extended complex systems [1,2]. Our results indicate that the phosphate group dramatically enhances charge transfer to the solvent (CTTS), as compared, for example, to sulfur-containing amino acids such as L-cysteine [3]. This finding highlights the role of solvation and, in particular, hydrogen-bond network effects in facilitating CTTS. Furthermore, the core-hole lifetime provides a natural timescale for electron dynamics, allowing quantification of CT rates. Our observations suggest that CT pathways are governed by the interplay between the phosphate moiety and the amino acid backbone in the hydrated environment around pTyr. Understanding CT in biomolecules is crucial for fields such as radiation chemistry, protein chemistry, and biophysics. Our findings contribute to a deeper understanding of early electronic processes in complex aqueous systems, paving the way for future studies of radiation-induced damage under biologically relevant conditions.

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