

SYML 1: Molecular Spectroscopy in Liquid Jets

Time: Monday 11:00–13:00

Location: HS 1+2

Invited Talk SYML 1.1 Mon 11:00 HS 1+2
The challenging road to work function measurements from aqueous solutions — ●BERND WINTER — Fritz-Haber-Institut, Faradayweg 4-6, 14195 Berlin

Electronic structure of liquid water and aqueous solutions is accessible by liquid-jet photoelectron spectroscopy (LJ-PES). Photoelectron spectra are typically referenced to the vacuum level which would be difficult to relate to explicit surface properties such as the work function of aqueous solutions. We discuss how the latter can be inferred from a LJ-PES measurement, based on an explicit consideration of a solution's Fermi energy / electrochemical potential. Competing surface-charging effects contributing to energy shifts of solute and solvent spectral features are important to be quantified and will be explored. This inherently connects to the ability to extract accurate electron binding energies from aqueous-solution microjets.

Invited Talk SYML 1.2 Mon 11:30 HS 1+2
Liquid Delivery Systems for Time Resolved X-ray Spectroscopy — ●ZHONG YIN — Tohoku University, Sendai, Japan

Advancements in modern light sources have transformed the study of matter, offering unparalleled brilliance, coherence, and ultrashort pulses [1,2]. These innovations have significantly enhanced our ability to explore electronic properties that are fundamental to bonding and reactivity in real time.

Time-resolved X-ray spectroscopy, with its exceptional element, site, and orbital specificity, has emerged as a key tool for probing electronic structures.

However, studying chemically and biologically relevant processes in the liquid phase presents significant experimental challenges, requiring advanced experimental setups and innovative sample delivery systems [3,4].

In this talk, I will highlight recent results from table-top sources, such as high-harmonic generation (HHG) [5,6], and free-electron laser (FEL) facilities that enable time-resolved X-ray spectroscopy of biochemical systems in the liquid phase. These advancements are opening new avenues for investigating ultrafast molecular dynamics in their native environments with unprecedented time resolution.

References [1] D. Pile, *Nat. Photon.* 18, 640 (2024). [2] C. Bostedt et al. *Reviews of Modern Physics* 88, 015007 (2016) [3] M. Faubel et al. *Z. Phys. D, Atoms, Mol. Clust.* 10, 269 (1988) [4] M. Ekimova et al. *Struct. Dyn.* 2, 054301 (2015) [5] A. Smith et al, *J. Phys. Chem. Lett.* 11 (6), 1981 (2020) [6] Z. Yin et al. *Nature* 619, 749 (2023)

Invited Talk SYML 1.3 Mon 12:00 HS 1+2
UV photoelectron spectroscopy of aqueous solutions — ●HELEN FIELDING, JOHANNA RADEMACHER, KATE ROBERTSON, and

EDOARDO SIMONETTI — Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, U.K.

Ionisation and electron transfer processes are ubiquitous in condensed-phase biology and atmospheric chemistry. It is, therefore, essential to measure the electronic structure and UV photoexcited state dynamics of biologically and atmospherically important chromophores in conditions similar to those encountered in nature, i.e. in aqueous solution. A direct way of probing electronic structure, and its evolution following photoexcitation, is through the measurement of electron binding energies using photoelectron spectroscopy. However, there are a number of practical challenges associated with carrying out such measurements in aqueous solution using UV light pulses. These include electrokinetic charging, vacuum level offsets, uncertainties in instrument functions at very low electron kinetic energies (< 1 eV), and the need to account for distortions of measured electron kinetic energy distributions arising from inelastic scattering of low energy electrons (< 5 eV) in liquid water. We will present our approach to accurate UV photoelectron spectroscopy measurements in aqueous solution and its application to biologically and atmospherically relevant chromophores.

Invited Talk SYML 1.4 Mon 12:30 HS 1+2
Decoherence and electron transport in liquid water observed with attosecond interferometric spectroscopy — ●HUGO MARROUX ET AL — Université Paris-Saclay, CEA, LIDYL, 91191 Gif-sur-Yvette, France

The dynamics of electron scattering in liquid samples are of fundamental importance. However, time resolved observations are difficult due to stringent experimental challenges as the process begins on the attosecond timescale [1] with an effective mean free path limited to about 8 \AA [2]. To investigate electron dynamics in water we perform RABBIT [3] experiments in both gas and liquid water over a photon energy range from 37 to 74 eV. The RABBIT technique is based on an interferometric scheme where the oscillation contrast can be used as an observable of decoherence phenomena [3], while its phase provides insight into electron's dynamics and transports. I will discuss recent results obtained using an experimental setup where a liquid micro-jet device is combined with a two foci geometry enabling referencing of the RABBIT trace against an atomic species.

We will discuss the role of inelastic scattering to interpret the large time delay (300 as) observed. Additionally, the analysis of the contrast over the energy range reveals the effect of decoherence in water. I will present our ongoing efforts to characterize the decoherence dynamics in terms of the dephasing of a representative density matrix.

References :[1] Jordan et al., *Science* 369 (2020), [2] Mondal et al., *Nat. Phys.* 19 (2023), [3] Paul et al., *Science* 292 (2001), [4] Bourassin Bouchet et al., *Phys. Rev. X* 10 (2020)