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Handedness in Space: Photons, Molecules, and Life's Chiral Signature

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Homochiral biomolecules such as amino acids, sugars, and lipids are fundamental to life, yet how their selective handedness emerged abiologically is still unclear. Abiotic l-enrichments of amino acids recurrently detected in carbonaceous chondrites—meteorites rich in organic carbon—suggest that the origin of life's homochirality may be linked to processes that occurred in space [1]. Among the possible mechanisms, stellar ultraviolet circularly polarized light (UV CPL) has been recognized as a promising candidate for triggering symmetry breaking in interstellar environments [2].

In this context, I will present our recent work on the asymmetric interaction of UV CPL with prebiotically relevant chiral molecules [3,4]. To understand how chiral asymmetry may be induced, amplified, or preserved, we investigate the electronic circular dichroism (CD) and anisotropy spectra of chiral complex organic molecules in both gas and condensed phases using the AU-CD beamline at the ASTRID2 synchrotron, supported by time-dependent density functional theory calculations. These measurements allow us to disentangle the intrinsic chiroptical response of isolated molecules from environment-induced effects arising from solvation, hydrogen bonding, and conformer redistribution within water-rich matrices. They also provide quantitative predictions of monochromatic and broadband UV CPL-induced enantiomeric enrichments, which we validate through asymmetric photolysis experiments using synchrotron radiation and in-house UV-tunable circularly polarized laser sources [4]. By combining gas-phase chiroptical spectroscopy, condensed-phase studies, quantum chemical simulations, and asymmetric photochemistry, this work provides a molecular framework for assessing how stellar UV CPL may generate chiral imbalances under astrophysical conditions. Together with experiments on the formation of chiral organic molecules in cosmic ice analogues [5] and the analysis of meteorites and asteroid-return samples [6], these results contribute to a broader understanding of the earliest stages of molecular asymmetry in space. Future work will further extend this approach to probe the role of amorphous water in interstellar ice analogues, bridging intrinsic molecular properties with astrochemical processes that may have shaped the pathways leading to biological homochirality.



Fig. 1 Did stellar circular polarization selectively enrich one enantiomer over the other in interstellar chiral molecules?

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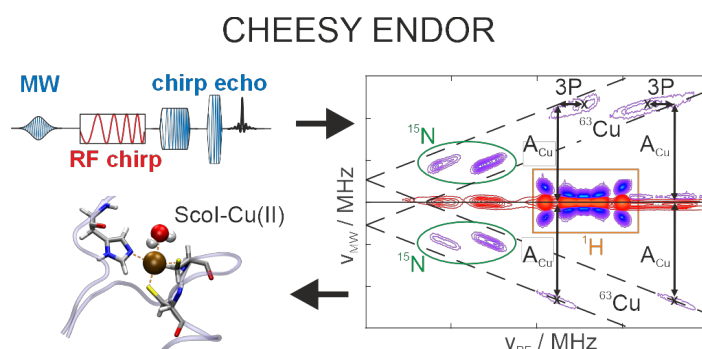
Acknowledgement

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Enhanced sensitivity and reduced spectral overlap in ENDOR spectroscopy with chirped pulses

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Electron–Nuclear Double Resonance (ENDOR) spectroscopy is a powerful magnetic resonance technique for probing the geometric and electronic structure of paramagnetic centers, including transition metal complexes and metalloproteins, through combined microwave (MW) and radiofrequency (RF) pulse sequences. Unlike conventional paramagnetic NMR, ENDOR selectively detects nuclei in the immediate vicinity of the unpaired electron spin, providing direct insight into catalytically and biologically active sites. This is particularly important for understanding structure–function relationships in transition metal catalysts, such as Ti(III)-based Ziegler–Natta systems, and metalloproteins such as ScoI-Cu(II). However, ENDOR studies of such systems are often limited by low sensitivity and severe spectral overlap arising from broad, anisotropic transitions and multiple interacting nuclei, especially for low- γ and quadrupolar nuclei commonly encountered in catalysis and biology.



In this talk, I will show how advances in instrumentation and pulse ENDOR methodology overcome these challenges by improving both sensitivity and spectral resolution. Inspired by NMR spectroscopy, we implemented chirped (frequency-swept) microwave pulses for broadband detection of electron spin transitions in CHEESY ENDOR, introducing a second spectral dimension that separates overlapping features and simplifies spectral analysis. [1] In addition, chirped RF pulses enhance sensitivity in frequency-domain ENDOR by exciting a larger fraction of nuclear spin transitions, particularly for broad resonances of low- γ nuclei such as Cu(II) and Ti(III). [2] Using ScoI–Cu(II), a metalloprotein essential for the biogenesis of mitochondrial complex IV in the respiratory chain, we demonstrate how these methods resolve overlapping signals from different nuclei (^1H , $^{14/15}\text{N}$, ^{63}Cu) and separate hyperfine from quadrupolar interactions, enabling a more accurate determination of spin Hamiltonian parameters and electronic structure. These developments significantly extend the applicability of ENDOR spectroscopy to challenging problems in transition metal catalysis and bioinorganic chemistry, enabling studies of previously inaccessible nuclei such as ^{27}Al , $^{47/49}\text{Ti}$, and ^{63}Cu . [3]

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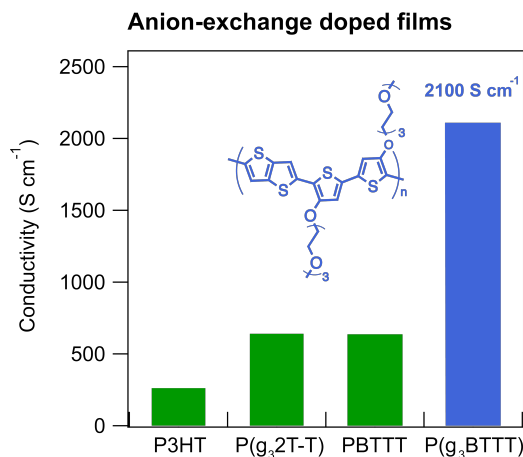
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Resistance to Overdoping Allows Over 2000 S cm⁻¹ Conductivity in P(g₃BTTT) With Anion-Exchange Doping

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Organic semiconductors have a wide range of near future applications, such as bioelectronics, thermoelectronics and optoelectronics^{1,2} where their low production cost and chemical tunability make them very attractive candidates for the aforementioned fields. Current challenges include the low conductivity which can be addressed *via* doping. In particular for conjugated polymers doping increases the conductivity by several orders of magnitude²⁻⁴. Recently, sidechain engineering has been shown to be a useful tool for the modification and improvement of conjugated polymers⁵. By exchanging the commonly used alkyl sidechains with glycol sidechains the dopant-polymer miscibility and the ionic uptake is improved⁶. Herein we investigate how these improvements affect chemical and anion exchange doping of thiophene and thienothiophene type polymers in respect to their conductivity. To characterize these changes, we use steady state absorbance spectroscopy, four-point probe, time domain THz spectroscopy, *in situ* absorbance measurements and chronoamperometry. For P(g₃BTTT), we find extraordinarily high conductivities of over 2 000 S/cm combined with a high charge carrier mobility. We show that transport involves delocalized charges, that all generated charges participate to the transport, and that the mobility is resilient over nanometer to micrometer length scales. However, the high-doping regime also shows a trade-off between high charge density and high mobility, limiting the conductivity at excess concentrations of doubly charged species. Surprisingly, P(g₃BTTT) is resistant to this ‘overdoping’ effect and sustains particularly high levels of doubly charged species without drop in mobility. The exceptional conductivity of doped P(g₃BTTT) can thus be related to the high doping level that is achieved thanks to the oligoether side chains, without significant trade-off on the concomitantly high mobility.



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- [2] B. Lüssem, M. Riede, and K. Leo. “Doping of organic semiconductors”. In: phys- ica status solidi (a) 210.1 (2013), pp. 9–43.
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- [5] Giovannitti, A. *et al.* Controlling the mode of operation of organic transistors through side-chain engineering. *Proc. Natl. Acad. Sci. U. S. A.* **113**, 12017–12022 (2016).
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Ligand-Dependent Lipid Bilayer Disruption by Atomically Precise Metal Clusters

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Atomically precise metal nanoclusters have emerged as highly promising nanomaterials for biomedical applications owing to their ultrasmall dimensions (<2 nm), atomically defined structures, tuneable ligand shells, and remarkable opto-electronic properties. Their structural precision and surface versatility enable the design of nanoclusters with tailored functionalities for therapeutic and diagnostic applications.

Despite these advantages, a comprehensive understanding of their interactions with biological membranes remains limited. Since the cell membrane represents the first biological barrier encountered by nanomaterials, elucidating nanocluster–membrane interactions are crucial for both the rational development of biocompatible nanomaterials and the assessment of potential nanotoxicological effects[1].

In this study, three different atomically precise metal nanoclusters, Au₂₅(GSH)₁₈, Au₂₅(Capt)₁₈, and Au₂₅(MHA)₁₈, were employed to investigate their interactions with POPC lipid bilayers as model cell membranes. The interactions between the nanoclusters and lipid bilayers were systematically analysed using ATR-FTIR spectroscopy, QCM, and AFM measurements.

The results revealed that although all nanoclusters possess the same Au₂₅ core, variations in the ligand shell led to significantly different interaction with the membrane. In particular, the Au₂₅(MHA)₁₈ nanoclusters induced complete disruption of the lipid bilayer, whereas the other ligand-protected clusters exhibited comparatively weaker effects on membrane integrity. These findings demonstrate that ligand shell chemistry plays a critical role in governing nanocluster–membrane interactions and membrane destabilization mechanisms.

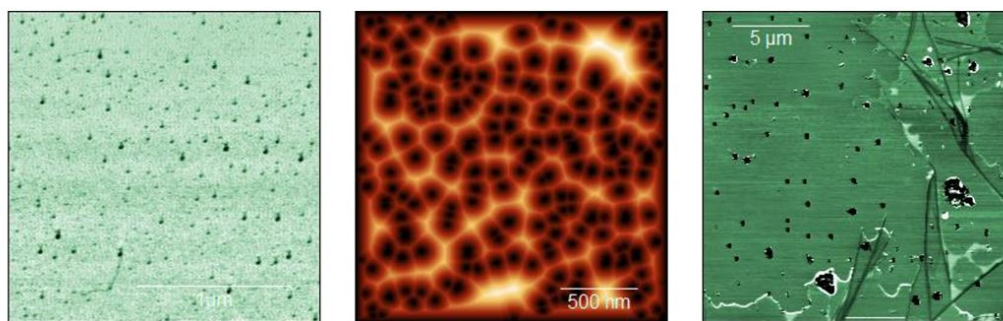


Figure 1. **Left.** Phase AFM image of Au₂₅(Capt)₁₈ on lipid bilayer. **Middle.** Voronoi diagram shows effective area per nanocluster for Au₂₅(Capt)₁₈ on lipid bilayer. **Right.** Phase AFM image shows disruption of the lipid bilayer by Au₂₅(MHA)₁₈.

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Progress on photo-CIDNP as a General Tool for Dye Sensitized Hyperpolarization in Solid-state NMR

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NMR spectroscopy is an extremely versatile technique for atomic level structural investigation. One of the major disadvantages of NMR spectroscopy is its poor sensitivity, due to the low polarization of nuclear spin-flip transitions. To address this, throughout the past decades, significant advances have been made to hyperpolarize nuclear spins.

Emerging pathways to generate bulk nuclear hyperpolarization are optically based techniques such as photochemically induced dynamic nuclear polarization (photo-CIDNP). Recently, we have shown that it is possible to generate bulk hyperpolarization using small donor-acceptor molecules (D-A) as polarizing agents (PAs).^{1,2} Following the initial demonstration of ¹H bulk hyperpolarization at low magnetic field, we extended the approach through rational design of small D-A systems to magnetic fields as high as 21.15 T, reaching enhancements up to a factor of 100.³

Using our recently the kinetic photocycle description of solid-state photo-CIDNP,⁴ we report a new generation of photo-PAs, which yield enhancements significantly in excess of what we have previously reported. Moreover, we also present novel results on bulk ¹H using standard DNP solvent formulations for generating ¹H nuclear hyperpolarization. Furthermore, we will also discuss theoretical and experimental progress on understanding polarization trans-fer via spin diffusion to the bulk to increase bulk enhancements.

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A Molecular Movie of Photoinduced Structural Dynamics in Diazocine Captured by Small-Molecule Time-Resolved Serial Femtosecond Crystallography

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Photochemistry is governed by coupled electronic and nuclear dynamics on femtosecond-to-picosecond timescales, where many product-determining steps occur. Conventional structural methods typically capture only static snapshots or long-lived intermediates. Time-resolved serial femtosecond crystallography (TR-SFX) overcomes this limitation by resolving structural change with femtosecond time resolution, complete reciprocal-space sampling, and sub-Ångström spatial precision, enabling real-space molecular movies. While TR-SFX has transformed the study of ultrafast biomolecular reactions, including light-induced isomerisation, bond formation and cleavage, and electron transfer,[1] it has until recently been largely restricted to large-unit-cell crystals such as photoactive proteins and, more recently, metal–organic frameworks.[2] Here, enabled by new analysis methods and indexing algorithms, we demonstrate TR-SFX on small-molecule, capturing an azobenzene derivatives[3] ultrafast structural dynamics and opening a route to molecular movies of small-molecule photochemistry.

I first give a brief overview of TR-SFX before presenting our analysis of diazocine photodynamics. We reconstruct a time series from extrapolated structures and difference electron density, with frames every 10 fs and an effective time resolution of ~150 fs. While a single 300 fs frame is shown below, the full time series follows the earliest structural response: N=N bond twisting within 150 fs, redistribution of distortion into the ethyl bridge, and progressive planarisation of the molecule. After ~1 ps, crystal disorder develops and diffraction intensity decreases, marking the loss of long-range structural order. These results demonstrate that small-molecule TR-SFX can resolve reaction pathways and help guide the design of solid-state photoactive materials.

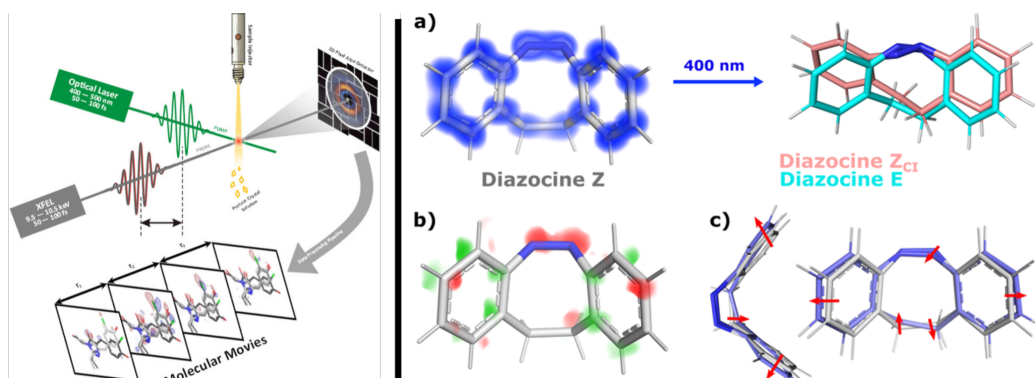


Fig 1. Left: Pump–probe TR-SFX schematic. An optical pulse excites microcrystals, and femtosecond X-ray pulses probe the structure at defined time delays. **Right: Structural dynamics of a sterically constrained bridged azobenzene.** a) Ground-state Z-diazocine electron density at 0.88 Å resolution, with TD-DFT E and Z_{Cl} structures.[3] b) Difference electron density at 300 fs (±3σ). c) Extrapolated 300 fs structure, revealing early N=N bond twisting, distortion of the ethyl bridge, and increased planarity of the aromatic ring.

[1] G. Khusainov, J. Standfuss, T. Weinert, *Structural Dynamics*, 2024, 11, 020901.

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Evolution of interference control in ICP-MS: From correction models to MS/MS

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Part 1 (G. Hudin): ICP-MS technology has evolved over recent decades into an indispensable tool for ultra-trace analytical applications. One of the key challenges, however, remains the effective elimination of spectral and non-spectral interferences, which can significantly impact accuracy and detection limits. This presentation highlights the critical turning points in the development of interference removal strategies in ICP-MS.

Starting from early approaches such as mathematical correction and the use of high-resolution ICP-MS, particular emphasis is placed on technological innovations that have enabled a paradigm shift. These include the introduction of collision and reaction cells (CRC), the use of kinetic energy discrimination, and the targeted implementation of chemical reactions for the selective removal of interfering species. Another major milestone is the establishment of triple quadrupole ICP-MS (ICP-QQQ), which offers unprecedented selectivity and robustness against complex matrices through controlled reaction chemistry.

Using selected case studies, the contribution demonstrates how these technological advancements have significantly improved analytical performance for greener chemistry and opened up new application areas—particularly in environmental and food analysis.

Part 2: Intelligence That Performs: The Next Generation of GC

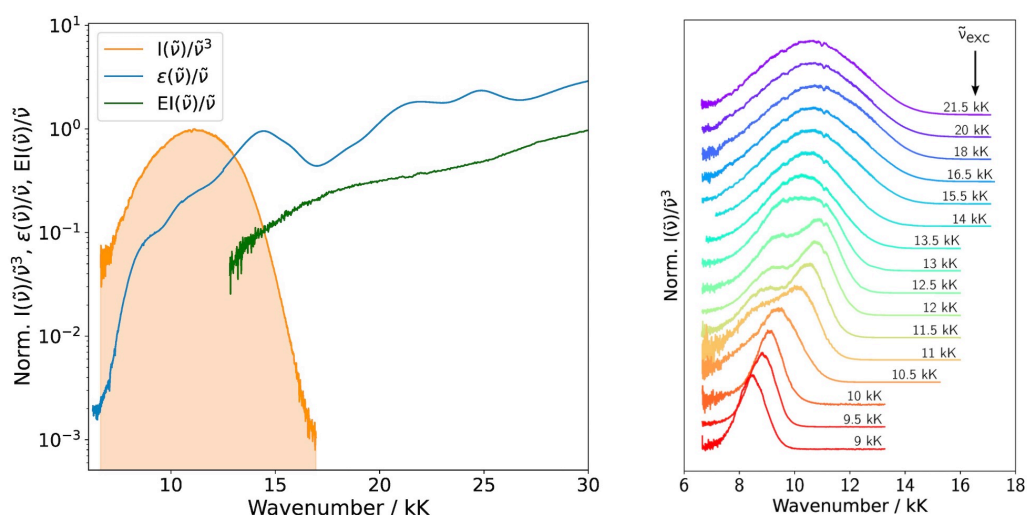
(Sarah Kubik): The growing need for higher throughput, improved efficiency, and reduced downtime is driving innovation in gas chromatography (GC). Agilent's new 8890B and 8860B GC systems feature a redesigned oven that delivers up to 30% faster cooldown times, reducing cycle times and increasing sample throughput. In addition, the 8890B and 8860B include smart features that simplify operation and maintenance. GC Assist provides continuous performance monitoring, parameter tracking, and user guidance, while Guided GC-MS Maintenance streamlines routine servicing and reduces downtime. Built-in gas and power consumption logging supports cost control and sustainability goals, making these systems efficient, intelligent solutions for modern analytical laboratories.

Breaking Kasha's Rule in Gold Nanoclusters: Unconventional Photophysics of $[\text{Au}_{25}(\text{SR})_{18}]$

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Atomically precise gold nanoclusters (NCs) are promising materials for photocatalysis, biosensing, and solar energy conversion, yet their fundamental excited-state dynamics remain poorly understood due to experimental limitations and incomplete spectral characterization.[1] Among the more than 100 structurally resolved metal NCs with ultra-small cores (<2 nm), $\text{Au}_{25}(\text{SR})_{18}$ (SR = PET, 2-phenylethanethiol) is the most extensively studied and typically exists in three oxidation states (-1, 0, +1). However, systematic photophysical investigations remain scarce because of limited NIR sensitivity in commercial fluorometers and the lack of accurate measurements.[2] Here, we present a combined steady-state and time-resolved spectroscopic study of neutral Au_{25} NCs using a custom-built setup with extended near-infrared sensitivity, emphasizing the importance of instrumentation design for reliable characterization.



Our results reveal a low-energy absorption band at ~9 kK (fig. 1), not previously reported, together with a pronounced excitation-energy dependence of both the emission profile and peak position (fig. 2), representing the first observation of such behavior in gold nanoclusters. Time-resolved measurements further show distinct temporal evolution for each excitation energy and highly distributed, strongly non-monoexponential photoluminescence decays over the ns– μ s timescale. Compared with the closed-shell anion, the neutral cluster displays clear deviations from Kasha's and Vavilov's rules. These observations support a working hypothesis involving dark states and delayed fluorescence to explain the unconventional emission pathways and relaxation dynamics of the neutral species. To gain deeper insight into these effects, comparative studies were performed on Au_{25} , Au_{38} , and $\text{Au}_{13^{2+}}$ nanoclusters, all of which are of interest due to the presence of Au_{13} icosahedral motifs in their cores. Complementary low-temperature and quenching experiments were also conducted to further clarify the nature of the excited states. Together, these results provide a basis for proposing a Jablonski diagram and a kinetic model to rationalize the observed relaxation dynamics.

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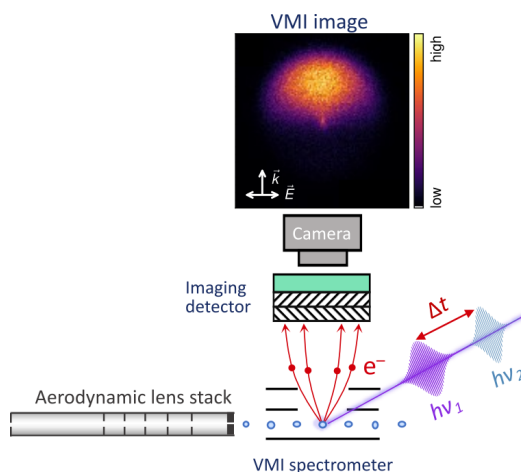
[2] L. E. Llanes-Montesino, G. Angulo, J. Zhao, T. Bürgi, A. Rosspeintner, Chimia, 2026, 80, 1–4

Time-resolved photoelectron imaging of photochemistry at aqueous droplet surfacesN. Kriūnas¹, J. Heitland¹, J. C. Lee¹, M. Wyrsh¹, B. L. Yoder¹, R. Signorell^{1*}¹Department of Chemistry and Applied Biosciences, ETH Zurich, 8093 Zurich, Switzerland

Photochemical reactions at the air–water interface can be accelerated by up to several orders of magnitude [1,2], a phenomenon with major impact on our understanding of atmospheric chemistry. However, the investigation of the mechanisms behind the rate increase remains challenging due to difficulties in correlating the observed changes in reaction rate to the underlying electronic structure.

Photoelectron spectroscopy, combined with a pump–probe scheme, enables temporal resolution of photoinduced dynamics through direct probing of the evolving electronic structure. We present preliminary data from surface-sensitive time-resolved femtosecond UV pump–probe photoelectron imaging (PEI) of aqueous submicron aerosol droplets. Phenol and phenolate were chosen as high-interest well-characterized model systems, given their role as aromatic chromophores in atmospheric aerosols. The experimental results show signatures consistent with hydrated electron formation from electron ejection into the solvent, revealing sub-ns timescale decays of 266 nm-photoexcited phenol and phenolate at the droplet surface.

Our technique (Fig. 1) benefits from the high surface-to-volume ratio of aerosols, and surface sensitivity, due to the limited escape depth of the probed low-kinetic-energy electrons. This enables us to resolve the electronic structure and photodynamics of molecules at the droplet surface [3,4], closely resembling real atmospheric conditions. Our work complements photoelectron spectroscopy with liquid jets [5,6], and sum-frequency generation techniques at air–water interfaces [2].



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- [6] K. Robertson et al., *Chem. Sci.*, **2023**, *14*, 3257–3264

Two molecular pathways for ion-driven "structure making / braking" in water revealed by Correlated Vibrational Spectroscopy

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Aqueous anions are commonly classified as "structure makers" or "structure breakers" based on how they affect water, which is deduced from macroscopic observables, yet the underlying molecular mechanisms remain debated because most spectroscopies do not directly isolate water–water hydrogen bonds. Here we use Correlated Vibrational Spectroscopy (CVS)¹, a hyper-Raman based approach that separates self-correlated (single-molecule / isotropic) from cross-correlated (collective / interacting) vibrational responses, thus isolating the cross-correlated water–water H-bond stretch near 205 cm⁻¹. Which allowed us to quantify the changes in strength of orientationally cross-correlated H-bonds, and the number of such interacting H-bonds. We apply CVS to 2 M sodium salt solutions². The data reveal two distinct pathways by which anions modify the water HB network. Soft, polarizable anions induce large red shifts (up to -62 cm⁻¹ for I⁻) together with strong increase in cross-correlated intensity (up to +56% interacting H-bonds), consistent with charge-transfer mediated weakening of individual H-bonds accompanied by an increased concentration of correlated water–water interactions. In contrast, hard anions show only small frequency shifts and modest intensity changes, consistent with predominantly electrostatic perturbations. These contrasting molecular responses are rationalized using Hard–Soft Acid–Base (HSAB) theory³, showing that similar macroscopic trends can arise from fundamentally different microscopic mechanisms due to compensation between H-bond strength and the number of H-bonds.

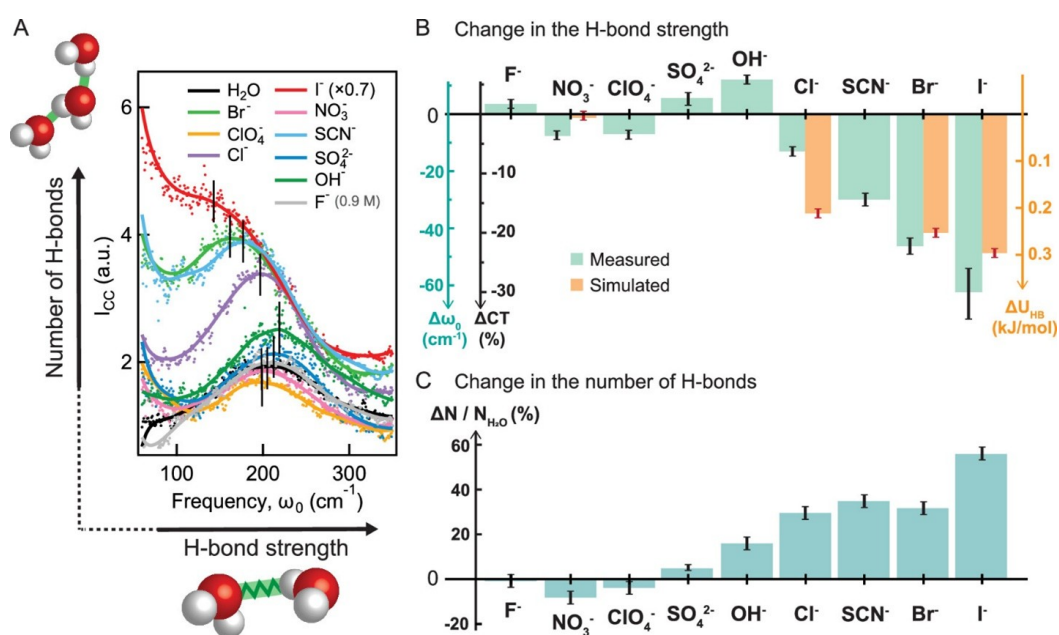


Figure 1: Ion-specific modification of the water–water H-bond network measured by CVS in concentrated sodium salt solutions. The cross-correlated H-bond stretch frequency shift reports changes in H-bond strength (and associated charge-transfer), while the intensity reports the relative change in the number of orientationally cross-correlated (interacting) H-bonds, revealing distinct behaviors for soft vs hard anions.

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Cold chemistry of single trapped H_2O^+ ions with neutral HD molecules in a cryogenic ion trap

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Precise quantum control of trapped molecules has emerged as a key technology in a wide range of applications such as precision spectroscopy, quantum computing, tests of fundamental physics, and state-to-state chemistry [1, 2, 3]. Trapped ions can also serve as an excellent platform for probing cold ion–neutral reactions, facilitating investigation at the low-temperature, low-density conditions characteristic of the interstellar medium (ISM).

In our recently developed cryogenic ion trap setup, we explored cold collisions between a single trapped H_2O^+ ion and cold HD molecules at a collision energy of 7 K. We demonstrated the isotope effect in this ion-neutral reaction by utilizing a single molecular ion, sympathetically cooled to a few millikelvin in a linear Paul trap, and non-destructively identifying its reaction products with the HD molecules. The experiments revealed a pronounced isotope effect at this low collision energy of 7 K, and were consistent with the computed values using the quasi-classical trajectories (QCT) method.

The current experimental setup is being developed with the primary goal of extending complex quantum logic spectroscopy (QLS) schemes to H_2O^+ ions. With the advancement in experimental techniques for the preparation, cooling, and coherent manipulation of molecular ions, precise quantum control of polyatomic molecular ions is feasible [2,4]. Such quantum control can open new prospects and allow state-selected chemistry studies in the future.

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Competition between photoionization and predissociation in electronically excited states of He₂ studied by simultaneous detection of metastable He fragments and He₂⁺ ions.

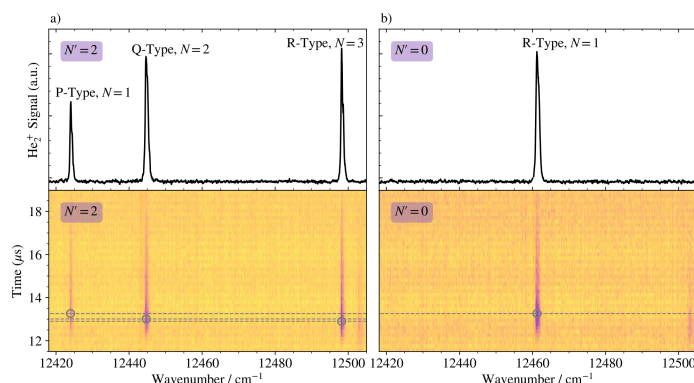
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He₂ has been called a "Rydberg molecule" because its ground electronic state is repulsive, whereas its electronically excited states are strongly bound and have Rydberg character [1,2]. In previous studies, only low vibrational levels ($v \leq 3$) of these electronic states have been studied, and almost no information is available on vibrational levels with $v \geq 4$.

We have recently demonstrated that 1+1' two-photon excitation via the $v = 3$ and 4 levels of the $c^3\Sigma_g^+$ state provides access to very high vibrational levels of high-lying Rydberg states of He₂ [3]. In the present work, we introduce an experimental approach to systematically study the high vibrational levels of electronically excited states of He₂ using 1+1' excitation via the $c^3\Sigma_g^+$ state. This approach relies on the simultaneous detection of photoionization and predissociation processes.

The well-characterized $c^3\Sigma_g^+(v = 4)$ [3-5] state was used to calibrate the experiment and demonstrate the very efficient detection of tunnelling predissociation in He₂ by monitoring the metastable He(1s2s) ³S₁ fragments on a microchannel-plate (MCP) detector. This detection method was then applied to study transitions to vibrationally excited levels of the $f'^3\Sigma_u^+$, $f'^3\Pi_u$, and $d^3\Sigma_u^+$ states. This contribution presents the main results of this study. As an example, the figure displays the spectra of the $f'^3\Pi_u(v = 3, N = 1, 2, 3) \leftarrow c^3\Sigma_g^+(v = 2, N = 0, 2) \leftarrow a^3\Sigma_u^+(v = 0, N = 1)$ transitions. In both panels, the upper spectrum corresponds to the He₂⁺ signal produced by photoionization, and the lower spectrum corresponds to metastable He* atoms produced by predissociation of the f' state. The maxima in the time-of-flight distributions are marked by open circles, and dashed gray lines indicate the corresponding flight times. The ability to detect dissociation products makes it possible to observe transitions to rapidly dissociating molecular states that cannot be observed by photoionization or laser-induced fluorescence.



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From Atomic Precision to Neuromorphic Computing: Ag₁₁ and Ag₁₂ Cluster-Based 2D Frameworks

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Assembling atomically precise metal nanoclusters into ordered low-dimensional solids remains synthetically challenging, yet it offers access to electronic materials with tunable properties at the atomic scale. We report 2D frameworks built from silver–thiolate cluster nodes, in which the cluster nuclearity is governed entirely by the choice of capping ligand. Benzenethiol affords a 2D framework material based on Ag₁₂ nodes, whereas the electron-poor 3,5-bis(trifluoromethyl)benzenethiol affords an analogous 2D framework material based on Ag₁₁ nodes; both structures were determined by single-crystal X-ray diffraction (Figure 1). Lateral two-terminal devices fabricated from the as-synthesized 2D framework materials exhibit resistive switching together with a region of negative differential resistance (NDR) and retain stable switching for more than 4000 cycles. The Ag₁₁-based device outperforms its Ag₁₂ counterpart, with a higher on/off ratio (≈ 600 versus ≈ 200) and a more pronounced NDR response. The Ag₁₁-based device was further examined for synaptic behaviour: under successive voltage pulses it shows analog potentiation and depression, and the experimentally measured conductance states, used as synaptic weights, allow an artificial neural network to reach a classification accuracy of about 84%, approaching the 93% obtained by conventional software training. These results show that ligand-directed control of cluster nuclearity is an effective strategy for tuning the electronic and neuromorphic response of cluster-based two-dimensional materials.

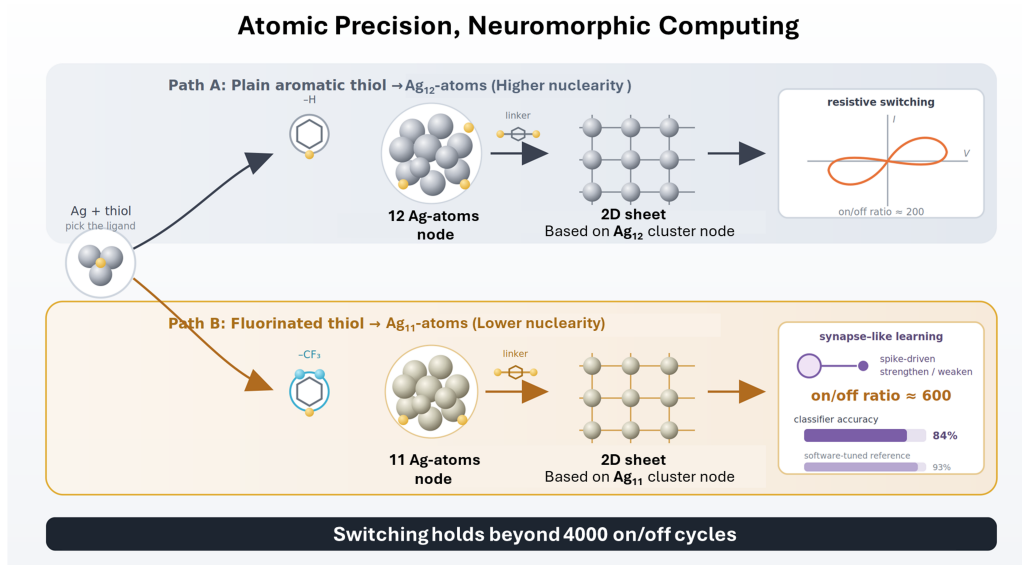


Figure 1. Schematic of ligand-controlled cluster nuclearity: a plain aromatic thiol yields Ag₁₂-based 2D frameworks, while a fluorinated thiol yields Ag₁₁-based 2D frameworks, and the resulting devices show resistive switching and synapse-like learning.

Nonadiabatic effects in spectroscopyK. Asnaashari¹, J. O. Richardson¹¹Department of Chemistry and Applied Biosciences, ETH Zurich

The breakdown of the Born--Oppenheimer approximation near avoided crossings and conical intersections leaves signatures in both frequency- and time-resolved molecular spectra. We present two complementary theoretical approaches for connecting electronic-state coupling to spectroscopic observables.

First, we introduce a nonadiabatic extension of ring-polymer instanton theory for calculating tunnelling splittings, which are observed directly in high-resolution rovibrational spectra. By treating the potential energy as an electronic operator, the method captures coupling between electronic states while requiring only adiabatic potentials, state overlaps, and nonadiabatic couplings from electronic-structure calculations. We benchmark the approach on a two-state model, where it reproduces exact quantum results, and apply it to ammonia inversion and tunnelling around the conical intersections of the allene cation.

Second, we introduce MASH-PLDM for simulating nonadiabatic dynamics and nonlinear optical spectra. The method uses two spin vectors to distinguish population and coherence contributions: populations evolve on individual adiabatic surfaces, while coherences evolve on the corresponding average surface. This allows the method to retain surface-hopping-like nuclear dynamics while improving the description of electronic coherence and recoherence compared with the original MASH method. We demonstrate the approach by simulating the pump--probe spectrum of a model of NaI.

Together, these methods enable the prediction of nonadiabatic signatures in both tunnelling splittings and nonlinear optical spectra.

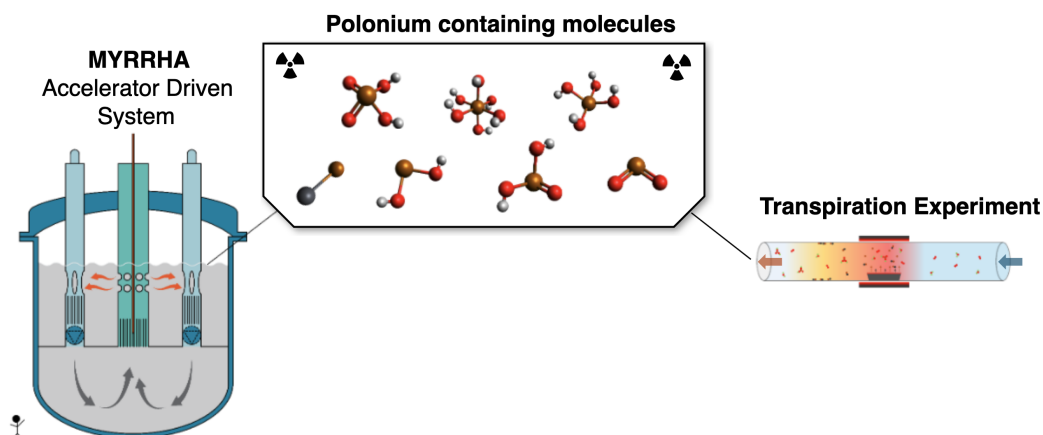
Elucidation of volatile Po species formed in liquid-metal-cooled nuclear reactors

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Polonium species are expected to be formed during operation of an accelerator driven system (ADS) within the framework of the MYRRHA nuclear reactor project and other liquid-metal-cooled nuclear systems. In ADS, the interaction of protons and neutrons with the coolant and spallation target material lead-bismuth eutectic (LBE) will generate hazardous amounts of $^{208-210}\text{Po}$. It is estimated that ca. 2 kg of Po will be present in LBE at the end of life, among other activation products. These radionuclides will be distributed between the liquid metal coolant and the cover gas of the reactor. The latter will consist of inert gases like N_2 or Ar but will also contain non-negligible amounts of $\text{O}_{2(\text{g})}$ and $\text{H}_2\text{O}_{(\text{g})}$ impurities. From literature it is known that ^{210}Po is released from LBE through at least 2 different mechanistic pathways.[1] At high temperatures (400 °C – 1000 °C), the logarithmic vapor pressure follows a linear trend with the inverse temperature. However, at lower temperatures (200 °C – 400 °C), the formation of Po-containing molecules with enhanced volatility occurs, being heavily influenced by $\text{O}_{2(\text{g})}$, $\text{H}_2\text{O}_{(\text{g})}$ and oxide layer formation on the liquid LBE. Elucidating the thermal release mechanism and finding ways of inhibiting Po release are not only crucial parts regarding the safe operation of MYRRHA but are also of importance for future Gen IV reactors, as well as small modular reactor designs.

In this work, we are developing a gas purification system capable of carefully controlling impurities such as $\text{H}_2\text{O}_{(\text{g})}$ and $\text{O}_{2(\text{g})}$ in the carrier gas at concentration levels in the ppb to ppm range, as well as O_2 dissolved in LBE. The latter will be measured with a custom-built oxygen-sensor, fabricated at SCK•CEN. Thus far, the system underwent several iterations of design and is in the final stages of construction with first experiments planned in summer 2026. This system will enable systematic control and variation of the carrier gas conditions in transpiration type evaporation experiments with Po-doped LBE.



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Cyclotron production of ^{44}Ti and gas-phase separation from bulk Sc in the context of $^{44}\text{Ti}/^{44}\text{Sc}$ generator system

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Scandium-44 (^{44}Sc) is a highly promising radionuclide for positron emission tomography (PET) due to its large positron-emission branching ratio of 94.278(11) %, a favourable half-life of 4.0420(25) h and its lanthanide-like coordination chemistry [1]. Furthermore, another scandium isotope, ^{47}Sc , has advantageous decay characteristics for targeted radionuclide therapy, making $^{44}\text{Sc}/^{47}\text{Sc}$ an ideal radiotheragnostic pair [2].

A promising production route of ^{44}Sc relies on the decay of the long-lived parent radionuclide titanium-44 (^{44}Ti , $t_{1/2} = 59.1(3)$ a). This decay chain forms the basis of a $^{44}\text{Ti}/^{44}\text{Sc}$ radionuclide generator system, enabling the continuous production and separation of ^{44}Sc . This generator can provide a long-term daily supply of ^{44}Sc without requiring an on-site cyclotron [2].

The development of such a generator system faces two major challenges: the cyclotron-based production of ^{44}Ti , which requires high proton flux and long irradiation time, and the optimisation of the radiochemical separation process [3]. The latter must ensure high molar activity of ^{44}Sc , minimal ^{44}Ti breakthrough, and long-term radiation stability of the separation phases [4].

Within this research project, the production of ^{44}Ti via the $^{45}\text{Sc}(p,2n)^{44}\text{Ti}$ reaction will be investigated. Thin scandium foils of 25 μm thickness will be irradiated at the IP2 72 MeV beamline of the Injector II cyclotron at the Paul Scherrer Institute (PSI). Here, an innovative liquid phase separation of titanium from the scandium targets is to be developed. Additionally, this research aims at developing a novel gas-phase separation process to isolate titanium, produced in high-energy spallation from irradiated bulk steel samples from PSI STIP-program in SINQ [5], as a source for the $^{44}\text{Ti}/^{44}\text{Sc}$ generator system [6]. The performance of this gas-phase approach will be evaluated against previously applied wet-chemistry separation processes.

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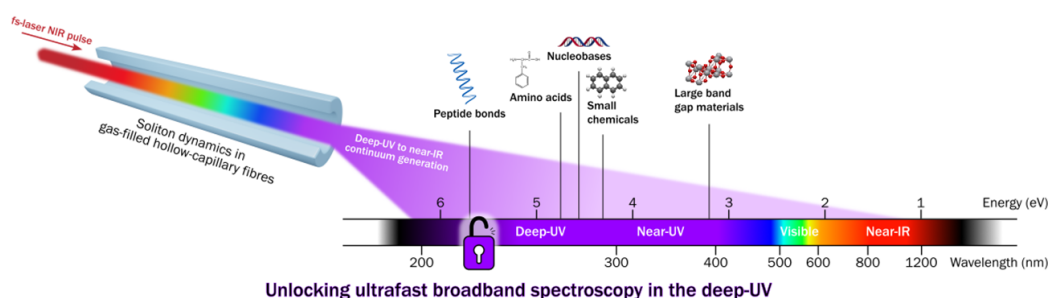
Mind the spectral gap: Extending ultrafast spectroscopy to the deep ultraviolet with stretched hollow-core fiber technology

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Ultrafast spectroscopy in the ultraviolet (UV) is an attractive tool to probe the dynamics of (bio)molecules via important UV-chromophores, such as peptide bonds, amino acids, nucleotides, and many organic ligands [1]. However, despite recent progress in photonic technology [2], the deep-UV region below 300 nm has remained largely unexplored, with only a few reports of broadband ultrafast spectroscopy setups and studies in this spectral region [3].

To extend the spectral range of ultrafast spectroscopy, we now employ a novel source of intense, broadband deep-UV pulses by exploiting soliton dynamics in gas-filled hollow capillary fibers (HCFs) [4,5]. Here, we present the implementation of an HCF-based transient absorption setup with ultra-broadband coverage (200-800 nm) that includes the entire deep-UV window (200-450 nm). We demonstrate the capabilities of this approach with a benchmark experiment on a well-studied Fe(II) spin-crossover complex that displays ultrafast dynamics encoded in the deep-UV. The results highlight the unique potential of HCF technology to extend ultrafast molecular spectroscopy to the deep-UV and expand its scope to study (bio)molecular dynamics in solution.



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Controlling Fe(II) spin-crossover dynamics through stereoselective ion pairing

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The spin-crossover dynamics of iron(II)-based coordination complexes have a tremendous potential for technological applications as switches and energy transducers [1]. To achieve this, a key challenge is to control the lifetime of the high-spin (HS) excited state in such complexes and suppress their fast ground-state relaxation [2]. In this respect, we have recently shown that controlling the chiral configuration of octahedral tris-chelate Fe(II) complexes through stereoselective ion pairing can extend their HS-state lifetime [3,4]. However the direct link between the stereoselective induction and HS-state relaxation has not yet been fully elucidated. To address this gap, we here investigate the HS state lifetime of iron(II)tris(4,4'-dimethyl-2,2'-bipyridine) ([Fe(II)(dm-bpy)₃]²⁺), associated for stereocontrol with the enantiopure TRISPHAT anions, and systematically tune the magnitude of the stereoselective induction via the solvent polarity. To this end, we measure the HS lifetime with femtosecond transient absorption in solvent mixtures of apolar chloroform and more polar DMSO. Varying the concentration of DMSO between 20% and 0% extends the lifetime of the HS state by multiple nanoseconds, more than a three-fold increase. These results provide an avenue for unravelling the direct coupling between the spin-crossover dynamics in Fe(II) complexes and their metal-centered chirality, with a view to control their HS state lifetimes.

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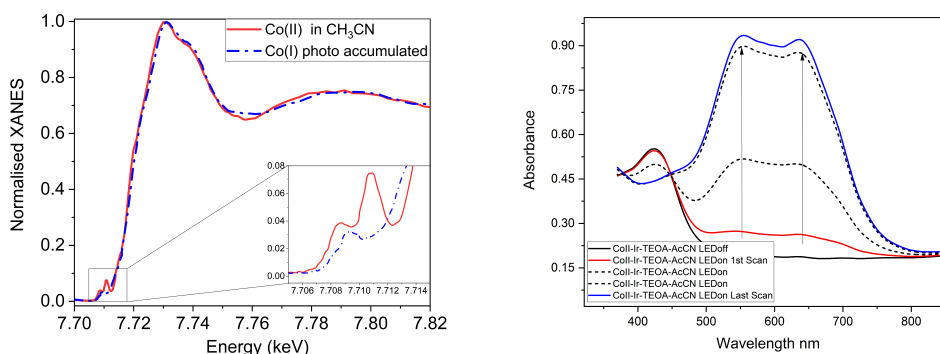
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Deciphering the Structure of H₂ Evolution Cobaloxime Photocatalysts with Multiconfiguration Calculations of Pre-Edge XAS

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Cobaloximes are widely studied as homogeneous catalysts for H₂ evolution^[1] and as biomimetic model molecules to study cobalamin-derived enzymes^[2]. Photocatalytic studies indicate the reduction of the initial Co(II) state to a transient, catalytically active Co(I) species^[3]. Solution-phase theoretical descriptions of both the resting and active state are highly inconsistent; reported Co co-ordination numbers range from 4-6 in literature resulting in competing mechanistic interpretations^[4]. Resolving this structural discrepancy is crucial to develop reliable theoretical reaction mechanisms and for rational catalytic design. We combine Co K-edge X-Ray Absorption Spectroscopy (XAS) with multi-reference Restricted Active Space Self Consistent Field (RASSCF) calculations^[5] to accurately describe the pre-edge region and enable structure-spectrum mapping of the photocatalyst Co(dmgbF₂)₂L_x (L: solvent, e.g. CH₃CN, x=0-2). A long-lived Co(I) state is photoaccumulated in the presence of a sacrificial electron donor. XAS of both states show a largely similar spectral shape, but the pre-edge region contains pronounced changes (Fig. 1).



Co(I) candidate structures have co-ordination numbers from 4-6; the 5-coordinated square-pyramidal model is found to be in best agreement with experiments. This is corroborated with Finite Difference Method (FDM) simulations of the XAS. Co(II) is found to be a similar square pyramidal geometry. However, large changes in Co-solvent bond length (0.2 Å) obtained from various density functionals are invisible to FDM simulations, but the minor changes in orbital covalency render them observable via RASSCF pre-edge simulations, highlighting the enhanced structural resolution possible from the pre-edge.

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A Rydberg-Stark single-beam approach to study the $\text{H}_2^+ + \text{H}_2 \rightarrow \text{H}_3^+ + \text{H}$ reaction

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The ability to control the translational motion of Rydberg atoms and molecules by Rydberg-Stark deceleration has enabled the study of several ion-molecule reactions at collision energies between $k_B \cdot 0$ K and $k_B \cdot 50$ K [1]. In these studies, a molecule or atom in a Rydberg state of principal quantum number $n \approx 30$ is employed in place of the ion. The Rydberg electron takes a “spectator role” [2] and at the same time shields the ion from stray electric fields, which allows one to precisely control the collision energies. An ion-molecule reaction of special interest is the $\text{para-H}_2^+(v^+ = 0, N^+ = 0) + \text{para-H}_2(v = 0, N = 0) \rightarrow \text{H}_3^+ + \text{H}$ reaction because it is a good candidate to study quantum effects caused by the wave character of the collision system at low temperatures. In particular, owing to its low reduced mass and strong exothermicity, it is an ideal reaction to verify the theoretical prediction of a twofold reaction-rate enhancement over the classical Langevin rate arising from s-wave scattering in the barrier-free charge-induced-dipole interaction potential of the collision partners [3]. This reaction-rate enhancement cannot be explained by classical capture models and is a signature of “quantum capture”.

The observation of quantum capture in an ion-molecule reaction was the main objective of a recent experimental study of the $\text{H}_2^+ + \text{H}_2 \rightarrow \text{H}_3^+ + \text{H}$ reaction by Höveler *et al.* using the Rydberg-Stark merged-beams approach [4]. However, a measurement of the full twofold rate enhancement was hampered by the collision-energy resolution of around $k_B \cdot 260$ mK of their experiment and by the para:ortho ratio of about 80 % : 20 % of their para- H_2 source. Here, we present a new experimental setup which relies on the Rydberg-Stark single-beam approach and features a high-purity continuous-flow para- H_2 source. This source allows us to realise a pulsed supersonic beam of H_2 in which more than 99 % of the H_2 molecules are in the rovibrational ground state. We show that, using a three-photon laser-excitation scheme, we can excite a fraction of the H_2 molecules in the supersonic beam to nf Rydberg states with a ground-state H_2^+ ion core and we demonstrate that, when exciting to the 31f Rydberg state, we can measure the rate of formation of H_3^+ ions with a collision-energy resolution of better than $k_B \cdot 10$ mK at a collision energy near $k_B \cdot 0$ K. Our current work focuses on measuring the rates of H_3^+ -ion formation at different collision energies by changing the relative velocities of the ground-state- H_2 and Rydberg- H_2 molecules in the supersonic beam with a Rydberg-Stark decelerator. We present possible electrode geometries for the Rydberg-Stark decelerator which aim at optimally controlling the relative translation motion of the reactants in our experiment.

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Photo-induced dynamics in liquid crystal chromophores investigated by UV-Vis femtosecond spectroscopy

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Abstract:

Photo-induced molecular reconfiguration in liquid crystal chromophores is a key factor influencing their excited-state behavior and electronic properties. Femtosecond UV-Vis transient absorption spectroscopy provide access to the controlled formation and concentration-dependent emergence of excimers in nCB liquid crystalline systems. This offer significant opportunities and allow in achieving a deep knowledge of the electronic processes guiding such molecular reconfiguration. This in turn will reveal new emergent electronic properties that such LC do not present in the ground state. for fundamental understanding and technological developments. In this work, we systematically investigate the ultrafast photophysical dynamics of cyanobiphenyl-based liquid crystals (5CB, 8CB & 8OCB), focusing specifically on the early-time molecular responses leading to structural changes and critical to excimer formation. Utilizing femtosecond transient absorption spectroscopy, we distinguish monomeric behavior from the onset of excimer formation, providing detailed insights into the underlying mechanisms and kinetics on the picosecond timescale. Our initial results emphasize the rapid isomerization and planarization processes occurring within the first tens to hundreds of picoseconds, forming a foundational understanding of how these structural changes facilitate subsequent excimer formation observed at longer timescales. Additionally, we examine the effect of increased concentration, which significantly enhances excimer formation, as evidenced by characteristic spectral shifts indicative of intermolecular interactions. This ongoing research aims to elucidate the relationship between molecular configuration, dynamics, and emergent photophysical properties in liquid crystals ultimately advancing liquid crystal-based photonic technologies.

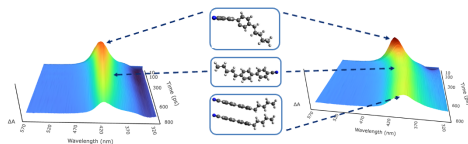


Fig: 3D transient absorption spectra of 5CB showing early-time isomerization in dilute solution (left) and concentration-dependent excimer formation at longer times (right), relevant for liquid-crystal photonics.

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Vibrationally Nonadiabatic Dynamics of (Floppy) Molecules in Liquid EnvironmentsH. Hoppe^{1,2}, J. O. Richardson¹, U. Manthe²¹ETH Zurich, Institute of Molecular Physical Sciences, Zurich, Switzerland, ²Bielefeld University, Theoretische Chemie, Bielefeld, Germany

Studying molecules in liquid environments is a powerful but challenging way to probe single-molecule properties and solvent-solute interactions. Sophisticated gas phase simulations of small molecules are commonly done in both chemistry and physics, while studies investigating the effect of liquid environments on dissolved molecules are scarce. Interesting solvent-solute systems include molecules dissolved in superfluid Helium, where it is assumed that the solvent interacts weakly with the solute. Another example is dissolving molecules in cold liquid Argon to study relaxation processes. In both regimes the accurate quantum mechanical treatment of the solute is required to obtain satisfying results, whereas the solvent can oftentimes be described classically^[1]. To this date, these simulations are very challenging due to the large number of degrees of freedom, the *floppiness* of both solute and solvent and the required accuracy of the interaction potentials.

This work is split into two parts: in the first part, a fully quantum-mechanical study of the interaction of Hydronium with Helium is presented. The solute-solvent interactions are described through a *vibrationally* diabatic representation, obtained via an *electronically* adiabatic interaction potential based on an accurate potential energy surface^[2]. Ro-vibrational energy levels of the H_3O^+ -He system are calculated and analyzed, revealing strong vibration-rotation coupling of the Hydronium with Helium.

In the second part, we investigate the dynamics of both HCl and DCl in liquid Argon. The relaxation rate of vibrationally excited HCl or DCl into their vibrational ground state is simulated. This project relies on a mixed quantum-classical description of the system treating the Argon classically and the HCl-subsystem quantum-mechanically. As before, the interaction between the two systems is modelled using a nonadiabatic representation based on an accurate electronic potential energy surface^[3]. The mixed quantum-classical dynamics are based on the *Mapping Approach to Surface Hopping*^[4]. The resulting relaxation rates are compared to experimental data.

In the future, both the methodology and the interaction potentials are to be used to further understand the dynamics of H_3O^+ in bulk Helium, as well as the properties of dissolved or confined molecules such as D_2O in H_2O .

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Accumulated Styrene Oligomers Suppress Divalent Cation Transport across Lipid Membranes Probed by Label-Free Second Harmonic Imaging

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Styrene oligomers are small hydrophobic degradation products of polystyrene that can accumulate within lipid membranes and alter their physical properties. While previous studies have shown that styrene oligomers affect membrane phase behavior and lipid packing, their effect on passive ion transport remains poorly understood. Here, we use wide-field second harmonic (SH) imaging to investigate how accumulated styrene oligomers influence divalent metal cation transport across model lipid membranes.

SH imaging is sensitive to interfacial water orientation and enables label-free visualization of membrane-potential heterogeneity and ion-induced changes in lipid bilayers. Building on recent work showing that divalent cations can permeate charged giant unilamellar vesicles through transient electrostatic-field-induced pores, we examine whether styrene oligomer incorporation alters this transport pathway. Lipid membranes containing increasing fractions of styrene oligomers were exposed to divalent metal cations, including Ca^{2+} , Mg^{2+} , Ba^{2+} , and Cu^{2+} , and the resulting SH intensity dynamics were monitored over time.

Preliminary measurements with Ca^{2+} show that styrene oligomers produce only modest changes in the average SH-derived membrane potential, but strongly suppress cation translocation. At high styrene oligomer loading, cation transport is nearly abolished. These results suggest that styrene oligomers impair membrane function not primarily by shifting the mean electrostatic potential, but by modifying the membrane's dynamic permeability landscape. We propose that styrene oligomer accumulation increases lipid packing and/or alters interfacial hydration, thereby inhibiting the transient defects required for divalent cation permeation.

This work provides a label-free physical-chemistry framework for understanding how plastic-derived molecular pollutants perturb membrane ion transport before causing gross membrane disruption.

Isotopic chirality, parity violation and structure of dichlorofluorophosphane from the analysis of high-resolution spectra and *ab initio* theory

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Parity violation leads to a fundamentally new isotope effect in molecules which are chiral by isotopic substitution [1–4]. In such isotopically chiral molecules electroweak quantum chemistry, which includes effects from parity violation of the weak nuclear interaction, predicts that the ground states are separated by a small parity violating energy difference D_{pv} on the order of aeV. This arises because different isotopes have different numbers of neutrons and thus have different weak nuclear charges. In contrast, ordinary quantum chemical theory, which is strictly parity conserving, predicts D_{pv} to be exactly zero by symmetry. The actual nonzero D_{pv} can be measured, in principle [5], but no successful experiment has yet been reported [3]. We have previously presented the first quantitative theoretical calculations of this effect for the isotopically chiral molecule $PF^{35}Cl^{37}Cl$ [2] as a prototype. In this context we have studied high resolution GHz and THz (FTIR) spectra of the isotopomers $PF^{35}Cl_2$, $PF^{35}Cl^{37}Cl$, and $PF^{37}Cl_2$ in natural abundance. We report here the results of an extended analysis of the GHz and THz (FTIR) infrared spectrum of dichlorofluorophosphane. The characterization of the ground state of $PFCl_2$ achieved through our study of the GHz spectrum [6] has made possible a detailed analysis of room temperature FTIR and supersonic jet cooled tunable diode laser spectra of the $PFCl_2$ isotopomers. The $PFCl_2$ spectra examined in the course of the present work have been measured with our Zurich GHz spectrometer, a Bruker IFS 125 HR(ZP 2001) Zürich Prototype Fourier Transform spectrometer (room temperature, 650–1000 cm^{-1} , resolution: 0.0015 cm^{-1}) and in a supersonic jet expansion ($T=15-20$ K) with our diode laser spectrometer between 830–834 cm^{-1} and 838–841 cm^{-1} . The results lead to a first accurate molecular structure of $PFCl_2$ and will be discussed in relation to our *ab initio* calculations and as they pertain to isotopic chirality, molecular parity violation, astrophysical spectroscopy, biomolecular homochirality, and the fundamental symmetries of physics and chemistry.

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Hydrogen Bond Cooperativity in Binary Liquids: A Spectroscopic and Molecular Dynamics Study of Formamide Mixtures

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Hydrogen bonds play a key role in stabilizing secondary structure of proteins, govern intermolecular interactions in solutions and solids, and underlie many of the chemical and physical processes that shape our world. While not as strong as covalent or ionic bonds, hydrogen bonds have a beautiful nature of being cooperative. Hydrogen-bond (H-bond) cooperativity is often studied in gas-phase clusters, where individual interactions can be isolated and analyzed.^[1] Bridging the understanding from gas-phase systems to condensed phases remains challenging, as local interactions in condensed phase are strongly coupled to the surrounding hydrogen-bond network and are continuously reshaped by thermal fluctuations and molecular dynamics.

By combining Raman spectroscopy, molecular dynamics simulations, and graph-theoretical analysis, we aim to probe and explore the structure, connectivity and complexity of hydrogen bond cooperativity in condensed phase. We use formamide as a model system, due to its complex hydrogen bond network^[2] and previously reported cooperativity^[3]. We explore how the introduction of a second component (methanol and acetone) perturbs intermolecular interactions and hydrogen bond cooperativity in formamide-based liquids.

We found that, hydrogen bonding in formamide forms a highly interconnected cyclic network that governs collective behavior. Methanol acts as an internal perturbation, integrating into the H-bond network and preserving its connectivity, hence produces uniform structural responses. In contrast, acetone behaves as an external perturbation, remaining outside the cyclic network and disrupting H-bond cooperativity, resulting in concentration-dependent structural changes. Local vibrations of formamide backbone probed by Raman spectroscopy show distinct response depending on the secondary liquid and its effect on hydrogen bond network, with acetone inducing red shift and a pronounced concentration dependence, while methanol produces concentration independent blue shift. Across all methods, the H-bond network response is governed by whether the perturbation is internal (integration) or external (disruption), rather than by simple changes in interaction strength.

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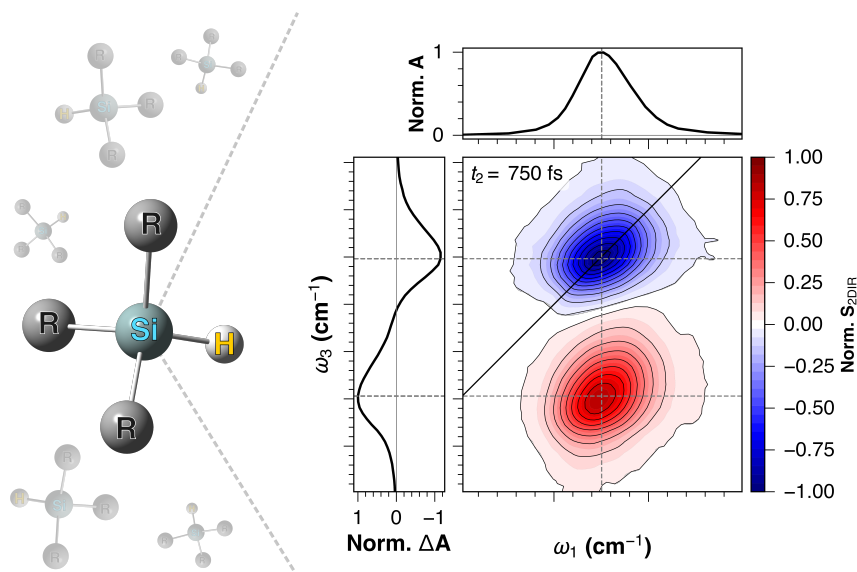
Vibrations Resolve Dissociations: A 2D-IR-Based Method to Determine Bond Dissociation Free Energies in Solution

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Accurate determination of bond dissociation free energies (BDFEs) is essential for the quantitative description of proton-coupled electron transfer (PCET) processes,¹ or the evaluation of hydricity.² Despite their fundamental importance, the direct determination of BDFEs remains experimentally and conceptually challenging. Conventional methodologies often rely either on equilibrium measurements employing reference compounds with established BDFEs, or on the construction of thermodynamic cycles.^{3,4} An alternative is to derive the BDFE from the corresponding bond dissociation enthalpy (BDE), however experimentally derived BDEs are typically obtained from gas-phase studies and therefore neglect solvation effects, whilst quantum-chemical predictions often show appreciable discrepancies relative to experimental benchmarks.¹

Our contribution to this field is a purely spectroscopic approach to the precise and easy estimation of BDEs in the solvents of interest. By employing two-dimensional infrared (2D-IR) spectroscopy, we successfully reproduced the BDEs of a range of silanes and subsequently expanded the available library by determining BDE values across multiple solvent environments. Furthermore, we report, for the first time, experimental BDEs for an additional derivative, showcasing the ability of our method to systematically investigate solvent and substitution effects on BDEs within and entire class of compounds. Given that specific solute-solvent interactions frequently limit the accuracy of purely computational methods or gas-phase measurements, this novel approach not only facilitates the identification of such interactions but also enables their direct characterization on picosecond timescales without the need for additional modifications.



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Investigations on Radionuclide Release Behavior for Lead-based Nuclear Reactors

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Lead-cooled fast reactors (LFRs) are one of the Gen-IV designs currently under development to address challenges such as reliability, proliferation resistance, economic competitiveness, and sustainability. Before their large-scale commercial deployment, comprehensive safety analyses are essential, including detailed evaluations of potential radioactive material dispersion during accident scenarios.

As a fission product, cesium (Cs) has been selected for detailed studies due to its significant radiological risk and volatility. The Henry's law constant for Cs in liquid lead (Pb) and lead-bismuth eutectic (LBE) has been determined using the transpiration method, providing critical data on the behavior of Cs under reactor conditions. Cs-134 was produced at PSI-SINQ's neutron irradiation facility and used as radioactive tracer during the transpiration experiments, allowing radioanalytical quantification of the evaporated Cs. The results obtained for the liquid Pb system are in very good agreement with the extrapolation of previously reported electromotive force data to the lower-temperature region. For LBE, our results show improved reproducibility compared to previously reported data. The thermodynamic data from this study enables a more quantitative assessment of radiocesium release potential and associated radiological impact.

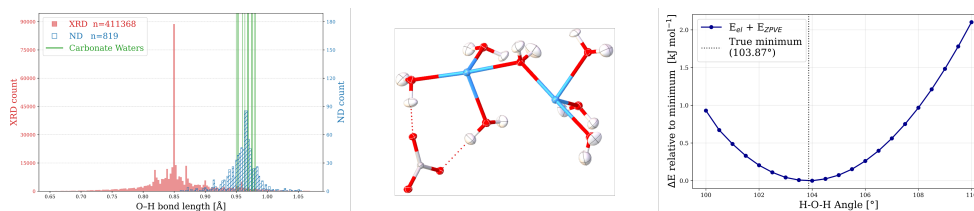
Furthermore, volatilization of polonium (Po) from Pb will be investigated due to its high radiotoxicity and its relevance for LFR safety assessments. Similar transpiration experiments are planned using Po-206 and Po-210 as radioactive tracers. Different methods for the preparation of homogeneous Po-Pb samples will be investigated, and the resulting thermodynamic data will be evaluated and compared with the reported data for similar LBE systems. In addition, the diffusion of Po in solid Pb and its segregation effect on Pb surface will be studied with advanced α -spectroscopy technique.

Overall, this research will provide critical insights into the behavior of Cs and Po in LFRs, supporting the development of robust safety protocols and improved reactor designs.

How Different Can Water Be?

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The distribution of covalent O–H bond lengths in water molecules within crystalline hydrates reported in the Cambridge Structural Database (CSD) demonstrates a significant discrepancy between the datasets of structures measured using Neutron Diffraction (ND, $0.961 \text{ \AA} \pm 0.024 \text{ \AA}$), and those determined by X-Ray Diffraction (XRD, $0.859 \text{ \AA} \pm 0.058 \text{ \AA}$), see Fig. 1a. Out of 220'000 hydrate structures in the CSD, 60'000 structures lie far outside the normal distribution of ND data, and are thus classified as artificially shortened bond lengths[1]. This is the result of the widespread use of the Independent Atom Model (IAM), which neglects chemical bonding. Therefore, these XRD structures are unfit for bonding analyses and necessitate re-refinement using Hirshfeld Atom Refinement (HAR). HAR is a refinement method, which is easily applicable to routine XRD data of sufficient quality. It yields hydrogen positions and anisotropic displacement parameters in agreement with ND results [1], and is therefore suited to be applied to a large number of the entries. Its effectiveness is exemplified by the crystal structure of sodium carbonate heptahydrate (Fig. 1b), which contains seven crystallographically independent water molecules coordinated to sodium, water, and carbonate ions. While all its water molecules differ substantially in their geometrical parameters (marked in green in Fig. 1a), all bond lengths are in agreement with ND results, highlighting the greater accuracy of HAR in comparison with the IAM used in standard XRD refinements.



At 104.27° , the equilibrium H-O-H bond angle of a water molecule in the gas phase, calculated at the gold-standard level of theory (CCSD(T)/def2-QZVP), does not reflect the observed H-O-H angle distribution found in water molecules within crystalline hydrates reported in the CSD ($107.57^\circ \pm 7.0^\circ$ for XRD and ND). This phenomenon was studied using potential energy surface (PES) scans of the H-O-H bond angle. A water molecule interacting with neighbouring water molecules through hydrogen bonding was scanned at CCSD/def2-QZVP (Fig. 1c). This PES proves water to be highly flexible, as distortion by $\pm 5^\circ$ of the optimal angle (103.87°) was associated with an energetic cost of 1.5 kJ/mol. When the effect of interactions with charged species is included, the PES plot changes significantly. Model systems were constructed based on the measured sodium carbonate heptahydrate. Calculations were performed at the B3LYP/def2-QZVP level of theory, which is planned to be increased to CCSD/def2-QZVP. When a formate anion is introduced to the system to approximate the interaction with carbonate, the H-O-H angle is compressed to $98.06^\circ (\pm 5^\circ \square 2.0 \text{ kJ/mol})$. This dramatic compression is the direct consequence of the negative charge of formate withdrawing electron density from the O-H bonds of water. In the case of Na^+ coordination, an optimised angle of 105.72° is calculated ($\pm 5^\circ \square 2.0 \text{ kJ/mol}$), producing a weaker distortion than formate. As Na^+ interacts with both oxygen lone pairs approximately symmetrically, it does not break the bilateral symmetry of the water molecule, and the angular potential is therefore not strongly perturbed. These results demonstrate that the H-O-H angle of water is not a fixed molecular constant but an environment-sensitive parameter of the intermolecular interactions.

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Internal conversion in naphthalene with non-adiabatic instanton theoryS. L. Krug¹, M. R. Fiechter¹, J. O. Richardson^{1*}¹Department of Chemistry and Applied Biosciences, ETH Zurich, Switzerland

Radiationless decay competes with light emission across many applied fields, such as organic electronics and photovoltaics. Whenever an excited molecule returns to its ground state, internal conversion drains population that would otherwise be emitted as light [1]. Controlling this loss channel is central to organic light-emitting diodes and light-harvesting materials, while the same process underlies the photostability of UV-absorbing molecules. Naphthalene is the parent of the acene family on which many of these materials are built and a prototypical aromatic for radiationless transitions, making it a natural model system.

I intend to approach the internal conversion in naphthalene from the perspective of instantons, and non-adiabatic instanton theory in specific: here, one locates an optimal, local tunneling path from a reactant to a product PES. This instanton can be characterized as a stationary-action path — minimal with respect to the hopping point from one PES to the other and a saddle point in the imaginary time it takes. Beyond a substantial reduction in computational complexity, it grants a physical interpretation in terms of classical mechanics and, by doing so, insight into the reaction mechanism [2]. However, locating an optimal tunneling path between two different surfaces even in simple systems can be very intricate. So intricate, in fact, that Ansari et al. [3] discovered a special instanton even just in case of a two harmonic oscillators. While fully analytical, this treatment restricts application and insight to systems that behave sufficiently harmonic.

Real systems, however, are rarely purely harmonic, and the internal conversion in naphthalene is such a case, where inherent anharmonicities appear to shape an instanton behavior different from those encountered previously. In this talk, I want to discuss the difficulties and insights from an analytical instanton treatment of two Morse oscillators, using the example of internal conversion in naphthalene.

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Stepwise ligand engineering on atomically precise gold nanoclusters

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Sequence defined materials^[1,2] are essential for a wide range of applications such as sensing,^[3] biocatalysis^[4] and drug delivery.^[5] Synthesis of these materials are executed either in solid phase (SPPS) or in solution through coupling reactions between a carboxylate (-COOH) and an amine (-NH₂) group to form an amide bond (-CONH-). Our group is interested in the physicochemical properties of water soluble atomically precise gold nanoclusters such as Au₂₅(SR)₁₈ (SR: captopril, L-glutathione) and its applications in (chiral) sensing^[6] and medicine.^[7] To investigate the fundamental concepts of chirality of the secondary coordination sphere of such atomically precise nanoclusters we propose a concept that relies on the building up of sequence defined oligopeptides on the surface of nanoclusters (Figure 1). In this poster presentation, I will discuss the synthetic route and some of our initial findings.

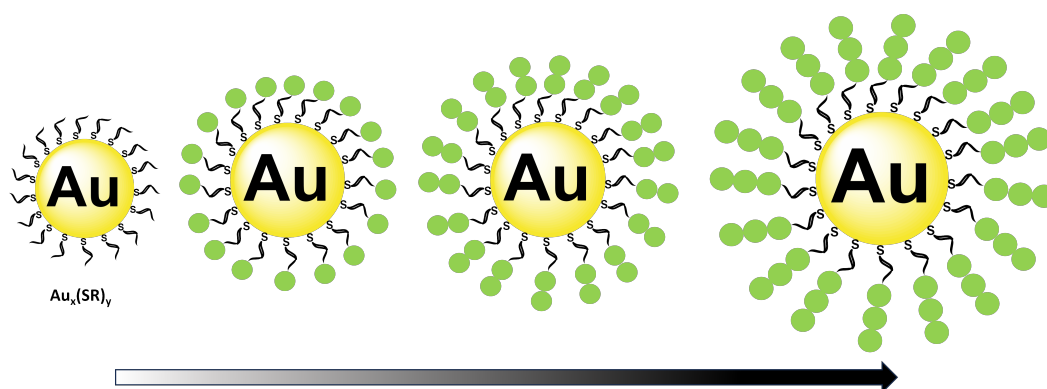


Figure 1. Sequence defined atomically precise gold nanoclusters

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>Mechanistical insights to optical hyperpolarization techniques for dye sensitized solid-state nuclear magnetic resonance

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Solid-state nuclear magnetic resonance (NMR) enables the study of complex systems ranging from membrane proteins over batteries to heterogeneous catalysts in their native environment. Its range of application could be widened even further if the sensitivity limitation, caused by the small energy gap of the probed spin states, could be overcome.^{1,2} One avenue to alleviate this issue is hyperpolarization. These techniques increase the sensitivity by transferring polarization from a highly polarized source to the nucleus of interest.

In this context, optically induced hyperpolarization techniques are particularly promising, since they can in principle yield a maximum ¹H NMR signal enhancement of a factor $\epsilon \sim 10400$ at 9.4 T and 100 K, i.e. 100% nuclear spin polarization. One of these methods is photochemically induced dynamic nuclear polarization (photo-CIDNP), which requires light irradiation of the sample, and can be active in crystalline and amorphous materials.^{3,4}

We recently demonstrated that photo-CIDNP can also be utilized to generate ¹H bulk hyperpolarization.⁵ Indeed, in these experiments ¹H hyperpolarization was generated locally using small molecular donor-acceptor molecules and distributed to the bulk via ¹H-¹H spin diffusion opening the perspective to take advantage of the same workflow today used in microwave driven MAS DNP.² We observed ¹H bulk hyperpolarization with enhancement factors of $\epsilon = 100$ at magnetic fields as high as 21.1 T.⁶

Following these milestone results, we have recently extended the theoretical photocycle description of photo-CIDNP in solids establishing a platform that allowed us the development of a series of design principles to improve future donor-acceptor systems.⁷ Building on this we have now introduced new dye molecules with improved performance, which led to ¹³C polarization levels of up to 16 % at 14.1 T corresponding to a signal enhancement of about 4500. Here, we will show these latest results and elucidate how theory and experiment can be combined to understand the mechanism of the photocycle, and use this knowledge to improve the performance of optical hyperpolarization via photo-CIDNP.

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Probing the supported Pt-H/solvent interface by in situ ATR-IR spectroscopy

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Hydride species represent the activated form of hydrogen on metal surfaces and provide a direct, sensitive probe of hydrogen activation, surface electronic structure, nano-particle dynamics, and hydrogen availability, making them central to understanding catalytic reactivity and stability in the heterogeneous hydrogenation and hydrogenolysis reactions of a wide range of organic molecules. It has been demonstrated that supported Pt nanoparticles (NPs) undergo electronic and morphological reconstruction which is related to the support, adsorbate, and reaction conditions. In this context, the Pt-hydride (Pt-H) system was extensively investigated both theoretically and experimentally, especially by means of X-ray absorption spectroscopy (XAS), Infrared and inelastic neutron scattering (INS) spectroscopy. While XAS provides direct information on the change of oxidation state and coordination environment of Pt in the presence of hydrogen H₂¹, vibrational spectroscopies have the capability to discern between different types of surface Pt-H surface species (i.e. linear, multicoordinated species). INS experiments had identified vibrational modes of linear and multicoordinated hydrides as a function of hydrogen coverage.² Attenuated total reflectance infrared (ATR-IR) spectroscopy was used to monitor adsorption-desorption of H₂ in liquid phase, using cyclohexane.³

In this work, ATR-IR spectroscopy was selected for its sensitivity to distinct Pt-H surface species, whose vibrational signatures reflect changes in local and electronic environment at the solid-liquid interface, where catalysis takes place.³ Using a custom flow cell (70 °C, 0.4 mL/min), H₂-saturated solvent was continuously flowed over Pt/Al₂O₃, enabling in situ observation of increasing coverage of Pt-H species at the solid-liquid interface. Pt-H species formed after a short induction time in which water formation was detected in the selected solvents (cyclohexane, isopropanol, and water), indicating the occurrence of reduction before hydride formation. During desorption in Ar-saturated solvent, hydrides rearranged before desorbing - a process that differed between apolar and polar solvents, consistent with preferential stabilization of polar Pt-H species in polar solvents. The results demonstrate that solvent nature plays a role in the distribution of hydride species and in maintaining Pt NPs in a partially hydrogen-solvated state. These effects are attributed to competitive adsorption, solvent polarity, and direct solvent-catalyst interactions⁴ - including the potential role of isopropanol as a hydrogen donor. These findings offer new insights into catalyst reactivity and stability under operando conditions, with implications for the broader understanding of liquid-phase heterogeneous catalysis.

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SAXS and SANS Guided Design of Biomimetic Lipid Nanoparticles

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Self-assembled structures at lipid–water interfaces play a central role in biological systems. These ordered phases can solubilize polar, nonpolar, and amphiphilic components, making them attractive for applications in nutrient and drug delivery. The project focuses on developing pH-responsive interfaces of oleic acid and dioleoylphosphatidylcholine (DOPC) that can be exploited for functional applications. The rational design of these self-assembled structures depends on a molecular-level understanding of structural response mechanisms. Beyond molecular composition, surface interactions, spatial confinement and hierarchical structuring play a decisive role in directing the functional behavior of these materials.

This presentation demonstrates pH- and composition-responsive lipid/water interfaces formed by dispersed oleic acid/DOPC self-assemblies in excess water. Using in situ SAXS and SANS, combined with selective deuteration and solvent-contrast variation, we analyze the formation of self-assembled structures with temporal and compositional resolution. Supported by numerical data modeling, we map the distribution of molecules within these systems, aiming to understand self-assembly mechanisms and create a multi-dimensional phase diagram with detailed structural assignments at the mesoscale.

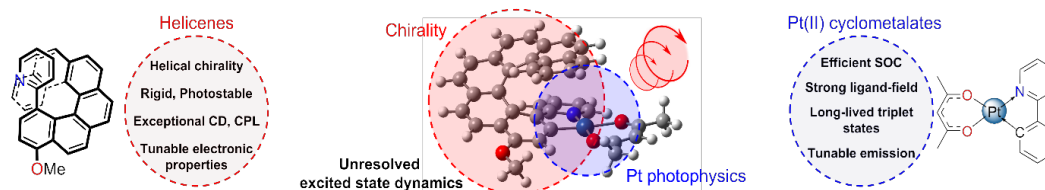
The structural transformations are interpreted within the critical packing parameter framework and correlated with intermolecular interactions. Building on these findings, we propose advanced design principles for creating adaptive, biomimetic nanomaterials with potential for application in nutrient and drug delivery.

Resolving the ultrafast spin-state dynamics driving the chiral luminescence of a Platinum-[6]helicene complex

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Cyclometalated Pt(II) complexes are highly efficient phosphorescence emitters with promising applications in organic light-emitting diodes and optical sensing.^[1] Importantly, the triplet-state dynamics that govern their luminescence properties sensitively depend on the ancillary and cyclometalating ligands,^[2] a feature representing both an advantage and a challenge. In fact, while selective ligand modifications enable tuning the relative energies and spin-orbit coupling constants between the involved singlet and triplet states,^[3] the complexity of the ensuing ultrafast spin-state dynamics continues to limit the mechanistic understanding and rational design of their emission properties.



To address this gap, we use broadband transient absorption (TA) spectroscopy (250 – 900 nm) from the femto- to the microsecond regime, together with extensive TD-DFT calculations, to map the complete formation and relaxation mechanism of the luminescent triplet state of a prototypical cyclometalated Pt(II) complex, (acetylacetonato)Pt-[6]helicene.^[4] The chirality of its ligand system induces circularly polarized phosphorescence, which, along with a strong mixing between ligand- and metal-based states, highlights the need to elucidate the coupling between structural and electronic degrees of freedom in the emission process. We find that its lowest-energy singlet state is deactivated on the 1-ps scale by an intersystem crossing (ISC) to the triplet manifold. Supported by the TD-DFT calculations and solvent-dependent TA measurements, we resolve a cascaded triplet-state relaxation on the 10-ps scale, from the first excited state T_2 to the lowest-energy state T_1 , followed by structural relaxation to its minimum-energy configuration, from where phosphorescence emission takes place on the 10- μ s scale. Notably, we find that photoexcitation of higher-lying singlet states enables access to a parallel sub-picosecond ISC to T_n , which converts to T_1 on the nanosecond timescale and thus acts as a triplet-state reservoir.

More generally, our results establish a comprehensive mechanistic picture of the ultrafast triplet-state dynamics that govern the luminescence properties of a prototypical cyclometalated Pt(II) complex. This opens the path to elucidate their dependence on structural ligand modifications, such as the extension of its chiral helicene ligands, with a view to further improving the rational design of their emission properties.

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Perturbative Treatment of Initial-State Anharmonicity in Vibronic Spectroscopy Using Hagedorn Wavepackets

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In the time-dependent approach, vibronic spectra are computed from the autocorrelation function of a nuclear wavepacket promoted from an initial to a final electronic state and subsequently evolved in time. While anharmonicity of the final-state potential energy surface is routinely included in these calculations, the initial surface is usually assumed to be harmonic, [1] crudely neglecting the additional structure of the anharmonic initial states. Here, we examine the role of initial-state anharmonicity within a perturbative framework: the vibrational wavefunction is corrected using time-independent perturbation theory and represented in the multidimensional Hagedorn wavepacket basis, [2-5] allowing systematic inclusion of non-Gaussian contributions with almost no additional computational overhead. Applications to realistic anharmonic systems show that even low-order corrections to the initial state markedly improve agreement with exact quantum or experimental spectra, particularly for single vibronic level transitions. These results demonstrate that weak-to-moderate anharmonic distortions of the initial potential energy surface can be captured accurately and efficiently within low-order perturbation theory using Hagedorn wavepacket dynamics.

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Thermoresponsive polymer nanoassemblies in complex biological media

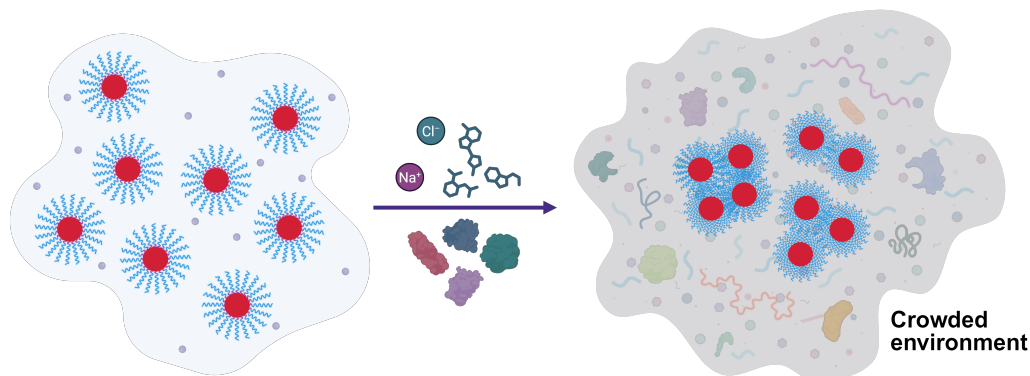
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Thermoresponsive polymers exhibiting lower critical solution temperature (LCST) behavior are widely explored for biomedical applications, yet their phase transitions are typically evaluated under simplified aqueous conditions which poorly mimic the complex biological environment. This overlooks the potential influence of biologically relevant ions, small molecules and macromolecules present at high concentrations in vivo.^{1,2} Here, we systematically investigate how polymer architecture and medium complexity jointly govern LCST in poly(di(ethylene glycol) methyl ether acrylate) (PDEGA)-based homopolymers and amphiphilic block copolymer nanoassemblies.

A library of PDEGA homopolymers and amphiphilic poly(butyl acrylate)-*block*-PDEGA (PBA-*b*-PDEGA) copolymers was synthesized using RAFT polymerization, enabling systematic variation of molecular weight, end-group functionality, and block composition. Thermoresponsive behavior was evaluated across environments of increasing complexity, from salts and small solutes to macromolecular crowders, human serum, and cell lysate.

Our findings reveal that the phase transition temperature determined in diluted aqueous solutions does not reliably predict phase transitions in self-assembled systems or biologically relevant environments. While molecular weight and end-group chemistry define baseline phase transition temperature of homopolymers, incorporation into amphiphilic block copolymers and subsequent self-assembly enhances sensitivity to the surrounding medium. Under biologically relevant conditions, the phase transition temperature of nanoassemblies can be reduced by more than 20 °C, effectively rendering these systems crowding-responsive. These results highlight the importance of evaluating thermoresponsive nanomaterials under conditions that more closely mimic physiological conditions.



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Organic Semiconducting Polymers as Photocatalysts for Green Hydrogen Production: Charge Dynamics in a PBDTTTPD:PNDI2HD-T Bulk Heterojunction

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With the depletion of fossil fuels and the growing impact of global warming, photoelectrochemical water splitting as a source of green hydrogen has gained significant importance as a renewable energy source. Historically, inorganic materials such as TiO₂ were employed, however, they have been proven inefficient due to their low absorption of visible light. Unlike inorganic materials, organic photocatalysts absorb significantly more visible light owing to their tunable bandgap. Furthermore, organic semiconductors are usually made of lightweight, low-cost raw materials with simple synthetic routes. Additionally, they allow for easy and accessible molecular modification to improve photoconversion by fine-tuning the levels of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) while posing a lesser environmental hazard.

In this study, the two semiconducting polymers PBDTTTPD and PNDI2HD-T were studied. When combined in a bulk heterojunction, they are promising candidates for photocatalytic water splitting. Transient absorption spectroscopy was employed to probe the nature and dynamics of charges generated upon photoexcitation under varying conditions. To identify the spectral signatures of polarons, the transient spectra were overlaid with those obtained from electrochemically doped films. Complementarily, photocurrent measurements under sustained illumination provided insight into the population of long-lived, mobile charge carriers.

Overall, these methods offered a comprehensive picture of the charge generation, separation, and transport dynamics governing the photocatalytic performance of the blend.

Mechanistic insights into oxidative and non-oxidative *n*-butane dehydrogenation over Cu-mordenite

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Selective dehydrogenation of light alkanes to terminal olefins remains a major challenge [1], as conventional catalysts typically require high temperatures and often suffer from limited regioselectivity, secondary isomerisation, cracking, and catalyst deactivation. Cu-exchanged zeolites have recently emerged as promising materials for low-temperature alkane dehydrogenation in chemical looping operation [2]. Here, we compare oxidative and non-oxidative dehydrogenation of *n*-butane over Cu-exchanged mordenite using *in situ* solid-state MAS NMR, FTIR spectroscopy and fixed-bed chemical looping experiments.

The use of ¹³C-labeled *n*-butane enables direct identification of butene isomers and Cu(I)-olefin π -complexes formed under reaction conditions. Two distinct dehydrogenation regimes are observed. Under oxidative conditions, Cu(II)-oxo sites initiate butane dehydrogenation at approximately 373 K and form 1-butene exclusively in the low-temperature regime. In contrast, non-oxidative dehydrogenation over Cu(I) sites becomes significant above approximately 448 K and produces a mixture of 1-butene, *cis*-2-butene, and *trans*-2-butene. These results show that 2-butenes are primary products of the Cu(I)-mediated pathway rather than products of rapid secondary isomerisation.

Spectroscopic evidence further indicates that butane forms pre-reaction complexes with copper sites, with preferential interaction involving terminal CH₃ groups, rationalising the high selectivity toward terminal C-H activation. Each oxidative dehydrogenation event reduces neighbouring Cu(II)-oxo sites to Cu(I), dynamically generating the active centres responsible for the non-oxidative pathway. Reactor experiments reveal that strong Cu(I)-olefin interactions can impose diffusion limitations in mordenite pores. These findings establish copper redox chemistry as a key factor controlling activity and regioselectivity and highlight Cu-mordenite as a platform for low-temperature, selective terminal olefin formation.

Does cholesterol distribute symmetrically across liposome leafletsC. Rani¹, P. Singh¹, S. Roke^{1*}

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Cholesterol is a key regulator of membrane structure and function, actively modulating lipid packing, phase behaviour, membrane rigidity. In plasma membranes, it also plays an important role in mechanical coupling between the two leaflets. However, how cholesterol distributes across the two leaflets of bilayer membranes remains debated. This is important because cholesterol asymmetry can generate differential stress across the bilayer, making one leaflet more ordered, more condensed, or more mechanically stressed than the other. The conventional picture is that cholesterol resides in a leaflet, with its -OH group positioned near the lipid headgroup and its sterol rings buried among the hydrocarbon chains. In a symmetric bilayer, cholesterol is generally expected to distribute symmetrically because of its rapid flip-flop between leaflets. In asymmetric membranes, however, cholesterol may preferentially partition into the leaflet where it relieves lipid packing stress or curvature imbalance. Its distribution is therefore expected to depend on lipid composition, leaflet stress, and curvature. Existing approaches to probe cholesterol placement like X-ray and neutron scattering, NMR, MD simulations, fluorescence-labelled cholesterol, supported bilayers, substrate-based AFM, and cyclodextrin-mediated exchange can be highly informative but many of these methods are either indirect, model-dependent, or perturbative. Ideally, cholesterol asymmetry should be measured non-perturbatively in freely suspended membranes that remain close to their native state.

Here, we use sum frequency scattering (SFS) spectroscopy to probe cholesterol-induced asymmetry in freely-suspended liposomes. Since second-order nonlinear optical responses vanish in centrosymmetric media, SFS is intrinsically sensitive to interfacial symmetry breaking, making it well suited for detecting leaflet-level molecular asymmetry in curved membranes without fluorescent labels, substrates, or immobilisation. We apply SFS to liposomes composed of one or two lipid types with cholesterol. For most lipid compositions studied, cholesterol appears to distribute predominantly symmetrically across the bilayer, as indicated by the absence of a measurable interfacial SFS response. In contrast, DOPC:DPPC liposomes, which form a symmetric bilayer in the absence of cholesterol, develop a strong cholesterol-associated SFS response upon cholesterol incorporation. This response closely resembles cholesterol SFS response, indicating asymmetric cholesterol across leaflets. We further examine this behaviour using curvature and packing arguments to understand why DOPC:DPPC:cholesterol membranes promote asymmetric cholesterol distribution, whereas other lipid combinations do not. Finally, we investigate the interaction of methyl- β -cyclodextrin with cholesterol-containing liposomes. Although cyclodextrin extracts cholesterol from the membrane, the SFS response shows that membrane asymmetry can persist, either because cholesterol extraction is incomplete or because lipid asymmetry remains after cholesterol removal. Overall, our results show that cholesterol distributes predominantly symmetrically in single-component lipid membranes, while in mixed membranes its transbilayer distribution depends sensitively on lipid-cholesterol interactions, packing stress, and curvature balance.

Controlled laboratory astrochemistry: Ion–molecule chemistry of CO^+ with neutral H_2O

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The chemistry and chemical composition of water-rich comets have long been of interest to planetary scientists and observational astronomers alike. Among the key processes in the coma of outgassing comets, the chemistry involving CO^+ and H_2O represents an important set of secondary reactions that contribute significantly to the overall chemical reaction network.^{1,2} The reaction also plays a major role in the carbon–oxygen chemistry of photodissociation regions (PDRs) in space.³ It proceeds via two competing pathways, charge transfer and bimolecular reaction, that produce H_2O^+ and HCO^+ , respectively. Both products may subsequently undergo further reactive collisions with neutral H_2O to form H_3O^+ . Under controlled laboratory conditions, we investigate the reaction rates and branching ratios of the $\text{CO}^+ + \text{H}_2\text{O}$ reaction, providing key constraints on the underlying chemistry with the aim of improving astrochemical models of these regions of space.

In this work, we use a linear Paul trap to confine CO^+ ions within a Ca^+ Coulomb crystal and subsequently react them with neutral H_2O , with control over its rotational temperature. Indeed, we compare reaction rates and branching ratios for water with thermal rotational distributions at 298 K and 13 K—representative of cometary comae and cold interstellar environments such as molecular clouds. We further refine our approach by separating *para*- and *ortho*- H_2O in a molecular beam using an electrostatic deflector, enabling state-resolved studies of the reaction.⁴ The kinetics and branching ratios are determined by analysing reactant and product ion signals following ejection of the ion crystals as a function of reaction time using mass spectrometry.

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Demonstration of sub-Doppler XUV spectroscopy with a spectral bandwidth of 20 MHz

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The ionisation energies of many atoms and molecules lie in the vacuum ultraviolet (VUV) and extreme ultraviolet (XUV) parts of the electromagnetic spectrum, which correspond to wavelengths (frequencies) of light of <200 nm ($>1.5 \times 10^{15}$ Hz) and <105 nm ($>2.9 \times 10^{15}$ Hz), respectively [1]. Laser radiation generated at these wavelengths can therefore be utilised to perform single-photon excitation from the ground electronic state of an atom or molecule to highly excited electronic states, including direct excitation to Rydberg states with a large value of the principal quantum number, n [1]. However, although VUV/XUV laser sources with < 250 MHz bandwidths have been achieved [2-6], large Doppler broadening of transitions at VUV/XUV wavelengths (with Doppler widths typically >100 MHz) often limit the achievable resolution of single-photon VUV/XUV spectroscopy. Additionally, large Doppler shifts can result in >100 MHz systematic shifts of measured transition frequencies in the VUV/XUV.

Here we demonstrate a technique for achieving sub-Doppler laser-bandwidth limited spectral resolutions in VUV/XUV spectroscopy. This method is based on combining an imaging-assisted single-photon Doppler-free spectroscopic technique, recently developed for precision Rydberg-state spectroscopy [7], with a long-pulse-length (50 ns) Fourier-transform limited pulsed VUV/XUV laser. Using (1+1') REMPI spectroscopy of the $(4p)^6\ ^1S_0 \rightarrow 6s'\ [^2P_{1/2}]_{J=1}$ transition of Kr, with XUV light generated at 95 nm, we observed spatially-dependent Doppler shifts using this imaging detection method, which arose from the interaction of the laser with a pulsed supersonic beam of Kr. The range of Doppler-shifts measured spanned 80 MHz. Additionally, in the different spatial detection regions of the imaging detection we could observed spectral lines with a sub-Doppler full-width half maxima bandwidths of down to 20 MHz, which was primarily limited by the Fourier-transform limited XUV laser pulse bandwidth.

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Investigating Solvent-Assisted and Design-Driven Proton Transfer Dynamics via Transient Vibrational Spectroscopy

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Photoinduced proton transfer (PT) was investigated in two molecular systems using transient vibrational spectroscopy supported by density functional theory calculations. In 1,1'-bi-2-naphthol (BINOL), PT is solvent-assisted, whereas in the designed molecular photoswitch 8-(benzo[d]thiazol-2-yl)quinolin-7-ol (HQBT), a proton crane enables long-range intramolecular PT.

Photoinduced reactions in BINOL have been linked to intramolecular PT processes, with previous studies suggesting a strong influence of solvent-mediated mechanisms and hydrogen-bonding networks [1]. We investigate the influence of solvent and isotopic substitution on these dynamics in acetonitrile-d₃, methanol, methanol-d₁, and mixtures containing controlled amounts of H₂O or D₂O. In methanol, relaxation of the sub-nanosecond fluorescent excited state leads to the formation of a long-lived intermediate for approximately one third of the initially excited population, with complete recovery of the ground state occurring within 100 ns. The intermediate population increases upon addition of H₂O. In methanol-d₁, a bleach feature in the OH bending region persists up to microseconds after the decay of the intermediate state. Addition of D₂O enhances both the intermediate population and the persistent bleach, indicating a common underlying process. In acetonitrile-d₃, both signals are observed but only after addition of D₂O in molar concentrations. We assign these observations to solvent-assisted PT from the alcohol to the naphthol moiety, followed by partial deuteration of the aromatic ring. Contrary to previous assumptions, our results indicate that H/D exchange can already occur in neat methanol and that the fraction of molecules undergoing transient PT is substantially larger than anticipated from steady-state measurements.

In contrast, HQBT is a molecular photoswitch in which a proton crane was designed to enable long-range intramolecular PT upon photoexcitation [2]. Excitation of the enol tautomer (off-state) initiates ultrafast intramolecular PT from the stator to the rotor moiety. Rotation of the rotor moiety in the electronically excited state subsequently enables efficient long-range intramolecular PT to the ketone form (on-state) of the molecule upon relaxation to the electronic ground state. Vibrational signals in combination with DFT-calculations indicate an equilibrium between two ketone forms in the switched state of HQBT, which re-tautomerizes back to the original enol form on a 10 second timescale at room temperature. These findings show how both solvent-assisted environments and molecular design can control PT pathways and transient-state populations in photoactive molecular systems.

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Electrochemistry of Homologs of Roentgenium – the ELCHOR project**L. Saxer^{1,2}**, P. Steinegger^{1,2}¹Laboratory of Radiochemistry, Paul Scherrer Institut, ²Department of Chemistry and Applied Biosciences, ETH Zürich

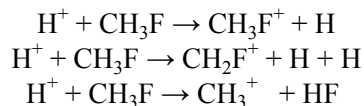
Research into the synthesis of new elements has expanded the periodic table with the currently heaviest element Oganesson (Og, $Z = 118$). Driven by technological advancements of accelerator facilities, the discovery of elements has outpaced their chemical characterization. Investigating these species is of great fundamental interest for furthering our understanding of relativistic effects. The chemical properties of so-called superheavy elements (SHEs, $Z > 103$) are most strongly affected by those effects.^[1] One major obstacle regarding the chemical characterization of SHEs has been the availability of suitably long-lived isotopes.^[2] Despite the continued discovery of new isotopes with longer half-lives, SHEs Meitnerium (Mt, $Z = 109$), Darmstadtium (Ds, $Z = 110$), and Roentgenium (Rg, $Z = 111$) remain a chemical blind spot in the periodic table of elements.^[3] This is also connected with their chemical characterization being inherently challenging in addition to the overall necessity of conducting experiment at the one-atom-at-a-time level. Since the lighter homologs of Rg are coinage metals, electrochemical deposition from aqueous solutions seem to be most promising. Investigating the electrochemical deposition behavior of radioactive silver (Ag) and gold (Au) isotopes will help develop an experimental approach employing a flow electrolytic cell (FEC) to probe the underpotential deposition (UPD) behavior of SHEs. UPD is particularly relevant for SHE research because it is confronted with single atoms interacting with the electrode surface. The first phase of experiments will include both offline experiments using longer-lived radioisotopes as well as thereof developed second-generation online experiments using short-lived radioisotopes. Here we will present the general experimental approach and discuss how one may arrive at well-defined thermochemical properties derived from single atoms only.

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Cold chemistry of the proton: The $\text{H}^+ + \text{CH}_3\text{F}$ reaction system below 10 KD. Schlander¹, J. A. Agner¹, H. Schmutz¹, F. Merkt^{1*}¹Department of Chemistry and Applied Biosciences, ETH Zurich, 8093 Zurich, Switzerland

The reactions of the proton are poorly characterised experimentally, especially at low temperatures and low collision energies [1]. To fill this gap, we use the Rydberg-spectator merged beam approach to study the reactions of H^+ with CH_3F :



at collision energies in the range between $k_B \times 0.2$ K and $k_B \times 10$ K. The reaction rate coefficient increases strongly as the collision energy is decreased below $k_B \times 10$ K but the branching ratios for the reactions above remain constant (see Figure).

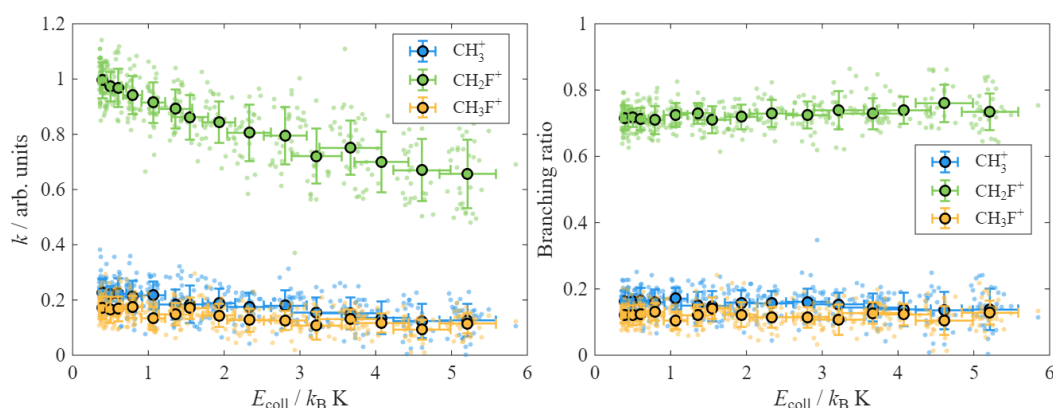
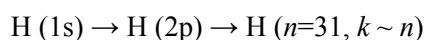


Figure: Collision energy dependence of the capture rate coefficient of the $\text{H}^+ + \text{CH}_3\text{F}$ reaction (left). Branching ratios for the same reaction (right).

The reactions are observed within the orbit of the $\text{H}(n)$ Rydberg electron after a Rydberg $\text{H}(n)$ atom beam is deflected and merged with a supersonic beam of CH_3F [2,3]. The $\text{H}(n)$ atom beam is generated from pure H_2 gas using a dielectric barrier discharge at the orifice of a pulsed valve and resonant two photon excitation



in a dc electric field (~ 50 V/cm). The poster will compare the experimental data with model calculations based on a rotationally adiabatic capture model [4-6].

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Towards Studying Rotationally State-Selective Ion-Molecule Reactions of ND₃ and He⁺ using an Electrostatic Hexapole Filter

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Over the past years, our group has developed a merged-beam method to study ion-molecule reactions at low collision energies (E_{coll} in the range $k_B \cdot 0.2 \text{ K} - k_B \cdot 15 \text{ K}$) [1,2]. To avoid undesirable heating of the ions by stray electric fields, the ions are substituted by Rydberg states of the parent neutral species, with principal quantum number n around 35. In these states, the Rydberg electron does not influence the ion-molecule reaction taking place within its orbit but shields the reaction system from stray fields. In the experiment (see Fig. 1), a beam of He(n) Rydberg atoms is merged with a supersonic beam of neutral molecules and their relative velocity is varied using a Rydberg-Stark deflector and accelerator [3]. We present the design and implementation of an electrostatic hexapole state filter to modify the number densities of the molecules in specific rotational levels with the goal of measuring state-specific rate coefficients. This hexapole filter has been used to alter the rotational-state population distribution in supersonic beams of ND₃ with initial rotational temperatures $T_{\text{rot}} < 25 \text{ K}$. Its effects were quantified by measuring the 2+1 REMPI spectra of the $B - X 2_0^{5,6}$ and $C' - X 2_0^{0,1}$ transitions of ND₃. Enhancements of the number densities of molecules in low-field-seeking rotational levels by factors up to four were observed. The hexapole state filter was used in a preliminary study of the reaction of He⁺ and ND₃ forming ND₃⁺, ND₂⁺ and ND⁺. This work was supported financially by ETH Zurich and the Swiss National Science Foundation (project number 200021-236716)

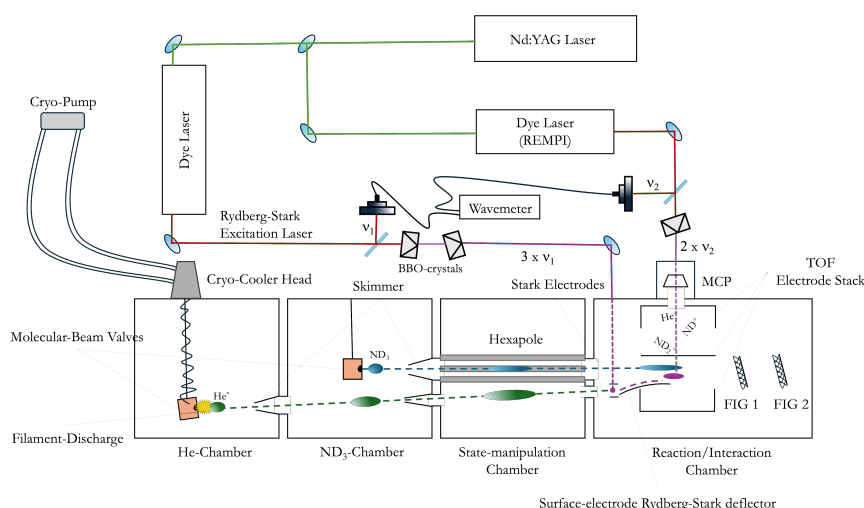


Figure 1: Schematic view of the experimental setup used to study ion-molecule reactions at low collision energies.

FIG: fast ionization gauge; MCP: microchannel plate

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Probing Solvated Electron and Dielectron Mediated Relaxation Dynamics in Sodium Doped Ammonia Clusters

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Slow unbound electrons, i.e., quasi-free or solvated electrons with kinetic energy less than 20 eV [1], have attracted interest due to their role in chemistry and medical physics. Notably, these low energy electrons act as potent reducing agents in the Birch reduction [2], a reaction widely employed in organic chemistry laboratories and in industrial processes, yet hazardous [3]. Moreover, slow solvated electrons have been identified as key components in the reaction cascade of DNA damage by ionizing radiation [1, 4]. In view of this, a detailed understanding of solvated-electron-mediated processes is particularly valuable, as it provides the necessary physical foundation for the development of safer, scalable reactions for chemical industry, radiation protection protocols and tailored radiation therapy.

To date, the challenge of performing controlled studies on slow solvated electrons *in situ* and the difficulty of deconvoluting complex multicomponent electron transfer mechanisms limit the understanding of reactions involving solvated electrons [5]. Sodium-doped ammonia clusters are, so far, the only system where the efficient formation of slow electrons from the relaxation of a solvated dielectron in an excited state has been observed, albeit without accessing the timescale of this process [5]. In this work, we utilize sodium-doped ammonia clusters ($\text{Na}(\text{NH}_3)_n$, $n \sim 100$) [6] as a model system and present the first time-resolved study of their photo-induced electron-transfer dynamics on the hundred-femtosecond timescale. We employ pump-probe photoelectron spectroscopy combined with velocity map imaging detection.

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Accurate size determination of proteins in 20 ms by Dynamic light scattering microscopy

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Dynamic Light Scattering (DLS) is widely used to characterize objects ranging from the nanometer to micrometer scale in solution. However, its application to systems undergoing rapid changes is limited by the need to maintain steady-state conditions throughout the measurement [1]. To address this limitation, we previously introduced a microscopy-based DLS (micro-DLS) platform based on time-correlated single-photon counting and a custom post-processing workflow. It was demonstrated that the setup was capable of performing autocorrelation analysis over arbitrarily selected time windows and particle sizing at sub-100 ms temporal resolution [2]. While this approach significantly improved the time resolution of DLS measurements, its performance remained limited for weakly scattering systems (size range below 10 nm, e.g. proteins) due to background contributions originating from reflections and other time-independent scattering sources.

Here, we present an improved micro-DLS configuration employing oblique illumination, where light enters the objective off-axis and illuminates the sample at an angle relative to the detection axis. In conjunction with a pinhole to spatially filter time-independent scattering, including reflections, this geometry substantially improves the signal-to-background ratio compared to conventional coaxial configurations. As a result, the coherence factor β of the autocorrelation function exceeds 0.9, approaching the ideal limit. Combined with the previously developed time-window analysis workflow, the method yields better-resolved size distributions and enables reliable measurements of weak scatterers such as bovine serum albumin (BSA), previously beyond the detection limits of coaxial micro-DLS, with temporal resolutions as short as 20 ms. Overall, the approach expands the range of systems accessible to DLS and provides a route toward time-resolved particle sizing of systems that are out of equilibrium processes.

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Multi-Scale Conductivity and Optical Characterization of Doped Thienothiophene-Based Conjugated Polymers

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Conjugated polymer semiconductors are promising materials for a wide range of organic optoelectronic applications due to their tunable electrical and optical properties. However, their relatively low electrical conductivity remains a key limitation for many applications.^{1,2} Molecular doping addresses this challenge through the formation of mobile carriers such as singly charged and doubly charged species, significantly enhancing conductivity by several orders of magnitude.¹⁻⁴ Despite these advances, a detailed understanding of how doping influences the electronic structure and transport properties of conjugated polymers remains essential for the development of highly conductive organic semiconducting materials.⁵

In this work, we chemically doped thienothiophene-based conjugated polymers and characterized them using steady-state UV-Vis-NIR absorbance spectroscopy, four-point probe measurements, and time-domain THz spectroscopy. We then investigated the evolution of optical signatures, charge-transfer interactions, and conductivity as a function of doping level and across different length scales. By correlating spectroscopic features with charge transport behavior, we aim to better understand carrier generation and transport in these materials, providing further insight into doping physics and structure-property relationships relevant for future organic optoelectronic and flexible device applications.

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From Excitons to long lived charges: Charge carrier dynamics in PCE10:ITIC Bulk heterojunction Nanoparticles for photocatalysis

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Photocatalytic hydrogen generation using donor–acceptor (D:A) bulk heterojunction(BHJ) nanoparticles has made significant progress in recent years. While previous studies have reported efficient charge generation and the presence of long-lived charge carriers in these systems, the fate of these charges following their initial separation remains poorly understood. Here, In this work investigate the charge carrier dynamics of a high-performing 3:7 blend of PCE10:ITIC^{1,2} using a newly developed transient absorption spectroscopy setup that synchronizes two ultrafast laser sources to generate electronically controlled delays extending up to 600 μ s, overcoming the limitations of conventional mechanical delay stages³. Transient absorption measurements reveal efficient exciton-to-charge conversion in both BHJ nanoparticle dispersions and spin-coated BHJ films. Furthermore, long-lived charge carriers are observed in nanoparticle dispersions in the presence of ascorbic acid as a sacrificial electron donor. While the ITIC exciton dynamics remain largely unchanged with and without cocatalyst, the nanoparticle dispersion containing ascorbic acid exhibits charge carrier lifetimes extending to approximately 100 μ s and a shift in exciton peak after 1ns. These results suggest that ascorbic acid facilitates efficient charge separation and suppresses charge recombination, leading to the generation of long-lived charge carriers that are potentially beneficial for photocatalytic hydrogen evolution.

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Correlating Zeolite Acidity with Framework Response Probed by IR Spectroscopy in Liquid Environment

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Surface acidity in solid acids is commonly characterized by adsorption of a basic probe molecule followed by desorption in controlled temperature ramp to quantify the amount of acid sites. Spectroscopic methods can also be applied to identify the nature of the acid sites, i.e. Lewis vs Brønsted acid sites. Infrared (IR) spectroscopy is the most used technique for characterization of acid sites in solid catalysts, where the shift of characteristic vibrational modes of the adsorbed base probe molecule with respect to the free molecule is observed. As a fundamental property of solid catalysts, characterization of acidity is well studied in gas phase experiments. However, it is poorly investigated in the liquid phase, where many catalytic reactions take place. There is thus a clear need in the development of acidity determination in liquid environments.

In this work, zeolite acidity is probed in liquid-phase conditions using in situ and operando spectroscopic techniques. By using pyridine as a probe molecule, the acidity of selected zeolites was studied by Attenuated Total Reflection Infrared (ATR-IR) and online UV-vis spectroscopy in liquid environments. The influence of solvent polarity, pore size, and presence of heteroatoms on probe-zeolite interactions was systematically evaluated, thus revealing key information on the presence and distribution of acid sites, as well as its correlation with the perturbation to zeolite framework during probe molecule adsorption. The approach can also be used to study reaction mechanisms of acid catalyzed reactions with the aim to selectively block acid sites.

Overall, this methodology establishes a versatile foundation for studying zeolite acidity under realistic liquid-phase conditions, with potential applications in mechanistic studies and process optimization in heterogeneous catalysis.

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Bridging interfaces in perovskite solar cells: band alignments from first principles calculations

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Molecularly engineered interlayers have emerged as a powerful strategy to enhance the efficiency and stability of perovskite solar cells. [1-2] These interfacial layers bridge structural and electronic mismatches between the perovskite and charge transport layers (CTLs), yet the underlying mechanisms of charge transport across such interfaces remain poorly understood. In particular, it is unclear whether photogenerated electrons and holes cross the interface via tunneling or hopping mechanisms. Tunneling occurs when carriers transfer across energy barriers between the perovskite and CTL, whereas hopping can proceed stepwise through the redox-active levels of the molecular layer or directly between the perovskite and CTL. Here, we investigate the relative band alignment across perovskite/molecular layer/CTL interfaces using large-scale density functional theory calculations. Our approach combines projected local density of states with real-space electron density maps to assess energy-level alignment and spatial charge localization at the interface. We apply this approach to experimentally realized perovskite devices incorporating naphthalene-imide based molecular interlayers [3], elucidating how molecular properties and interfacial interactions affect the relative band alignment between the materials stack in the device. Our results provide a picture of interfacial charge transfer mechanisms from a first-principles perspective, offering guidance for the rational design of molecular interlayers in perovskite photovoltaics.

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Water Confinement and Hydrogen-Bond Network Disruption in LiTFSI Water-in-Salt Electrolytes

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Water-in-salt electrolytes enable high-voltage aqueous batteries by extending the electrochemical stability window of water, yet the molecular origin of this stabilization remains debated [1]. In concentrated LiTFSI electrolytes, previous studies have shown extensive ion–water restructuring, reduced water activity, and nanoscale heterogeneity, but conventional structural probes do not directly isolate collective water–water hydrogen-bond dynamics [2]. Here we use Correlated Vibrational Spectroscopy (CVS), a hyper-Raman-based approach that separates self-correlated single-molecule responses from cross-correlated intermolecular vibrational signals [3], to probe how concentrated LiTFSI electrolytes restructure the hydrogen-bond network of water. By tracking the cross-correlated hydrogen-bond stretch near 205 cm^{-1} and the collective librational band between ~ 400 and 900 cm^{-1} , we show that increasing LiTFSI concentration progressively suppresses both water-network modes. At the water-in-salt limit, 21 m LiTFSI, these collective water signatures become indistinguishable from experimental noise, indicating collapse of the extended hydrogen-bond network and strong confinement of water in ion-rich solvation environments. In contrast, concentrated LiCl solutions retain and even enhance cross-correlated water modes, revealing a polarized but still collective hydrogen-bonded network. In LiTFSI, the disappearance of water-network modes is accompanied by the emergence of sharp TFSI-associated cross-correlated bands near 528 and 641 cm^{-1} , which red-shift upon H/D substitution, showing that these ion-network vibrations remain coupled to the local solvent environment. These results provide direct experimental evidence that the expanded stability of LiTFSI water-in-salt electrolytes originates from molecular-scale water confinement and hydrogen-bond network disruption, rather than from interfacial solid-electrolyte-interphase formation alone.

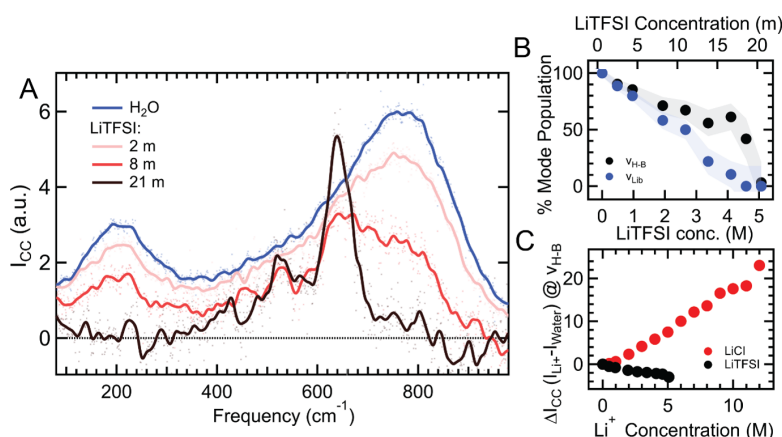


Fig. 1. Concentration-dependent changes in collective hydrogen-bonding and water structure in aqueous LiTFSI solutions revealed by cross-correlated CVS. (A) Cross-correlated CVS spectra of aqueous LiTFSI solutions. (B) Relative populations of v_{HB} (blue symbols) and v_{LB} (red symbols) modes as a function of LiTFSI concentration. (C) Change in cross-correlation intensity (ΔI_{cc}) at the hydrogen band stretching mode frequency (v_{HB}) between Li salts and bulk water plotted as a function of Li^+ concentration.

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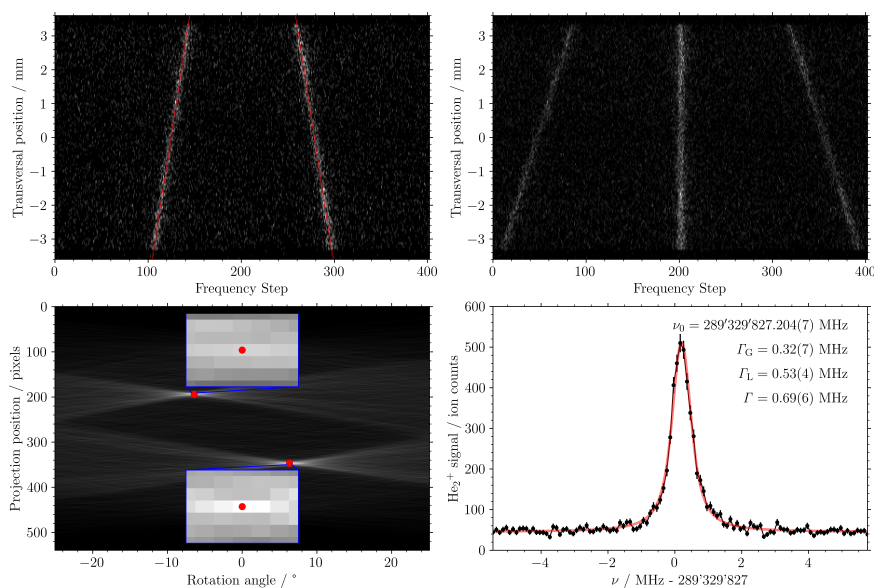
Metrology of the Helium Dimer with a Spectral Resolution of 2.5 ppb and a Precision of 17 ppt

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The helium dimer (He_2) serves as a benchmark system for testing ab initio calculations. Recently, highly accurate first-principles calculations that include relativistic and quantum-electrodynamical (QED) effects have become feasible for this six-particle, four-electron molecule [1-3]. Accurate experimental data on the low-lying triplet electronic states of He_2 are needed to validate the current theoretical advances.

We report on a high-resolution spectroscopic study of the fine structure of the $b^3\Pi_g(v=3) - a^3\Sigma_u^+(v=0)$ transition of He_2 in the near infrared (NIR) around 1040 nm. The measurements employed the recently developed Doppler-free method of imaging-assisted single-photon spectroscopy (IASS) [4] and applied it for the first time to a molecule. A narrowband continuous-wave laser locked to a frequency comb referenced to an SI-traceable frequency standard [5] was used in combination with an automatic interferometric alignment of the two counterpropagating laser beams using a Michelson-type interferometer featuring a corner cube, as described in Ref. [6]. With this setup, each spectral line was split into a red-shifted (ν_r) and a blue-shifted (ν_b) component with the first-order-Doppler-free line center $\nu = (\nu_r + \nu_b) / 2$. To optimize the spectral resolution, each Doppler component was further split into sub-Doppler components by imaging the photoexcited molecules in the direction perpendicular to both the laser and the molecular beams. Integration of the recorded signal along the forward propagation axis of the molecular beam led to images as shown below. The Doppler-free transition frequency was extracted using a Radon transform and a cross-correlation analysis, leading to full widths at half maximum of only 700 kHz and the determination of line centers with a precision of a few kHz.



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Chiral Induction by Ligand Exchange: Enantiopure Au₂₄Pt Nanoclusters from an Achiral PrecursorM. Zanjani¹, J. Zhao¹, T. Bürgi^{1*}¹University of Geneva

The development of enantiopure metal nanoclusters is essential for chiral catalysis, sensing, and biomedical applications, yet strategies to achieve absolute stereochemical control remain scarce. We report a facile, stereospecific ligand exchange protocol that converts the racemic Au₂₄Pt(TBBT)₁₂(PDT)₃ cluster^[1] (where TBBT = 4 tert butylbenzenethiol, PDT = propane 1,3 dithiolate) into an enantiopure Au₂₄Pt(TBBT)₁₂(1,3 butanedithiol)₃ species by replacing the three achiral PDT ligands with either (R)- or (S)- 1,3 butanedithiol. High performance liquid chromatography shows a single, well-resolved peak for each product, and MALDI TOF mass spectrometry confirms the expected composition. UV–vis absorption spectra of the enantiomers are virtually identical to those of the parent cluster, indicating that the electronic structure of the Au₁₂Pt core is retained. Circular dichroism measurements reveal perfectly mirrored spectra for the (R) and (S) derived clusters, demonstrating complete transfer of chirality from the surface dithiol to the metal framework. This work establishes that the handedness of an Au₂₄Pt nanocluster can be dictated solely by the chirality of only few ligands on its surface, providing a simple, general route to enantiopure atomically precise nanoclusters and deepening our understanding of ligand driven chiral control in metal nanoclusters.

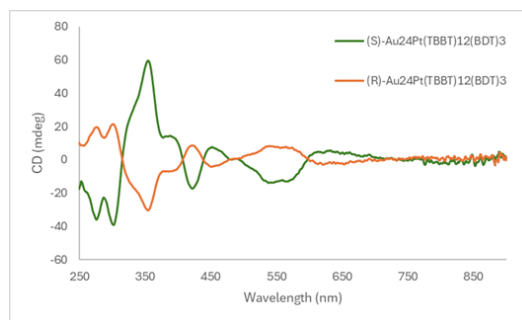


Figure1. CD spectra of (R)/(S)-Au₂₄Pt(TBBT)₁₂(BDT)₃ enantiomers

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Velocity Map Imaging of Carbonyl Sulfide Ionization: From Strong-Field Fragmentation to Chemi-Ionization

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Velocity map imaging (VMI) represents an important method for probing ionization and fragmentation dynamics through product kinetic energy and angular distributions.[1] Here, VMI is used to investigate the ionization dynamics of carbonyl sulfide (OCS) under two different conditions: femtosecond-laser-induced strong-field ionization and chemi-ionization with metastable neon atoms.

In strong-field ionization, OCS monomers and dimers produce a range of ionic fragments, revealing dissociation pathways of singly and doubly ionized OCS as well as charge-separation channels in weakly bound OCS dimers.[2,3] Our results highlight how ionization-induced fragmentation evolves from intramolecular dissociation in isolated molecules to intermolecular charge redistribution in molecular clusters.

This work was further extended to the chemi-ionization reaction between OCS and metastable neon atoms. Time-of-flight mass spectrometry and ion imaging reveal product channels associated with Penning ionization and dissociative ionization, providing insight into collision-induced ionization and fragmentation dynamics.[4,5]

Our apparatus is currently being extended towards coincidence velocity map imaging (CVMI)[6] through the addition of an electron detection system. This development will enable future measurements in which ion and electron products from the same ionization event can be correlated. Such measurements will provide additional information on the energy and momentum distributions of both products, as well as on the ionic states originally produced in the chemi-ionization, offering a more complete picture of the product states and dynamics in molecular ionization reactions.

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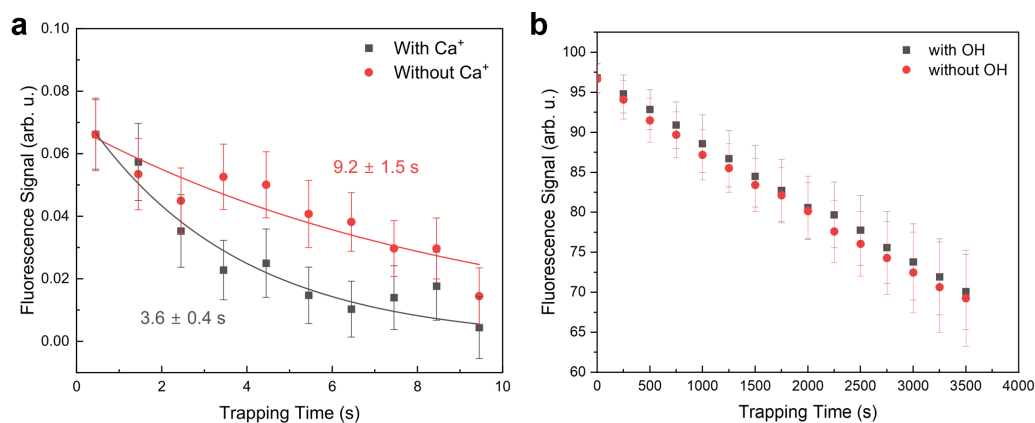
Cryogenic hybrid trapping of Ca^+ ions and OH molecules for cold ion-molecule collision studies

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Collisions between ions and molecules at very low temperatures are essential for understanding fundamental physical and chemical processes [1-2]. At low collision energies, only a few partial waves contribute, providing a clean regime for examining cold-collision mechanisms at the quantum level [3]. Such processes also play a key role in interstellar environments, where ion–molecule reactions govern molecular evolution [4].

In this work, we present a new experimental approach in which quantum-state–selected and phase-space–controlled OH radicals are produced with a Stark decelerator and confined in a magnetic trap and combined with cold Ca^+ ions prepared by laser cooling in a linear Paul trap [5-7]. Shuttling the Ca^+ ions brings them into spatial overlap with the trapped OH molecules, enabling the study of controlled cold collisions between Ca^+ and OH. The OH lifetime in the magnetic trap is measured by laser-induced fluorescence, and comparison of the measured lifetimes with and without Ca^+ ions reveal the effect of ion–molecule interactions. First results indicate that the Ca^+ ions reduce the trap lifetime of the OH radicals, indicating trap loss by either elastic or inelastic collisions.



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When Coolants Capture Fission Products: Tellurium Speciation and Retention in Liquid Lead–Bismuth

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Lead–bismuth eutectic (LBE) is a candidate coolant for lead-alloy fast reactors, where understanding the volatility and speciation of fission products such as tellurium (Te) is essential for source-term and safety assessments. We studied Te behavior in LBE using thermosublimatography to resolve gas-phase speciation and deposition. Using radioactive tracers produced at PSI allowed to quantify ultra-low vapor pressures between 300 and 700 °C through the transpiration technique. For Te-doped LBE ($x_{Te} = 1 \times 10^{-3}$) in He atmospheres (dry, humidified, and 10% H₂O admixture), thermosublimatography in fused-silica columns showed a high-temperature deposition zone (~500 °C) consistent with PbTe deposition and a low-temperature zone (~200 °C) of crystalline Te, indicating partial PbTe decomposition and release of a volatile Te fraction. This decomposition was promoted by trace water vapor and suppressed under reducing conditions. In stainless-steel columns only PbTe deposition was observed. Transpiration results a Henry's constant indicating stronger Te retention in LBE than predicted by an ideal-solution model.

Overall, Te volatilizes predominantly as PbTe, reducing Te release to the cover gas by a factor of approximately 10^3 at 380 °C compared to the ideal solution of Te in LBE. The sensitivity of PbTe decomposition to surface material and moisture highlights the importance of cover-gas conditioning and selection of trapping materials in LBE systems.

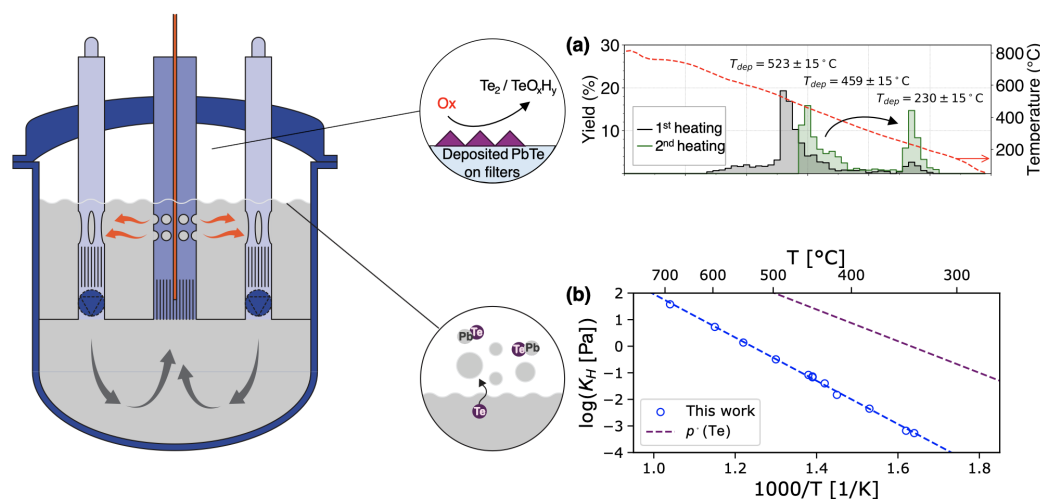
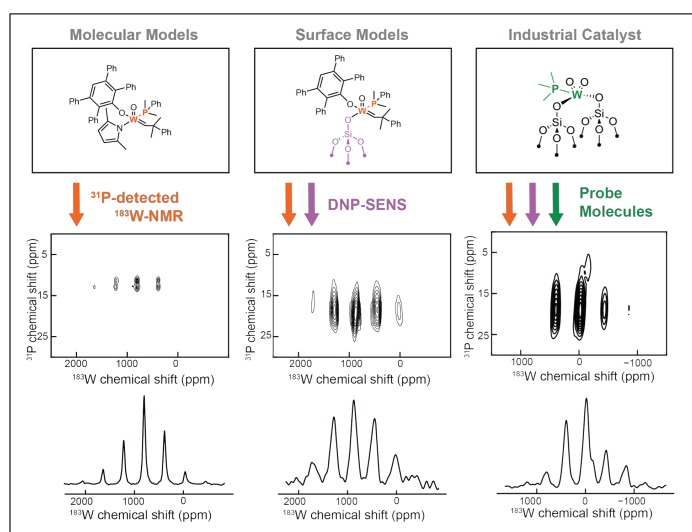


Figure 1. Evaporation behavior of Te in an LBE-cooled system: (a) PbTe deposition and its decomposition on a fused silica surface studied by thermosublimatography, (b) temperature dependence of Henry's constant for Te in LBE determined by transpiration method.

(Core scheme of MYRRHA is adapted from A. Aerts)

^{31}P -detected ^{183}W -NMR Signatures of Molecules and Surface SitesM. Z. Seidel¹, F. J. De Zwart¹, A. Yakimov¹, C. Copéret^{1*}¹ETH Zürich

Solid-state NMR of ^{183}W ($I=1/2$) is extremely challenging due to its low gyromagnetic ratio (1.796 MHz/T) and 14.3% natural abundance resulting in a receptivity $\sim 90\,000$ times lower than that of ^1H . Conventional approaches to boost sensitivity, such as ^1H - ^{183}W Cross-Polarization (CP-MAS) are limited by the typically weak ^1H - ^{183}W dipolar couplings requiring long contact times (>20 ms), as well as by proton relaxation. These challenges are further exacerbated for surface sites that suffer from low spin concentrations ($<1\ \mu\text{M}$), inhomogeneous broadening and the absence of spatially close protons.



Here, we present a strategy of utilizing indirect detection via J-coupled ^{31}P as a high- γ "spy" nucleus to enable efficient ^{183}W detection. Using a molecular system and recording 2D ^{31}P - ^{183}W -Heteronuclear Multiple Quantum Coherence (HMQC) spectra we demonstrate the validity of the approach, which also enables us to extract the ^{183}W chemical shift anisotropy (CSA) and to thereby understand the W local environment. The application on a well-defined surface complex containing a phosphine ligand is further demonstrated, thanks to the implementation of Dynamic Nuclear Polarization Surface Enhanced NMR Spectroscopy (DNP-SENS).

Finally, we apply this approach to silica-supported tungsten oxide (WO_3/SiO_2), a key catalyst of the chemical industry, with poorly understood surface sites. Using trimethylphosphine (TMP) as a probe molecule, to introduce the required ^{31}P - ^{183}W interactions enables us to record 2D ^{31}P - ^{183}W -NMR spectra and to distinguish two surface sites. Further extracting their CSA parameters provides detailed information and enables us to determine the local environments of the W sites. Overall, this work demonstrates the first successful application of surface-sensitive ^{183}W solid-state NMR spectroscopy, thus providing a blueprint for characterization of low- γ nuclei in heterogeneous materials.