BOOK OF ABSTRACTS

MOLEC 2026

25th European Conference on the Dynamics of Molecular Systems

September 6th to 11th, 2026

University of Freiburg
Kollegiengebäude I
Platz der Universität 3
D-79098 Freiburg

MOLEC 2026

universität freiburg

Imprint

25th European Conference on the Dynamics of Molecular Systems (MOLEC2026)

MOLEC is held by the *Molecular and Chemical Physics Group* (MCPG) of the *Atomic, Molecular and Optical Physics Division* (AMOPD) of the European Physical Society (EPS)

Local organizing committee:

Frank Stienkemeier, Lukas Bruder, Sebastian Hartweg, and Simone Ortolf

University of Freiburg
Institute of Physics
Hermann-Herder-Straße 3
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MOLEC

The European Conference on the Dynamics of Molecular Systems was first introduced in 1976 and since was held biennially.

- Trento (Italy), 1976.
- Brandbjerg Hojskole (Denmark), 1978.
- Oxford (UK), 1980.
- Nijmegen (The Netherlands), 1982.
- Jerusalem (Israel), 1984.
- Aussois (France), 1986.
- Assisi (Italy), 1988.
- Bernkastel-Kues (Germany), 1990.
- Prague (Czech Republic), 1992.
- Salamanca (Spain), 1994.
- Nyborg Strand (Denmark), 1996.
- Bristol (UK), 1998.
- Jerusalem (Israel), 2000.
- Istanbul (Turkey), 2002.
- Nunspeet (The Netherlands), 2004.
- Trento (Italy), 2006.
- St. Petersburg (Russia), 2008.
- Curia (Portugal), 2010.
- Oxford (UK), 2012.
- Gothenburg (Sweden), 2014.
- Toledo (Spain), 2016.
- Dinard (France), 2018.
- Hamburg (Germany), 2022.
- Aarhus (Denmark), 2024

The newest installment of the MOLEC will be held Sept 6th – 11th, 2026
in Freiburg im Breisgau, Germany.

MOLEC is held by the ***Molecular and Chemical Physics Group*** (MCPG) of the ***Atomic, Molecular and Optical Physics Division*** (AMOPD) of the **European Physical Society** (EPS)

MOLEC Board Members

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Claire Vallance
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[1] Representative of the AMOPD division of EPS

Local MOLEC2026 Organizers

Sebastian Hartweg
Lukas Bruder
Frank Stienkemeier
Simone Ortolf

General Information

Duration

Sunday, September 6th , 2026, 5:30 p.m. – Friday, September 11th , 2026, 2:00 p.m.

Venues

Sunday, September 6th , 2026

Welcome Evening

University of Freiburg
Institute of Physics – Großer Hörsaal
Hermann-Herder-Str. 3
D-79104 Freiburg

Institute of Physics

Monday, September 7th – Friday, September 11th , 2026
Conference

University of Freiburg
Kollegiengebäude I – Aula & Prometheushalle
Platz der Universität 3
D-79098 Freiburg

Entrance KG I

Prometheushalle KG I

Kollegiengebäude I (KG I)

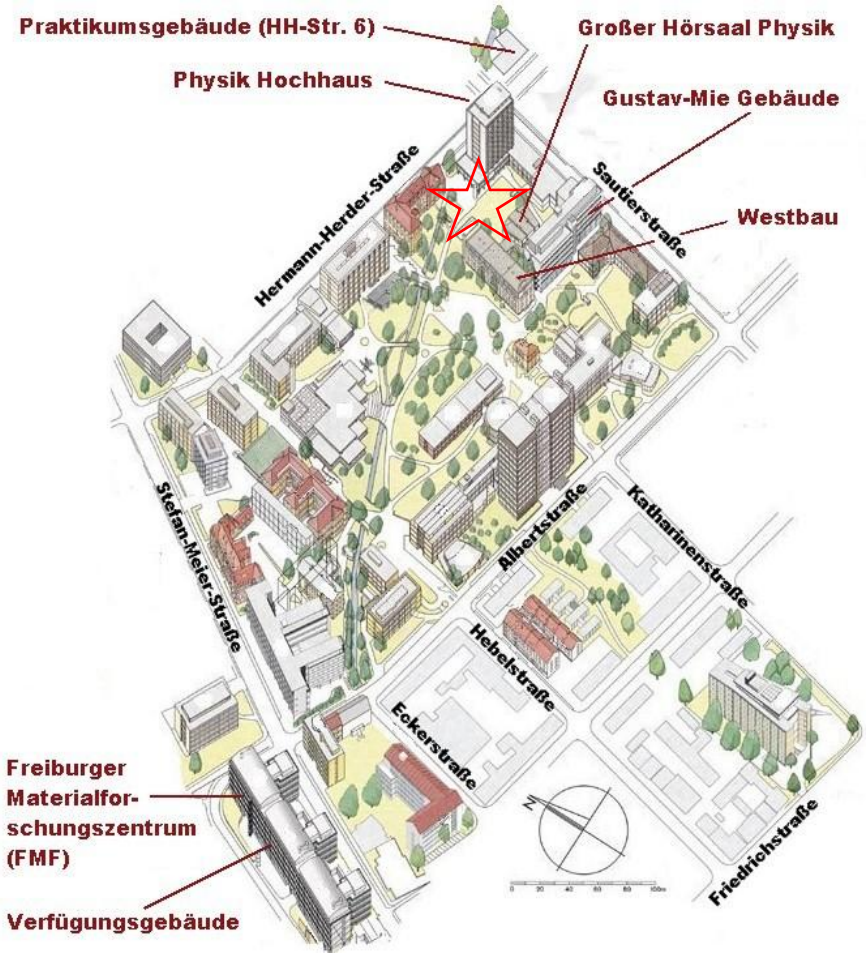
Map – Kollegiengebäude I

Lab tours

Tours are offered in the laboratories of:

Sansone (attosecond science and reaction microscopes)
von Issendorff (cluster physics and photoelectron detectors)
Stienkemeier/Hartweg (cluster isolation spectroscopy, femtosecond spectroscopy, TRPES)
Bruder (coherent multidimensional spectroscopy)

The meeting point for the lab tours is *in front of the physics high rise*:
Hermann-Herder-Str. 3, 79104 Freiburg.



Meals & Drinks

During the workshop, lunches, coffee breaks (morning & afternoon), as well as a welcome evening and a conference dinner will be provided.

Welcome Evening on September 6th , at 5:30 pm

University of Freiburg – Institute of Physics
Hermann-Herder-Str. 3
D-79098 Freiburg

Lunch from September 7th to 11th

Mensa Rempartstraße
Rempartstraße 18
D-79098 Freiburg

You will receive vouchers for each lunch at Mensa Rempartstraße, available are Meals I and II.

Conference Dinner on September 10th at 7:00 pm at

Dattlers Schlossberg Restaurant
Am Schlossberg 1
D-79104 Freiburg
https://dattler.de/

Program

Assigned time slots:

Keynote talk	50 min. + 10 min. discussion
Invited talk	25 min. + 5 min. discussion
Hot topic talk	15 min. + 5 min. discussion

Sunday, September 6th, 2026

From 5:00 p.m.	Arrival on site: Institute of Physics, Herrmann-Herder-Str. 3, 79104 Freiburg Registration
5:50 p.m.	**Welcome** (Sebastian Hartweg, Lukas Bruder, Frank Stienkemeier)
	Chair: ***Lukas Bruder***
6:00 p.m.	**Toshinori Suzuki** EUV Time-Resolved Photoelectron Spectroscopy of Liquids: From Interfacial Dynamics to Nucleic Acid Photodamage
7:00 p.m.	**Welcome Evening**

Monday, September 7th, 2026

	Chair: ***Gereon Niedner-Schatteburg***
9:00 a.m.	**Takamasa Momose** Asymmetric Photolysis of Amino Acids and Its Relation to the Origin of Homochirality
10:00 a.m.	**Jennifer Noble** Physics and Chemistry of Ices in Star Forming Regions: Interpreting JWST Observations of the Chamaeleon I Molecular Cloud via Laboratory Astrophysics
10:30 a.m.	Coffee Break
11:00 a.m.	**Evan Bieske** Carbon Clusters: Infrared and Electronic Spectra of Chains, Rings and Fullerenes
11:30 a.m.	**Jascha Lau** Towards State- and Time-Resolved Fluorescence Spectroscopy of Astrochemically Relevant Ions
11:50 a.m.	**Anthony Meijer** Formation of Uracil and Thymine in the ISM
12:10 p.m.	**Amit Debnath** The Infrared Fingerprints of Cosmic Carbon Chains
12:30 p.m.	Lunch Break
	Chair: ***Jennifer Noble***
2:00 p.m.	**Mischa Bonn** Confined and Interfacial Water: Insights from Surface Vibrational Spectroscopy
2:30 p.m.	**David Nesbitt** Chemical Physics at the Gas-Liquid Interface: From Liquid Microjets to Molten Metals
3:00 p.m.	**Wutharath Chin** High-resolution 2D-IR Spectroscopy in Low Temperature Solids: Symmetry-Breaking and Anharmonic Coupling Maps
3:20 p.m.	**Leeyeong Kim** Exploring Photochemistry for Quantum Optics with Large Organic Molecules
3:40 p.m.	Coffee Break

4:10 p.m.	**Kirsten Schnorr** Using Soft X-rays to Unravel Light-Induced Dynamics in Gas-Phase Systems
4:40 p.m.	**Daniela Rupp** Imaging Nano-Samples in Free Flight with Intense X-ray Pulses: Probing Highly Excited Matter with Extreme Precision
5:10 p.m.	**David Picconi** Simulating the ultrafast dynamics of multi-mode multi-state molecular systems coupled to a dissipative environment
5:30 p.m.	**Lok Yiu Wu** Observation of thermal non-equilibrium in uniform supersonic flows
5:50 p.m.	**Laura Pille** UV to Far-UV Photodissociation Reveals the Role of Sulfur–Aromatic Interactions in Peptides

Tuesday, September 8th, 2026

	Chair: ***Bas van der Meerakker***
9:00 a.m.	**Henrik Stapelfeldt** Real-time observation of the diffusion-limited formation of an ion-molecule complex
10:00 a.m.	**Stefanie Gräfe** Strong-field many-body dynamics in confined systems
10:30 a.m.	Coffee Break
11:00 a.m.	**Andrew Orr-Ewing** Photochemical Dynamics in Aerosol Microdroplets
11:30 a.m.	**Steen Brøndsted Nielsen** Gas-Phase FRET at Cryogenic Temperatures: Talking to Specific Conformers
11:50 a.m.	**Brendan Wouterlood** Local and Non-Local Double Ionisation of Micro-Solvated Nucleobases
12:10 p.m.	**Sebastian Trippel** Unraveling the early-stage dynamics of ionized water dimer in energy and time
12:30 p.m.	Lunch Break
	Chair: ***Daniel Neumark***
2:00 p.m.	**Bas van de Meerakker** Cold and Controlled Collisions using Tamed Molecular Beams
2:30 p.m.	**Xingang Wang** State-to-State Reaction Dynamics Using Velocity Map Ion Imaging
3:00 p.m.	**Andrea Orban** Quantum study of ultracold atom-ion excitation exchange
3:20 p.m.	**Nanditha Sunil Kumar** Cold chemistry of single trapped H_2O^+ ions with neutral HD molecules in a cryogenic ion trap
3:40 p.m.	Coffee Break
4:10 p.m.	**Marcel Mudrich** Penning ionization electron spectroscopy of atoms and molecules in or on helium nanodroplets
4:40 p.m.	**Elisabeth Gruber** Exploring Molecular Ions and Cryogenic Chemistry in Charged Helium Nanodroplets
5:10 p.m.	**Poster session 1** Entrance Hall KG I

Wednesday, September 9th, 2026

	Chair: ***Francesca Calegari***
9:00 a.m.	**Daniel Neumark** Spectroscopy and Scattering Experiments on Flat Liquid Jets
10:00 a.m.	**Thomas Allison** Imaging Exciton and Charge-Transfer Dynamics at Surfaces with Time-resolved Momentum Microscopy
10:30 a.m.	Coffee Break
11:00 a.m.	**Rebecca Ingle** Chemical Insights from Resonant Auger Spectroscopy
11:30 a.m.	**Jemma Gibbard** Visible Light Photochemistry of IO_2^-
11:50 a.m.	**Mathew Costen** Near-Surface Velocity-Map Imaging of Rotationally Inelastic Gas Surface Scattering
12:10 p.m.	**Wim van der Zande** The Advanced Research Center for NanoLithography: an example of a public-private partnership in the MOLEC field
12:30 p.m.	Lunch Break
1:30 p.m.	**Excursions** - Black Forest Hike - Wine Tasting
5:10 p.m.	**Lab visits**

Thursday, September 10th, 2026

	Chair: ***Rebecca Ingle***
9:00 a.m.	**Francesca Calegari** Tracking electron charge migration in molecules using attosecond FEL pulses
10:00 a.m.	**Giuseppe Sansone** Three-path attosecond interferometry
10:30 a.m.	Coffee Break
11:00 a.m.	**Alicia Palacios** Attosecond non-linear dynamics in molecules: correlation, coherences and entanglement
11:30 a.m.	**Hugo Marroux** Attosecond spectroscopy of electronic decoherence in liquid water
11:50 a.m.	**Maria Richter** High-order harmonic generation in an organic molecular crystal
12:10 p.m.	**Karin Sarah Thalmann** Quantum dynamics of singlet fission, charge transfer, and triplet-triplet annihilation
12:30 p.m.	Lunch Break
	Chair: ***Toshinori Suzuki***
2:00 p.m.	**Daniel Rolles** Imaging Ultrafast Dynamics in Gas-Phase Molecules with Coulomb Explosion Imaging
2:30 p.m.	**Daniel Strasser** Ionization / neutralization induced Dynamics
3:00 p.m.	**Lorenzo Iori** Tracking Ultrafast Electron Dynamics in Acetylacetone with 3-fs-resolved UV/XUV Photoelectron Spectroscopy
3:20 p.m.	**Arnab Sen**

	Probing ultrafast molecular dynamics with few-fs VUV pulses
3:40 p.m.	Coffee Break
4:10 p.m.	**MOLEC Prize session**
5:10 p.m.	**Postersession 2** Entrance Hall KG I
7:00 p.m.	**Conference Dinner** at Dattlers Schlossberg Restaurant

Friday, September 11th, 2026

	Chair: ***Alicia Palacios***
09:00 a.m.	**Christiane Koch** Quantum effects in cold and controlled molecular dynamics
10:00 a.m.	**Andrés Ordóñez** Theory of multi-photon excitation of chiral molecules with tailored light
10:30 a.m.	Coffee Break
11:00 a.m.	**Iain Wilkinson** High-Throughput Electron-Momentum Imaging from Liquids
11:30 a.m.	**Letizia Fede** Controlling Chiral Light-Matter Interactions with Tailored Multi-Color Laser Fields
11:50 a.m.	**Andrea Annunziata** High-order Harmonic Spectroscopy in Chiral Liquid Crystals
12:10 p.m.	**Nicolas Ladda** Real-Time Observation of a Controlled Femtosecond Enantiomeric Conversion
12:30 p.m.	**Concluding remarks**
12:40 p.m.	Lunch, Departure

ABSTRACTS

Program

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5:50 p.m.	**Welcome** (Sebastian Hartweg, Lukas Bruder, Frank Stienkemeier)
	Chair: ***Lukas Bruder***
6:00 p.m.	**Toshinori Suzuki** EUV Time-Resolved Photoelectron Spectroscopy of Liquids: From Interfacial Dynamics to Nucleic Acid Photodamage
7:00 p.m.	**Welcome Evening**

EUV Time-Resolved Photoelectron Spectroscopy of Liquids: From Interfacial Dynamics to Nucleic Acid Photodamage

Toshinori Suzuki
Department of Chemistry, Graduate School of Science, Kyoto University, Japan
suzuki.toshinori.2n@kyoto-u.ac.jp

Extreme ultraviolet time-resolved photoelectron spectroscopy (EUV-TRPES) is a powerful technique for investigating electron dynamics and chemical reactions in pure liquids and solutions. I present a few examples of recent progress.

The structures and dynamics at the gas–liquid interface have mainly been studied using nonlinear optical spectroscopies, whereas EUV-TRPES provides complementary information on electronic dynamics. Although the probing depth of EUV-TRPES extends to approximately 1 nm below the interface and is not strictly limited to the topmost molecular layer, hydrophobic molecules are preferentially localized at the interface, allowing the photoelectron signal to originate predominantly from the interfacial region. This enables photoelectron spectroscopic studies of interfacial reactions. Our experiments revealed that the electronically excited state of phenol at the gas–liquid interface deactivates one order of magnitude faster than in bulk solution. However, this deactivation involves no charge separation, but rather internal conversion to the ground state. The proximity of the electron binding energies of the excited state of phenol and the hydrated electron makes it difficult to distinguish them based on energetics; however, observation of vibrational quantum beats induced by sub-10-fs pulse excitation confirmed that the observed signal originates from phenol [1,2]. These results demonstrate the further potential of EUV-TRPES for studies of gas–liquid interfaces.

The second example concerns chemical dynamics in aqueous solution. Photolesion of nucleic acids is primarily associated with pyrimidine bases, which are more vulnerable than purine bases. EUV-TRPES studies of pyrimidine nucleobases, nucleosides, and nucleotides revealed that they disappear from the excited-state manifold within 1 ps through internal conversion to the ground state [3]. To obtain complementary structural information, we combined timeresolved infrared spectroscopy, which showed that a fraction of the internally converted molecules forms intermediates featuring a trans-twisted C5=C6 bond, and that these intermediates mediate the addition of water to C5=C6 [4-6]. This process is directly related to RNA photodamage, while extension of these studies to oligonucleotides and duplexes remains an important challenge for understanding photolesion in DNA.

Acknowledgements. This work has been supported by the Japan Society for the Promotion of Science (21H04970).

[1] Yamamoto and Suzuki, JACS **148**, 1524 – 1537 (2026).
[2] Yamamoto, Neumark, and Suzuki, *in preparation*.
[3] Miura et al., JACS **145**, 3369–3381 (2023).
[4] Obara et al., JACS **147**, 15077–15087 (2025).
[5] Obara et al., JACS **147**, 41284–41296 (2025).
[6] Ghosh et al., JACS **148**, 18903–18918 (2026).

Program

Monday, September 7th, 2026

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9:00 a.m.	**Takamasa Momose** Asymmetric Photolysis of Amino Acids and Its Relation to the Origin of Homochirality
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5:50 p.m.	**Laura Pille** UV to Far-UV Photodissociation Reveals the Role of Sulfur–Aromatic Interactions in Peptides

Asymmetric Photolysis of Amino Acids and Its Relation to the Origin of Homochirality

Takamasa Momose
Department of Chemistry, The University of British Columbia,
2036 Mail Mall, Vancouver BC, V6T 1Z1, Canada

Objects are chiral when they cannot be superimposed on their mirror images, such as our left and right hands. All proteinogenic amino acids, except glycine, are chiral molecules. In living organisms, proteinogenic amino acids are almost exclusively of one chirality, a phenomenon known as homochirality. However, the origin of homochirality in biological systems remains an open question. Some suggest that its origin might be extraterrestrial, specifically due to the exposure of chiral molecules to circularly polarized photons in interstellar space. This exposure could cause an initial population imbalance leading to the homochirality observed today. However, this extraterrestrial hypothesis has not been widely accepted, largely because molecular absorption anisotropy is believed to be too small to create the substantial imbalance required for homochirality.

Our group has investigated the photolysis of amino acids in their non-zwitterionic form using matrix-isolation spectroscopy. Recently, we found that some conformers of non-zwitterionic amino acids exhibit significant asymmetry in the rate of chirality-destroying dissociation induced by circularly polarized photons. The observed anisotropy factor for the lowest-energy conformer of leucine was remarkably large, reaching 0.1, approximately 40 times larger than the anisotropy value reported for the electronic absorption of a gas-phase leucine ensemble. Although the origin of this large asymmetry is not understood, this experimental evidence indicates that even if the reported anisotropy values in electronic absorption spectra are low, the dissociation asymmetry of certain conformers can still be substantial. An anisotropy factor of 0.1 could result in an initial enantiomeric excess exceeding 10%, even at a 90% extent of reaction. This result suggests that asymmetric photodissociation of amino acids may have been a crucial factor in the emergence of biological homochirality. Details of our experiments will be discussed.

[1] B. Moore et al. J. Am. Chem. Soc. 146, 34253 (2024).

Physics and chemistry of ices in star forming regions: interpreting JWST observations of the Chamaeleon I molecular cloud via laboratory astrophysics

J. A. Noble[1], for the IceAge and Cheerio teams [1]PIIM Laboratory, CNRS / Aix-Marseille Université, Avenue Escadrille Normandie-Niemen, 13013 Marseille, France

Understanding the chemical mechanisms involved in star and planet formation requires knowledge of the composition of the initial molecular inventory, formed in the molecular cloud phase. Much of the carbon, oxygen and nitrogen budget resides in molecular solids, or "ices", that form on dust grains under the cold, relatively dense conditions in molecular clouds. The JWST programs IceAge (PID 1309, PI McClure) and Cheerio (PID 4358, PI Smith) observed ices in the molecular cloud Chamaeleon I. IceAge observed principally the densest central region, using a combination of pointed and survey spectroscopic modes to reveal the presence of new molecules[1] and spectral absorption features,[2] while also unveiling physical processes including grain growth.[3] Spectra towards hundreds of new lines of sight have been measured with the Cheerio program, which will complement the tens of lines of sight mapped towards the cloud centre with IceAge.[4] The new data probe less dense regions of Cha I in order to determine the ice onset thresholds at the edges of the cloud. Laboratory astrophysics and astrochemistry are critical in the interpretation of this large dataset. Optical constants allow the analysis of observed spectra to determine abundances of icy molecules, while experiments can give insight into molecular-level processes at play on and in dust grains. Ultimately, to understand the system it is necessary to constrain the dynamics at play, notably between the accretion of atoms and molecules from the gas phase, the surface chemistry occurring on dust grains to form icy molecules, and the desorption of complex molecules into the gas phase.

[1] McClure et al., Nat. Astron. 7, 431 (2023).
[2] Noble et al., Nat. Astron. 8, 1169 (2024).
[3] Dartois et al., Nat. Astron. 8, 359 (2024).
[4] Smith et al., Nat. Astron. 9, 883 (2025).

Carbon Clusters: Infrared and Electronic Spectra of Chains, Rings and Fullerenes

Chang Liu, Patrick Watkins, Evan Bieske
School of Chemistry, University of Melbourne, 3010, Australia

Small carbon clusters play important roles in a variety of contexts, and are present in flames and discharges, and in interstellar space. Although buckminsterfullerene (C60) is well characterized, much less is known about smaller carbon clusters, which progressively adopt structures as chains, rings, bi-rings, and fullerenes.1 As shown in Figure 1, carbon clusters are part of an extended hydrocarbon landscape, that includes partially hydrogenated clusters and molecules and polycyclic aromatic hydrocarbons (PAHs). PAHs can be progressively dehydrogenated when energised by light or collisions to eventually produce bare carbon clusters, including cyclocarbons.2, 3

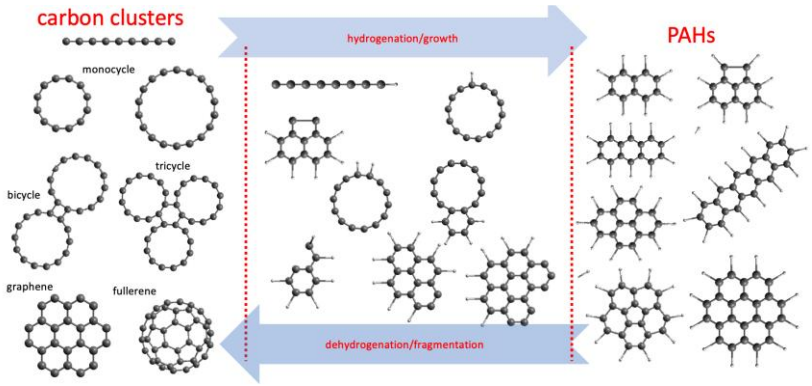

Figure 0-1: Bare carbon clusters, partially hydrogenated carbon clusters, and polycyclic aromatic hydrocarbons (PAHs).

To learn more about carbon clusters we have measured electronic and infrared spectra for clusters of different sizes and isomeric structures. To avoid isomeric ambiguities, we employ a strategy whereby the target isomer (linear, ring, bi-ring, or fullerene) is preselected using ion-mobility and mass spectrometer stages prior to spectroscopic interrogation with beams of tunable light in a cryogenically cooled ion trap.4 Narrow electronic transitions of charged cyclocarbons (cations and anions) occur in the visible and near-IR spectral regions, with a progressive shift of the main band to longer wavelength with increasing ring size.5 The C4n+rings possess sharp, intense IR transitions that are at least 50 times stronger than transitions of corresponding bi-ring and fullerene isomers, and which are associated with a single vibrational mode that propels charge back and forth across the ring.6 These intense vibrational transitions may serve as a signature for carbon rings in remote or hostile environments and may also provide a means for energised rings to dissipate energy through IR emission.

[1] G. von Helden, M-T. Hsu, P. Kemper, M. Bowers, *J. Chem. Phys.* **95**, 3835-3837 (1991)
[2] C. Lifshitz, T. Peres, I. Agranat, *Int. J. Mass. Spectrom. Ion Proc.* **93,** 149-163 (1989)
[3] H. Hrodmarsson, J. Bouwman, A. Tielens, H. Linnartz, *Int. J. Mass Spectrom.* **476,** 116834 (2022)
[4] J. Buntine, *et al. Rev. Sci. Instrum.* **93,** 043201 (2022)
[5] S. Marlton, *et al. J. Phys. Chem.* **127,** 1168–1178 (2023)
[6] C. Liu, P. Watkins, P. Taylor, E. Bieske, *J. Phys. Chem. Lett.*, **16**, 12989–12996 (2025)

Towards State- and Time-Resolved Fluorescence Spectroscopy of Astrochemically Relevant Ions

N. Asanova[1], S. Gupta[1], S. Swain[1], H. Haak[1], G. Meijer[1], and J. A. Lau[1]
1*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany*

In the interstellar medium, where collisional stabilization after chemical reactions or photoexcitation is unlikely, unimolecular stabilization channels—such as radiative cooling—become increasingly important. An improved understanding of radiative emission may further help in identifying additional molecules in space. While most molecules in the interstellar medium have been detected through a combination of radioastronomy and microwave spectroscopy, numerous molecular emission lines observed with telescopes in the visible and infrared are so far unassigned [1,2]; laboratory emission spectra measured under comparable conditions are, however, rarely available.

Especially recurrent fluorescence has received significant attention as an efficient radiative cooling mechanism for isolated gas phase molecules throughout the last decade and has been shown to play a role in many polycyclic aromatic hydrocarbons and carbon chains [3]. Its mechanism involves inverse internal conversion, populating an excited electronic state, followed by visible/near-IR fluorescence [4], thereby leading to efficient relaxation of highly vibrationally excited molecules on µs-ms timescales.

To overcome the limitations of current experimental approaches and measure the dispersed emission spectra and rates of molecules showing recurrent fluorescence, my group at the Fritz Haber Institute is currently building a new experimental setup that is specifically designed for fluorescence spectroscopy under the relevant conditions and timescales. Bursts of molecular ions, prepared in a pulsed ion source, will be efficiently loaded into a cryogenic, linear Paul trap at high density, in which they are cooled to ~10 K through a pulse of buffer gas. Following nanosecond laser excitation, the emitted light is then spectrally dispersed and detected with single-photon sensitivity through either a photomultiplier tube or an intensified CCD camera.

Recent advances in our experimental design addressing multiple challenges of this experiment, such as maximizing the number of stored ions, avoiding collisional quenching and reducing unwanted background light, will be presented.

[1] S. Kwok, Astrophys. Space Sci. 367, 16 (2022).
[2] T. S.-Y. Lai et al., Mon. Not. R. Astron. Soc. **469**, 4933-4948 (2017).
[3] H. B. Pedersen, L. H. Andersen, Phys. Rev. A 112, 022820 (2025).
[4] A. Léger et al., Phys. Rev. Lett. 60, 921-924 (1988).

Formation of Uracil and Thymine in the ISM

Reetu,[1] Rue Cavanagh[1], Andrzej Machowski[1], Alasdair J. Massey[1], and Anthony J. H. M Meijer[1]
[1]Chemistry, School of Mathematical and Physical Sciences, University of Sheffield, Western Bank, Sheffield S3 7HF, United Kingdom

The interstellar medium contains vast dust clouds, which can be chemically incredibly diverse. The grain species in these clouds are covered by a variety of small ice species, include H2O, CO, H2CO, CO2, MeOH, CH4, and NH3. These ices can photodissociate to generate radicals, which can lead to further, more complex molecules. Of particular interest is the formation of molecules that are potentially important for the abiotic origin of life, such as urea or nucleobases. In particular, the detection of uracil and thymine in equal measure on the asteroid Bennu[1] is notable, as the preferential formation of uracil over thymine is used as a starting point for the RNA world hypothesis. Hence, we have investigated the potential formation of uracil and thymine, based on previous work on the formation of urea.[2] Based on that work, we have now investigated new pathways for the formation of urea and thymine, based on the double addition of isocyanic acid to acetylene and propyne, respectively.

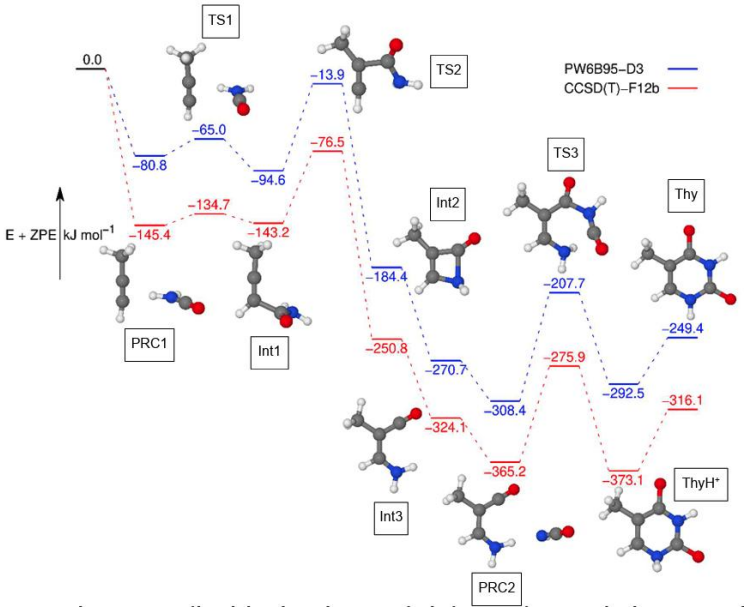

Figure 1: Energy (E + ZPE) profile for the formation of thymine within the ISM, via initial addition of propyne and N-protonated isocyanic acid.

[1] D. P. Glavin et al., Nat. Astron., 9, 199 (2025).
[2] E. C. S. Slate et al., Mon. Not. Roy. Astron. Soc., 497, 5413 (2020).

The Infrared Fingerprints of Cosmic Carbon Chains

T. E. Doglas-Walker, A. Debnath, O. O'Neill and E. K. Campbell
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Laboratory astrochemistry provides a controlled route to probe the formation, stabilisation, and fragmentation dynamics of pure-carbon molecular ions under astrochemically relevant conditions, enabling direct identification of unresolved spectral features. The Diffuse Interstellar Bands (DIBs) and the Unidentified Infrared (UIR) emissions are among the longest unexplained astronomical observations. Only the fullerene cation (C60+) has been conclusively identified as a carrier of some DIBs, leaving polycyclic aromatic hydrocarbons and carbon-chain species as prime candidates. UIR emissions spanning 3.3–11.3 µm are associated with sp2-carbon containing molecules, motivating the investigation of pure-carbon molecular ions. This study focuses on the infrared spectroscopic characterisation of C-chain cations, particularly 4n+ systems with n = 2-7, alongside an exploration of previously studied Giant Infrared Resonance.1 The experiments employ Laser Vaporisation Radio Frequency Trap Action Spectroscopy2, in which carbon clusters are generated via laser ablation of graphite, trapped, and cooled to ~3 K in a quadrupole ion trap. The formation of weakly bound He-tagged complexes provides a sensitive probe of cationic C-clusters through the resonant infrared excitation, leading to He detachment. This process provides insight into how low-energy vibrational excitation couples with weak intermolecular bonding in cold-ion environments.

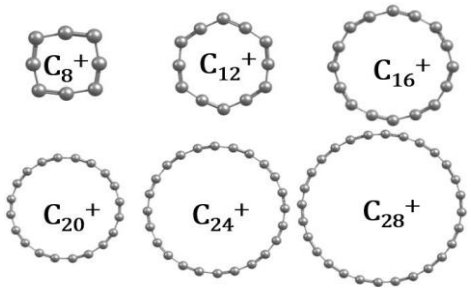

Figure.1 Structures of cyclic carbon clusters C4n+ (n = 2-7)

The measured spectra for cyclic-C8+-C28+ reveal a pronounced linear trend in vibrational behaviour for larger systems (C16+-C28+), while smaller chains exhibit clear deviations, indicating size-dependent structural effects. Additional spectral features, including shoulder peaks attributed to Fermi resonance, are observed in a few clusters, alongside enhanced absorption intensity and a broader asymmetric peak in C8+ compared to C12+. Computational analysis using several density functional and non-empirical methods shows strong agreement with experiment, confirming that these ions predominantly adopt polyynic-type structures. The deviation in position of the band maxima and intensities of these carbon-chain molecules is explained in terms of the bond length and angle alteration in the polyynic chain. While these spectral data do not yet enable a definitive assignment of these clusters as UIR carriers, they strongly indicate that these species may collectively contribute to the observed features alongside known carbon-chain molecules, including C2, C3, C5, $C60^+$, C60 and C70. These findings reinforce the growing evidence for carbon-chain systems as structurally and dynamically active contributors to unresolved interstellar signatures and mark a step forward in identifying UIR carriers. This study gains additional significance in the era of unprecedented infrared sensitivity and resolution offered by the James Webb Space Telescope (JWST), which provides new opportunities to connect laboratory spectroscopy and dynamics with astronomical observations.

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Confined and Interfacial Water: Insights from Surface Vibrational Spectroscopy

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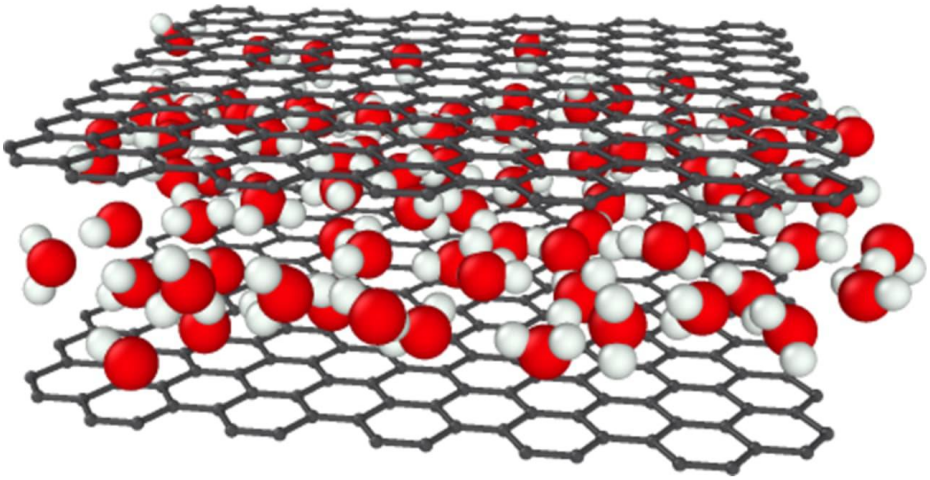
Understanding how water, ions, and surfaces interact across length scales is central to electrochemistry, nanofluidics, and catalysis. In particular, the impact of hydrogen-bond network termination and interfacial charges on the arrangement of counterions and water has been the subject of intense debate. Across three studies, we have established a molecular-level picture of structure and dynamics at aqueous interfaces under confinement and electrostatic perturbation. At angstrom-scale confinement, interfacial effects dominate water structure, disrupting bulk hydrogen bonding and creating asymmetric environments governed by surface interactions. [1] Extending this, we show that even nominally neutral materials, such as hexagonal boron nitride, spontaneously acquire surface charge upon contact with water, indicating that electric doublelayer formation is nearly universal at solid–liquid interfaces. [2] Finally, femtosecond spectroscopy reveals that ionic rearrangements in the electric double layer occur on tens-of-picoseconds timescales, faster than diffusion-limited expectations but consistent with classical Debye theory. [3] Together, these results provide a unified molecular understanding of how confinement, interfacial polarization, and charge govern water behavior in nanofluidic and electrochemical systems.



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[2] Y. Wang et al., J. Am. Chem. Soc. 147, 30107 (2025).
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Chemical Physics at the Gas-Liquid Interface: From Liquid Microjets to Molten Metals

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There is a particularly challenging “phase” of matter associated with the microscopically thin interface (< 10 molecules thick) *between* gases and liquids which is poorly understood and yet plays a crucial role in diverse chemical scenarios ranging from atmospheric aerosol chemistry to transpiration of O2/CO2 in alveolar sac lung tissue. Work in our group has recently been focused on exploring the dynamics of collisional interactions at such interfaces from a fundamental chemical physics perspective. Time permitting, this talk will present results from our group in three different complementary areas: i) liquid microjet studies of quantum state resolved NO solute evaporation dynamics at the gas-water, gas-benzyl alcohol, and gas-butanol interface, ii) rovibrational inelastic scattering of supersonically cooled HCl from liquid like self-assembled monolayers (SAMs) via resonance-enhanced photoionization (REMPI)/velocity map imaging (VMI), and iii) rovibronic thermalization of supersonically cooled NO in collisions at the gas-hot molten metal (Ga, Au) interface. As one recurring theme, we find that molecular projectiles inelastically or evaporatively scatter from these gas-liquid interfaces into internal quantum state distributions that can be substantially *out of equilibrium* with respect to the bulk (TS). By detailed balance considerations, these data unambiguously indicate that even simple molecules can exhibit a strong rovibronic state dependence to how they “stick” to accomodate with,and eventually solvate into the liquid phase. Such results highlight the surprising ubiquity of ***non-equilibrium effects*** in collisional energy transfer dynamics at the gas-liquid interface.

High-resolution 2D-IR Spectroscopy in Low Temperature Solids: Symmetry-Breaking and Anharmonic Coupling Maps

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Current affiliation: CNRS - Université de Strasbourg, Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS), Strasbourg, France.

We report 2D-IR spectra of molecules trapped in cryogenic matrices at very high spectral resolution, measured by a combination of a 320 pixel detector and >30 ps coherence time scanning [1].
The T1u asymmetric C≡O stretch vibrations of W(CO)6 give rise to a single band in the liquid phase IR spectrum, but multiple bands are observed in solid nitrogen [2, 3]. In this matrix, the 3-fold degeneracy is fully lifted for approximately two thirds of the trapped molecules, while the remaining ones maintain the Oh symmetry and exhibit a single T1u transition. Cross-peaks between the three orthogonal modes of lower symmetry reveal weak negative anharmonic coupling (-1 cm-1). The same coupling also gives rise to a cross-peak on the diagonal for the degenerate T1u band (Figure 1). Waiting time- and polarization-dependent experiments evidence excitation transfer between the non-degenerate modes on a timescale of tens of picoseconds at 20 K, which becomes slower and mode-dependent at 6 K. On the other hand, energy redistribution among the components of the high-symmetry modes (T1u) shows no variation with temperature.
Next to providing such textbook examples of symmetry-breaking, our high-resolution 2D-IR spectra of matrix-isolated molecules can directly map the anharmonic coupling between normal modes in the fingerprint region, or, in rare-gas solids, resolve mode-connectivity for different trapping sites and site-dependent anharmonic couplings.

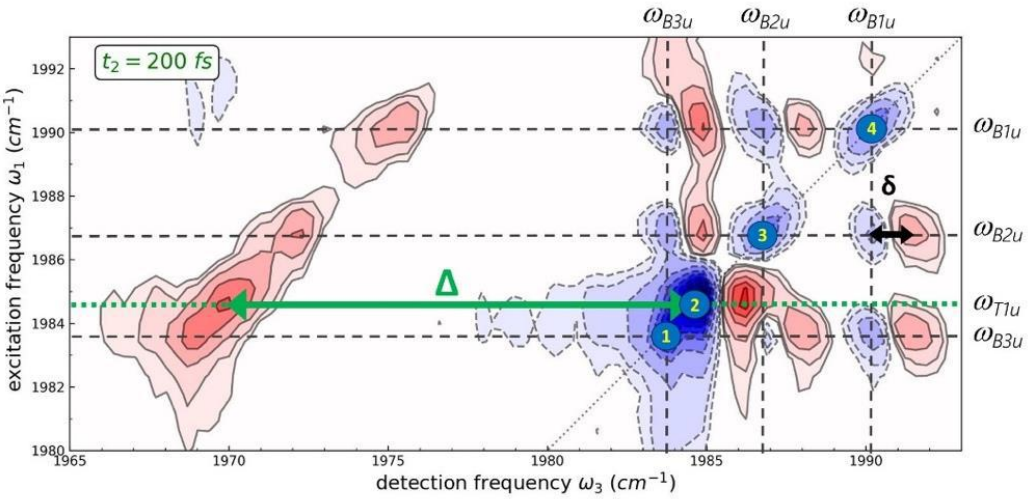

Figure 1. 2D-IR spectrum of W(CO)6 in solid nitrogen at 20 K showing the asymmetric stretch signals for both the degenerate (2) and low-symmetry sites (1,3,4).

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Exploring Photochemistry for Quantum Optics with Large Organic Molecules

Leeyeong Kim,[1] Olga Rybakova,[1] Josef Reisinger[1], Marcel Strauß[1], Philipp Geyer[1], Stefan Gerlich[1], Amal Kumar[2], Valentin Köhler[2], Markus Arndt[1*]

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Demonstrating superpositions of distinct states of massive, warm, organic, or inorganic systems remains a long-standing goal at the quantum-classical boundary. Over the past decades, numerous experimental setups were capable of demonstrating the quantum delocalization of massive objects across distances many times their own diameter. These range from far-field diffraction of carbonaceous molecules [1] to near-field interferometry with atoms, vitamins, peptides [2], as well as massive nanoclusters exceeding 170 kDa [3].

Large neutral biopolymers represent a challenging material class for such studies, still lacking well-defined, low-velocity molecular beams, coherent beam splitters or soft ionization for mass detection. Here, we discuss in particular the use of photocleavable tags: molecules of interest are synthesized with a covalently attached photocleavable tag that absorbs photons at a target wavelength. Upon photoexcitation, the tag cleaves from the parent molecule, optionally carrying charge and momentum. This enables charge-state control, and the separation of parent and fragment can induce a recoil that shall be exploited in photodepletion beam splitters. Recent work demonstrates that tags can be cleaved from biomolecules in the gas phase by a single or two photon, and that molecules can be tailored to respond to different wavelengths from ultraviolet to visible light [4]. Here, we will discuss the processes involved in the photochemistry and how they appear promising in a novel light-grating mechanisms for matterwave interferometry with organic molecules that cannot be simply photoionized.

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Using Soft X-rays to Unravel Light-Induced Dynamics in Gas-Phase Systems

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Understanding ultrafast molecular dynamics on their intrinsic femtosecond timescales is essential for revealing microscopic mechanisms governing charge transfer and structural transformations. X-ray Free-Electron Lasers (XFELs) provide unique capabilities to probe such processes by combining femtosecond pulse durations with element specificity to access electronic and nuclear dynamics in real time. The soft X-ray branch Athos of SwissFEL provides photons in an energy range from 350 to 1800 eV, covering essential K-edges of the light elements nitrogen and oxygen and the metal L-edges. In addition to standard SASE millijoule level operation, Athos also provides special beam modes, such as short pulses down to the attosecond regime and multi-color X-ray pulses. The Maloja endstation is one of the experimental stations located at Athos and specializes on atomic, molecular, non-linear and chemical sciences. Maloja supports a wide range of experimental techniques ranging from electron, ion and X-ray spectroscopy to single-particle imaging. This talk will focus on light-induced dynamics of gas-phase molecules and clusters obtained by X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy (XAS). Time-resolved XPS is a highly sensitive probe to the chemical environment, which will be illustrated by tracing prototypical reactions in gas-phase molecules and nanoplasma ignition in seeded helium droplets. The use of special beam modes, specifically two-color X-ray pulses, in combination with XAS will be introduced as a powerful tool to study core- and inner-shell dynamics in molecules.

Imaging nano-samples in free flight with intense X-ray pulses: probing highly excited matter with extreme precision

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Single-particle Coherent Diffraction Imaging (CDI) allows us to take snapshots of individual nanoscale objects and create movies of their ultrafast dynamics, revealing structures and processes that no other method can access. Intense and short pulses of X-ray free-electron lasers (XFELs) or intense high-harmonic generation (HHG) based sources are diffracted by a free-flying nanostructure, forming an interference pattern that is captured with a large-area detector. With computer-based iterative phase-retrieval [1] or forward-fitting methods [2] we reconstruct a snapshot of the object and follow its transformations after laser excitation in real time [3].
In my talk I will present our recent findings on superheated silver nanoparticles and discuss the novel opportunities for tracking ultrafast electron dynamics in nanoscale matter with two-color X-ray CDI [4, 5].

[1] A. Colombo, et al., SPRING, an effective and reliable framework for image reconstruction in single-particle Coherent Diffraction Imaging, npj Computational Materials 11, 265 (2025).
[2] A. Colombo, et al., Three-dimensional femtosecond snapshots of isolated faceted nanostructures, Science Advances 9, eade5839 (2023).
[3] Dold et al., Melting, Bubblelike Expansion, and Explosion of Superheated Plasmonic Nanoparticles, Physical Review Letters 134, 136101 (2025).
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Simulating the ultrafast dynamics of multi-mode multi-state molecular systems coupled to a dissipative environment

David Picconi[1]
[1]*Institute of Theoretical and Computational Chemistry Heinrich Heine University Düsseldorf, Germany*

Ultrafast processes in condensed phase photoexcited molecular systems involve the transition from a coherent dynamical regime – where a precise phase relation exists between different wave packet components – to incoherent "classical-like" dynamics. The decoherence process is driven the dissipation due to the surrounding molecular environment.
From the computational viewpoint, modelling the dynamics of nonadiabatic vibronic quantum systems interacting with fluctuating environments becomes especially challenging when the system' s high dimensionality precludes the calculation of its eigenstates. To overcome this limitation, a novel eigenstate-free formalism is introduced. This approach represents the open quantum system as a mixture of high-dimensional, time-dependent wave packets, governed by coupled Schrödinger equations [1], while the environment is modeled using a multi-component quantum master equation [2]. A computationally efficient implementation of this formalism employs a variational Gaussian/ multiconfigurational time-dependent Hartree (G-MCTDH) ansatz for the wave packets and propagates the environment dynamics using hierarchical equations truncated at the first or second level.
The methodology is validated through simulations of the dynamics in vibrationally excited adsorbates [2], multichromophoric aggregates, and symmetry-breaking donor-acceptor systems [3,4], explicitly incorporating multiple vibrational modes and accounting for the effects of the residual bath in full dimensionality.
These results demonstrate the potential of the approach as a powerful quantum dynamical method for modeling complex system–bath interactions involving numerous degrees of freedom across multiple time scales.

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Observation of thermal non-equilibrium in uniform supersonic flows

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Reactions occurring in the interstellar medium and other cold environments (10 – 200 K) are of considerable interest to both theoreticians and experimentalists, especially ion–neutral and neutral–neutral reactions that exhibit non-Arrhenius behaviour at low temperatures. Many such reaction rate coefficients have been measured with the CRESU (*Cinétique de Réaction en Ecoulement Supersonique Uniforme*) technique over the last 40 years, contributing to international astrochemical databases [1]. Crucial to this experimental methodology is the uniformity of the gaseous flow in terms of both temperature and density, and an assumption of local thermal equilibrium, where all degrees of freedom are thermalised. In this work, we present a comprehensive investigation using multiple measurement techniques, including infrared frequency comb spectroscopy, laser-induced fluorescence, impact pressure measurements, and computational fluid dynamics simulations. We report the observation of a vibrational hot band, with an intensity inconsistent with the rotational temperature under all conditions of flow [2]. Deviations between the rotational temperature and the Pitot temperature from conventional impact pressure measurements are also observed. These results indicate that a single temperature is insufficient to describe the internal energy distributions possessed by molecules undergoing reaction in the uniform supersonic flow, and consideration must be given to the energy present in different modes when incorporating experimentally measured reaction rate coefficients into astrochemical kinetic databases.

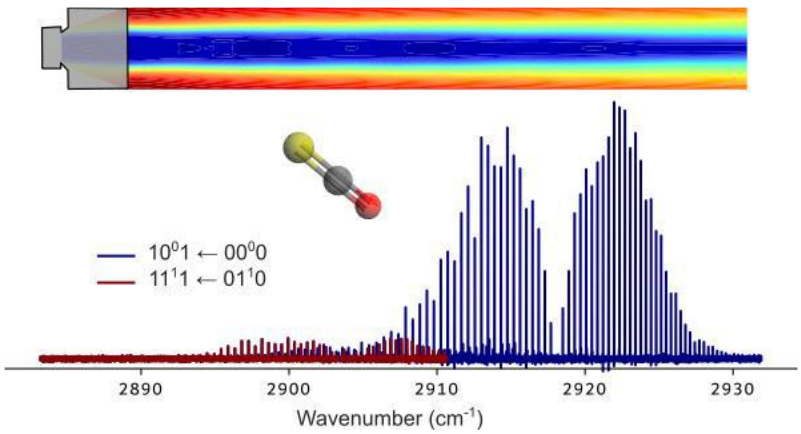

Figure 1. CFD simulations of temperature within the uniform supersonic flow (top) and an infrared frequency comb absorption spectrum (bottom) of OCS in an argon flow.

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UV to Far-UV Photodissociation Reveals the Role of Sulfur–Aromatic Interactions in Peptides

Laura Pille[1], B. Oostenrijk[1], J. Leroux[2], L. MacAleese[3], M. Girod[4], A. Giuliani[5], L. Nahon[5], D. Scuderi[6], S. Bari[1,7], L. Schwob[1]

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While ultraviolet photodissociation (UVPD) at fixed photon energy is commonly used for peptide sequencing and structural characterization in mass spectrometry, extending this approach into action spectroscopy spanning from UV to Far-UV provides a more comprehensive picture of peptide fragmentation. Since each amino acid in the Far-UV region exhibits a unique spectral fingerprint [1] and aromatic residues can be selectively excited in the UV region, this technique enables residue-specific identification.

In biological systems, aromatic amino acids frequently engage in non-covalent interactions—such as π-π, cation-π, or sulfur-π (S-π) interactions—which are crucial for stabilizing tertiary structures. Among these, S-π interactions involving methionine (Met) and aromatic residues like tyrosine (Tyr) or tryptophan (Trp) have gained significant attention. Protein database analyses have identified these motifs in one-third of all known proteins [2, 3], highlighting their abundance in nature. Furthermore, the disruption of these interactions is associated with neurodegenerative diseases, such as Alzheimer's [4, 5].

This study demonstrates how photodissociation across the UV to Far-UV range can be used to identify spectroscopic fingerprints of sulfur–aromatic interactions in peptides. By systematically varying the proximity between the aromatic residue and the sulfur atom, as well as the nature of the aromatic residue and the peptide size, we show how specific structural motifs modulate dissociation pathways. Our findings demonstrate that these non-covalent interactions significantly dictate the resulting fragmentation patterns, emphasizing the importance of these weak interactions on peptide characteristics.

[1] T. Goto, A. Ikehata, Y. Morisawa, Y. Ozaki, J. Phys. Chem. A **117**, 2517 (2013).
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Program

Tuesday, September 8th, 2026

	Chair: ***Bas van der Meerakker***
9:00 a.m.	**Henrik Stapelfeldt** Real-time observation of the diffusion-limited formation of an ion-molecule complex
10:00 a.m.	**Stefanie Gräfe** Strong-field many-body dynamics in confined systems
10:30 a.m.	Coffee Break
11:00 a.m.	**Andrew Orr-Ewing** Photochemical Dynamics in Aerosol Microdroplets
11:30 a.m.	**Steen Brøndsted Nielsen** Gas-Phase FRET at Cryogenic Temperatures: Talking to Specific Conformers
11:50 a.m.	**Brendan Wouterlood** Local and Non-Local Double Ionisation of Micro-Solvated Nucleobases
12:10 p.m.	**Sebastian Trippel** Unraveling the early-stage dynamics of ionized water dimer in energy and time
12:30 p.m.	Lunch Break
	Chair: ***Daniel Neumark***
2:00 p.m.	**Bas van de Meerakker** Cold and Controlled Collisions using Tamed Molecular Beams
2:30 p.m.	**Xingang Wang** State-to-State Reaction Dynamics Using Velocity Map Ion Imaging
3:00 p.m.	**Andrea Orban** Quantum study of ultracold atom-ion excitation exchange
3:20 p.m.	**Nanditha Sunil Kumar** Cold chemistry of single trapped H2O+ ions with neutral HD molecules in a cryogenic ion trap
3:40 p.m.	Coffee Break
4:10 p.m.	**Marcel Mudrich** Penning ionization electron spectroscopy of atoms and molecules in or on helium nanodroplets
4:40 p.m.	**Elisabeth Gruber** Exploring Molecular Ions and Cryogenic Chemistry in Charged Helium Nanodroplets
5:10 p.m.	**Poster session 1** Entrance Hall KG I

Real-time observation of the diffusion-limited formation of an ion-molecule complex

Henrik Stapelfeldt
Department of Chemistry, Aarhus University, Denmark

Time-resolved studies of bond making between two molecules or atoms are notoriously difficult due to the challenge of measuring when the two reactants meet. This is determined by diffusion – a process that is typically not controllable on ultrafast time scales. Previous works used a weakly-bonded precursor complex of the two reactants to eliminate diffusion or introduced one of the reactants in a dense environment of reactants to minimize diffusion or allow it to be simulated by models. I will present real-time measurements of the bimolecular reaction where a Li+ ion diffuses towards a benzene dimer and forms a Li+Bz2 complex, a textbook cation-π-system, inside a liquid helium nanodroplet [1]. After formation at the droplet surface, Li+ solvates [2-3], then diffuses ballistically with a velocity of 43 m/s and finally binds to Bz2 near the droplet center to form Li+Bz2. The experimental findings are compared to and rationalized by ring-polymer molecular dynamics simulations. Results from ongoing studies of real-time imaging of stereodynamics, i.e. how the molecular orientation changes as the ion approaches, will also be presented.

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complex. Nature Comm. **17**, 1249 (2025).
[2] S. H. Albrechtsen *et al.*, Observing the primary steps of ion solvation in helium droplets. *Nature* **623**, 319 (2023).
[3] J. K. Christensen *et al., Time-resolved solvation dynamics of Li+, Na+ and K+ ions in liquid helium nanodroplets.* Phys. Chem. Chem. Phys., **27**, 24184 (2025).

Strong-field many-body dynamics in confined systems

M. Thümmler[1], A. Croy[1], D. Kartashov[2,3], U. Peschel[3,4] and Stefanie Gräfe[1,3,5]

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Recent experiments have demonstrated high-order harmonic generation (HHG) in confined systems, such as 2D materials or semiconductor quantum dots (QDs) [1,2]. These experiments have shown surprising effects such as, e.g., strong spin or valley (de)polarization, signatures of the Berry phase (for 2D materials), or a very strong dependence of the harmonic signal strength on the quantum dot's size. A thorough theoretical description of HHG in confined systems constitutes many challenges: (i) QDs consist of many hundreds to thousands of atoms, exhibiting structural disorder, surface roughness, surfactants and other contributions. Consequently, the dots' electronic states form – due to their finite and irregular structure – discrete electronic levels rather than electronic bands, precluding a direct application of the semiconductor Bloch equations (SBE). At the same time, atomistic *ab initio* real-time time-dependent density functional theory (rtTDDFT) remain computationally demanding. (ii) for 2D materials, both the SBE and rtTDDFT can be employed, require, however, a dephasing time to obtain meaningful harmonic spectra. The commonly utilized phenomenological values range between 2-10 fs, are shorter than the optical cycle of the driving laser field and are an order of magnitude faster than the corresponding values in the perturbative regime. Moreover, the physical origin of ultrafast decoherence processes leading to these values has remained unclear until now.

In this talk, we present our joint experimental-theoretical work on HHG in confined systems [1,3,4]. In QDs, we observed a strong suppression of the intensity for above-bandgap harmonics for dots below 3 nm diameter [1]. We developed a real-space tight-binding model, explaining the suppression due to scattering of the laser-driven electron-hole motion off the dot's boundary and the corresponding loss of coherence [3]. In 2D semiconductors, via wavelength-dependent HHG measurements and simulations, we identified electron-phonon scattering as the dominant ultrafast dephasing mechanism. Our SBE-based calculations quantitatively reproduce the experiment when incorporating a momentum-dependent dephasing time, derived from first principles scattering rates [4]. Allover, we identify various mechanisms leading to ultrafast dephasing, providing a framework for understanding coherence in strongly driven confined many-body systems.

[1] H. Gopalakrishna, et al., Phys. Rev. Research. **5**, 013128 (2023).
[2] K. Nakagawa, et al., Nature Phys., **18**, 874–878 (2022); I. Tyulnev, et al., Nature **628**, 746 (2024).
[3] M. Thümmler, A. Croy, U. Peschel, S. Gräfe, J. Chem. Phys. **164**, 094114 (2026).
[4] V. Korolev T. Lettau, V. Krishna, A. Croy, M. Zuerch, C. Spielmann, M. Wächtler, U. Peschel, S. Gräfe, G. Soavi, D. Kartashov, Nature Comm., accepted (2026); arXiv:2401.12929.

Photochemical Dynamics in Aerosol Microdroplets

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The photochemistry occurring in aerosol particles and droplets dispersed in the Earth's atmosphere impacts both the chemical composition of the troposphere and the global climate. Ultrafast transient absorption spectroscopy methods can explore the photochemical pathways taken by the organic constituents of these aerosols, but these laboratory measurements typically use sample solutions with volumes of a few millilitres [1-4]. When the solute is instead confined in picolitre aerosol droplets, the photochemistry is expected to be impacted in numerous ways. For example, the water-air interface becomes increasingly important because of the large surface-area to volume ratios of the droplets. In addition, the solutes may aggregate or reach supersaturated concentrations as the droplet water content evaporates, and coupling to whispering gallery modes of spherical droplets can modify excited-state radiative lifetimes.

Results will be presented from recent measurements of fluorescence lifetimes for dye molecules confined in microdroplets, and interpreted in terms of the effects of the droplet environment. The aqueous photochemistry of pyruvic acid, an important contributor to secondary organic aerosol growth in the atmosphere, will be contrasted in bulk and microdroplet environments.

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Gas-Phase FRET at Cryogenic Temperatures: Talking to Specific Conformers

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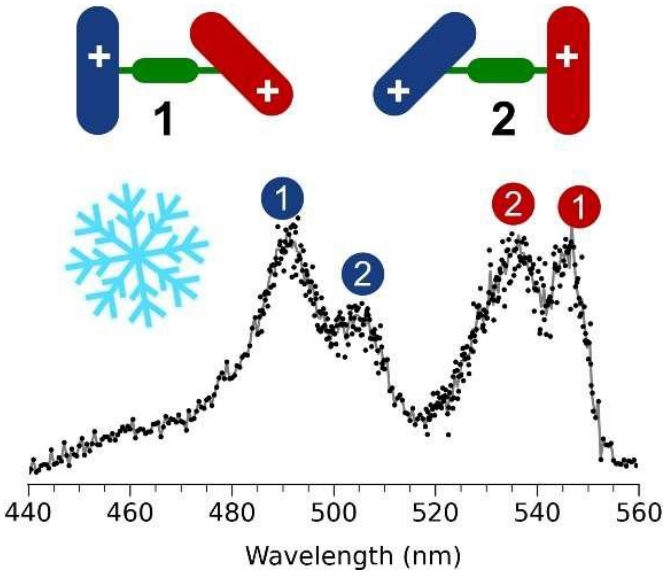
Various techniques are available to illuminate geometric structures of molecular ions in gas phase, such as Förster Resonance Energy Transfer (FRET) informing on distances between two dyes covalently attached to a molecule [1]. Typically, cationic rhodamines, which absorb and emit visible light, are used for labelling. Extensive work has revealed that the transition energy of a rhodamine is intricately linked to its nearby microenvironment, with nearby charges causing Stark-shifted emission. This occurs because the inter-dye Coulomb interaction is weaker in the excited state (S1) than in the ground state (S0) due to the increase in polarizability upon excitation. Therefore, absorption and emission spectra, along with FRET efficiencies, provide insights into structural motifs. At room temperature, multiple conformers often coexist, leading to overlapping absorption bands among different conformers and broad spectra.
To study specific conformers, it is necessary to isolate them, for example, using ion-mobility spectrometry. Another approach is to reduce temperature, which results in spectral narrowing and distinct absorption bands (cf., figure below for a molecule in green tagged with two dyes, colored blue and red), allowing for the selection of specific conformers through selective excitation. Here, I will describe the instrumentation used for cryogenically cold FRET experiments [2] and discuss recent results for small model systems [3-5], as well as future directions for a technique still in its infancy.



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Local and Non-Local Double Ionisation of Micro-Solvated Nucleobases

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Secondary ionisation mechanisms are an important source of low kinetic energy electrons, which can cause mutagenic DNA damage in biological systems. In the condensed phase, non-local processes, such as ICD (inter-molecular Coulombic decay), significantly contribute to the abundance of low energy electrons and can also affect the presence of molecular cationic fragments and radicals. An understanding of radiation damage, thus requires understanding the effects that the solvated aqueous environment has on the dynamical relaxation processes triggered by ionisation.

By limiting the condensed phase environment to only a few molecules in a micro-solvated system, the study of both local and non-local relaxation processes is possible, along with the implementation of gas phase detection techniques such as electron-ion-ion coincidence spectroscopy. We present an electron ion (multi-)coincidence study of the micro-solvated nucleobase, thymine, and its analogue, pyridine, doubly ionised by synchrotron radiation in the XUV. The detection of both cationic fragments in coincidence with a photo-electron, makes it possible to disentangle signals arising from differing double-ionisation processes of the micro-solvation complexes. We found that processes which create local doubly ionised moieties, such as Auger-Meitner decay and direct double ionisation of the biomolecule, stabilise by proton transfer reactions from the doubly-ionised biomolecule to the solvent water. This experimental apparatus enables us to distinguish these signals from charge separated states produced by ICD, that undergo Coulomb explosion without prior proton transfer. The branching ratios between local and non-local double-ionisation processes can thus be determined, along with their dependence on the photon energy and the molecular species in question.

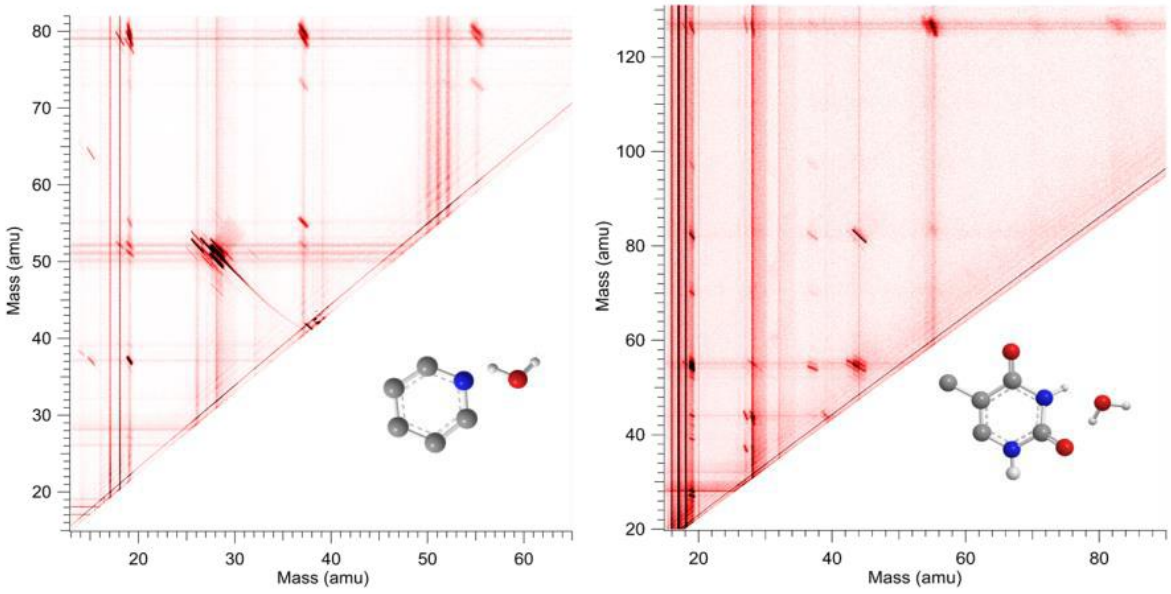

Figure 1. Left (right) ion-ion coincidence map of pyridine (thymine) – water complexes after ionisation by synchrotron radiation at 36 eV

Unraveling the early-stage dynamics of ionized water dimer in energy and time

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Radiation chemistry in aqueous systems initiated by ionizing radiation is primarily governed by the ultrafast dynamics of water molecules. The prompt response of the aqueous environment involves the formation of hydrated electrons and proton transfer on femtosecond timescales [1]. We employed a disruptive-probing scheme [2] on a purified ensemble of water dimer to investigate the prompt dynamics after strong-field ionization [3]. Investigating the relation of the hydronium fragment kinetic-energy release with the observed timescales reveals a coupling between proton transfer and fragmentation. With the observation of water-dimer-cation stabilization, this provides new insight into the ultrafast post-ionization dynamics underpinning radiation chemistry in aqueous environments.

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Cold and Controlled Collisions using Tamed Molecular Beams

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The study of molecular collisions with the highest possible detail has been an important research theme in physical chemistry for decades. Experimentally, the level of detail obtained in these studies depends on the quality of preparation of the collision partners before the collision, and on how accurately the products are analyzed afterward.
Over the last years, methods have been developed to get improved control over molecules in a molecular beam. With the Stark decelerator, a part of a molecular beam can be selected to produce bunches of molecules with a computer-controlled velocity and with longitudinal temperatures as low as a few mK. The molecular packets that emerge from the decelerator have small spatial and angular spreads, and have almost perfect quantum state purity. These tamed molecular beams are excellent starting points for high-resolution crossed beam scattering experiments.
I will illustrate the possibilities this technology offers to study molecular collisions with unprecedented precision and at low collision energies. I will discuss our most recent results on the combination of Stark deceleration and velocity map imaging. The narrow velocity spread of Stark-decelerated beams results in scattering images with an unprecedented sharpness and angular resolution. This has facilitated the observation several quantum effects in state-to-state cross sections, such as diffraction, scattering resonances and product pair correlations in bimolecular collisions. Finally, I will present recent results on bimolecular collisions at collision energies down to 0.1 cm-1 obtained by merged beam configurations, featuring novel effects induced by the dipole-dipole interaction.

State-to-State Reaction Dynamics Using Velocity Map Ion Imaging

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Crossed molecular beam scattering, combined with modern laser-based detection, has become a pivotal tool for unraveling the quantum dynamics of chemical reactions. Recent advances in velocity map ion imaging and state-selective ionization now provide unprecedented access to state-to-state dynamics, yielding fully resolved differential cross sections for elementary reactions [1-3].
In this talk, I will first outline the methodology established in our state-to-state studies of the H + HD/D_2 benchmark systems [4-6], and then present our recent, preliminary imaging measurements on two challenging reactions, from which quantum-state-resolved differential cross sections have been extracted for both systems. The first is $N(^2D) + D_2 \rightarrow ND + D$, a prototypical elementary reaction proceeding via a deep potential well. The second is $H + O_2 \rightarrow OH + O$, an endothermic and strongly activated reaction of central importance to combustion chemistry, for which the extremely low reactivity and the difficulty of product detection have long hindered state-resolved measurements.
Taken together, these measurements could provide stringent benchmarks for ab initio potential energy surfaces and full-dimensional quantum dynamics calculations, and offer a deeper mechanistic picture of elementary reactions at the quantum level.

Acknowledgements: This work was supported by the National Natural Science Foundation of China (Grant No. 22125302).

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Quantum study of ultracold atom-ion excitation exchange

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We present a full quantum model for the dynamics of cold collisions between a groundstate Rb atom and a metastable excited Sr+ ion [1]. Despite the apparent simplicity of such diatomic systems, our work highlights the complexity of the dynamics induced by non-adiabatic coupling terms, for which a specific theoretical treatment based on original quasi-diabatic models [2] had to be developed.
Starting from our calculated Hund‘s case (a) potential energy curves where molecular spin-orbit interaction has been introduced via a quasi-diabatic transformation, we calculated cross sections and reaction rates for two processes, namely electronic excitation exchange (EEE) and fine-structure quenching (FSQ), while no charge exchange is expected to happen. Our results are in satisfactory agreement with the experiment [3] for the EEE process, confirming the quality of our molecular data not only for the excited electronic manifold, but also with respect to the modeling of spin-orbit interaction. In contrast, a significant discrepancy in the FSQ rates is obtained, which is assigned to a presumably pronounced dependence of the process on the initial Zeeman sublevels in which the reactants are prepared in the experiment. This represents a natural extension of our formalism by including the corresponding quantum numbers in the basis set chosen for the dynamical calculations.

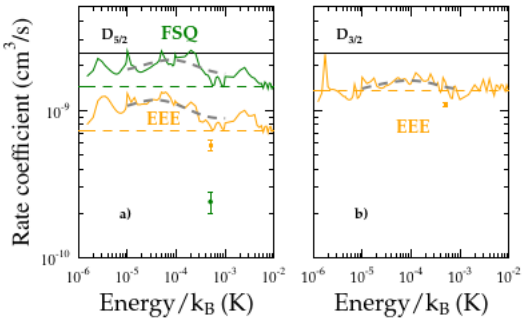

Figure 1: Computed rate coefficients for the Rb(5S1/2)+Sr+(4D5/2) (panel a) and Rb(5S1/2)+Sr+(5D3/2) (panel b) incoming channels. Green solid line: FSQ. Orange solid lines: EEE. Black solid line: Langevin rate. Colored dashed lines: scaled Langevin rates

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Cold chemistry of single trapped H2O+ 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 H2O+ 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 H2O+ 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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Penning ionization electron spectroscopy of atoms and molecules in or on helium nanodroplets

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He nanodroplets are widely used as cold and inert spectroscopic matrices of embedded "dopant" molecules and clusters. Especially the ability of He nanodroplets to form unusual atomic and molecular complexes by aggregation inside the ultracold droplet environment makes them attractive „nano-cryo reactors" for spectroscopic and mass spectrometric studies [1]. However, upon electronic excitation or ionization of either the dopant or the He droplet, the latter itself becomes a reactive environment that can induce severe perturbations of spectra due to strong guest-host interactions. To date, only few photoelectron spectroscopy studies of dopants in He nanodroplets have been reported and significant line shifts and broadenings were observed.
An alternative method is Penning ionization electron spectroscopy (PIES). This method has its merits for its sensitivity to the spatial electron distribution of molecules, clusters, and surfaces and to vibrational and electronic excitations of the product ions. Traditionally, a rare gas atom, most often He due to its extremely high excitation energy, is prepared in an excited metastable state and collides with the target atom or molecule, M, to induce the ionization of the latter in the reaction He* + M → He + M+ + e-. In a series of recent experiments [2-5] we have shown that this reaction can be very efficient for M embedded in He nanodroplets that are resonantly excited by synchrotron radiation. By detecting the emitted electron e- using various techniques, we measure Penning ionization electron spectra which reveal valuable information about the electronic structure of the dopant M [3], its interaction with the local environment [5], and the excited states of its ion M+, see e.g. Fig. 1.

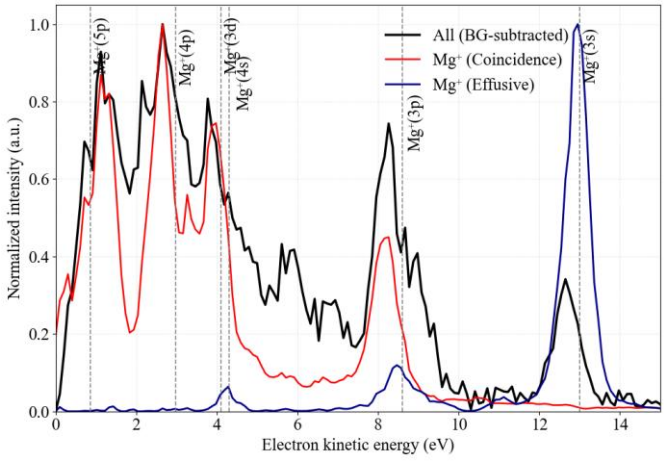

Figure 1 Photoelectron spectrum of free Mg atoms (blue line) and Penning ionization electron spectra of Mg atoms embedded in He nanodroplets. The spectrum in black is for all emitted electrons, the one in red shows the spectrum of electrons detected in coi

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Exploring Molecular Ions and Cryogenic Chemistry in Charged Helium Nanodroplets

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Helium nanodroplets provide a versatile platform for trapping, cooling, and stabilizing dopant species at ultralow temperatures. When these droplets carry multiple charges, they offer unique opportunities to investigate fundamental physical and chemical processes that are otherwise difficult to access. In addition, they enable the efficient production of helium-tagged molecular ions of both polarities, which serve as ideal targets for messenger spectroscopy [1].

We currently employ this approach to record absorption spectra of cold molecular ions of astrochemical relevance. By directly comparing laboratory spectra with astronomical observations, we seek to identify and characterize molecular ion species present in the interstellar medium [2–4].

Beyond spectroscopy, the ultracold and weakly perturbing environment of helium nanodroplets provides an attractive setting for studying chemical reactions under cryogenic conditions. As an example, I will discuss the formation of benzene through the sequential addition of two neutral acetylene molecules to the acetylene cation. The production of benzene is confirmed by helium-tagging spectroscopy in the visible spectral region [5].

To investigate reaction dynamics on extended timescales, ranging from seconds to minutes, we have recently begun trapping charged helium droplets in ion traps. In particular, we have successfully coupled a helium droplet source to a multi-reflection time-of-flight mass spectrometer operated as an electrostatic ion trap [6]. I will present the first results from these trapping experiments and conclude with an outlook on the future prospects and opportunities offered by this emerging approach.

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Program

Wednesday, September 9th, 2026

	Chair: ***Francesca Calegari***
9:00 a.m.	**Daniel Neumark** Spectroscopy and Scattering Experiments on Flat Liquid Jets
10:00 a.m.	**Thomas Allison** Imaging Exciton and Charge-Transfer Dynamics at Surfaces with Time-resolved Momentum Microscopy
10:30 a.m.	Coffee Break
11:00 a.m.	**Rebecca Ingle** Chemical Insights from Resonant Auger Spectroscopy
11:30 a.m.	**Jemma Gibbard** Visible Light Photochemistry of IO_2^-
11:50 a.m.	**Mathew Costen** Near-Surface Velocity-Map Imaging of Rotationally Inelastic Gas Surface Scattering
12:10 p.m.	**Wim van der Zande** The Advanced Research Center for NanoLithography: an example of a public-private partnership in the MOLEC field
12:30 p.m.	Lunch Break
1:30 p.m.	**Excursions** - Black Forest Hike - Wine Tasting
5:10 p.m.	**Lab visits**

Spectroscopy and Scattering Experiments on Flat Liquid Jets

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The dynamics of photoexcited solute molecules and the properties of liquid interfaces are studied by carrying out spectroscopy and scattering experiments on flat liquid water jets. In one set of experiments, solute dynamics are probed using time-resolved photoelectron spectroscopy in which molecules are photoexcited with a femtosecond UV pulse and photoionized with a time-delayed femtosecond XUV pulse (at 21.7 eV). The time-dependent photoelectron spectra provide a unique probe of the relaxation of photoexcited neutral and anionic species in aqueous solution. Results will be presented for several negative ions including phenolate,1 bromophenolate,2 and nitrophenolate. These experiments probe the competition among the various relaxation pathways including internal conversion, dissociation, and electron ejection.
In complementary experiments, the liquid interface is explored in molecular beam scattering experiments from flat liquid jets of cold salty water (-50 °C, 8 m LiBr). In contrast to cylindrical jets, flat jets provide a large target area and well-defined surface normal, both of which are highly advantageous for scattering experiments. Product angular and translational energy distributions for rare gas and molecular scatterers will be presented.3, 4 The competition between impulsive scattering (IS) and thermal desorption is measured, and the energy loss in the IS channel is characterized using a soft-sphere model. Results are sensitive to both the scatterer identity and its collision energy. Possible effects of surface roughness on the product angular distributions will be discussed.

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Imaging Exciton and Charge-Transfer Dynamics at Surfaces with Time-resolved Momentum Microscopy

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Many of our current technological ambitions hinge on our ability to engineer and control the light-driven dynamics of energy, charge, and spin at the nanoscale. Prominent examples occur in the development of photovoltaics and photocatalysts, for the conversion of abundant sunlight into electrical power or chemical fuels, and the development of optoelectronics for information technology. The coherent manipulation of excited states also lies at the heart of emerging quantum information technology, in the context of quantum memories and quantum repeaters which work with photons as mobile qubits. The excited states created by optical excitation of matter are inherently complex, with many strongly-coupled degrees of freedom and dynamics ocurring over a wide range of time and length scales. Ultrafast spectroscopy can in principle be used to dissect these complex interactions. However, most ultrafast spectroscopy measurements involve drastic averaging over many quantum states, which reduces the information content of the data and obscures its meaning. Optical spectroscopy methods are also blind to “dark states” that cannot be probed due to selection rules. So while the time resolution of ultrafast spectroscopy is often sufficient to resolve dynamics in complex systems, the interpretation of the observables remains a major challenge. I will present recent results on advancing the sensitivity of time- and angle-resolved photoemission (tr-ARPES) from surfaces and applying these methods to exciton and charge-transfer dynamics in quantum materials and molecule-surface interfaces. The unique combination of an XUV light source based on cavity-enhanced high-order harmonic generation at 60 MHz repetition rate [1, 2] and time-of-flight momentum microscopy [3] enable experiments to be conducted under low excitation fluence – which is critical for studying the intrinsic dynamics of the system – while still varying many parameters.

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Chemical Insights from Resonant Auger Spectroscopy

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For larger and more complex molecules, one of the biggest challenges for experimental spectroscopy is in the interpretation of heavily convoluted spectra. X-ray spectroscopies and their element and site-selectivity can help address this challenge by providing observables that are uniquely related to particular atomic sites or functional groups in a system.
In this talk, I will discuss how, with combinations of complementary X-ray methods, it is possible to extract information on both electronic structure and dynamical processes on a series of molecular systems. I will look at how our recent developments for resonant X-ray techniques1-3 are extending the chemically relevant information that can be extracted from these methods for polyatomics in the gas and solution phase as well as providing insights into the few femtosecond processes following core-hole excitation.

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[3] E. Muchová, et al., 2023, *Phys. Chem. Chem. Phys.*, 2023, 25, 6733-674

Visible Light Photochemistry of IO_2^-

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IO2– has been observed in the atmosphere and suggested as a reaction intermediates in the destruction of ozone. The photoelectron action spectrum of IO2– provides evidence for a vibrational progression of anion resonances, characterized by a vibrational frequency of ~0.03 eV, originating from a weakly bound (close to the photodetachment threshold) electronically excited state of IO2–. Photoelectron spectroscopy of IO2 at similar wavelengths shows autodetachment of the vibrational resonances leading to internally excited IO2, as well as direct detachment. As the excited state has a vertical excitation energy in the visible portion of the solar spectrum, this photoprocess is likely occurring in nature, providing a mechanism for the formation of internally excited IO2 and electrons in the atmosphere.

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Near-Surface Velocity-Map Imaging of Rotationally Inelastic Gas-Surface Scattering

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Velocity-map imaging (VMI) is probably the most widely used technique in gas-phase photodissociation and scattering dynamics, providing precise measurements of quantum-state-resolved velocity distributions. However, the application of VMI to gas-surface scattering is complicated by the presence of the surface, with previous reports either limited by the detectable scattering-angle range or by imaging a plane orthogonal to the scattering plane. We have recently reported a new gas-surface scattering apparatus that overcomes these limitations, enabling scattering-plane imaging with > 120□ of angular range, symmetric around the surface normal.1 We present measurements of the dynamics of rotationally inelastic scattering of HCl from alkane-thiol self-assembled monolayers (SAMs) on Au(111)/Si substrates. HCl (incident angle □*i* = 45□, *E*k = 55 kJ/mol) scatters from both -CH3 and -CH2OH terminated SAMs with strong correlations between speed, angle and final rotational state. Fast specular scattering is observed for all final rotational states, but slower products are also observed with broad angular distributions that peak backwards of normal, even for rotational states that would not be significantly populated at the surface temperature. Scattering from -CH2OH terminated SAMs displays consistently higher final speeds than from -CH3, consistent with a more rigid surface arising from inter-chain H-bonding. Significantly, we see no clear evidence for a simple binary division of the scattered products into impulsive scattering and thermal desorption.

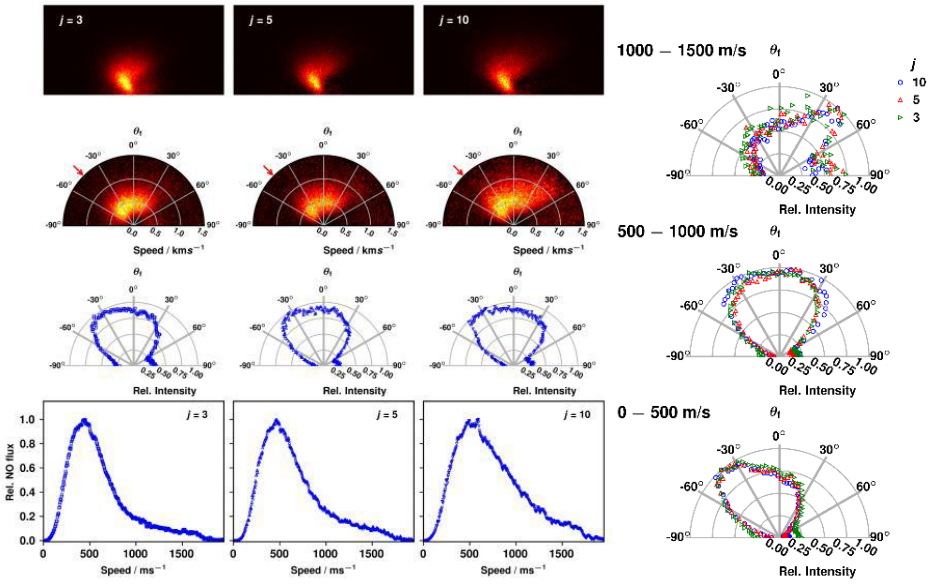

Figure 1. HCl scattering from a -CH2OH terminated SAM, for three final rotational states *j* = 3, 5 and 10. Left top to bottom: raw velocity-map images, density-to-flux corrected velocity distributions, angular distributions integrated over all speeds, speed distributions integrated over all angles. Right top to bottom: angular distributions integrated over 3 different speed ranges as a function of final rotational state.

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The Advanced Research Center for NanoLithography: an example of a public-private partnership in the MOLEC field

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ARCNL, the Advanced Research Center for NanoLithography, was founded in 2014 upon an initiative of ASML. ASML produces highly advanced lithography tools for the semiconductor industry. The tools have been called the most complex machines made by mankind. Creating many hundreds of Watts of 13.5 nm radiation, imaging sub 30 nm lines on a wafer and allowing the production of 1010 transistors on a single chip requires limits in many dimensions. Inside the tool wafers and reticles (containing the information for each layer of a chip) move with m/s-speed, tens of g acceleration and single nanometer precision. The 13.5 nm radiation creates not only the desired structures but also a reactive mostly hydrogen plasma resulting in subtle surface chemistry. Wafers need to be clamped on the moving tables. Understanding friction and clamping requires molecular understanding.
In my talk, I will present the why, how and what of the ASML initiative and the path from a single academic project way of public private projects to a collaboration between an industrial and academic team understanding and respecting each other's drivers including examples recognizable by the MOLEC community.

[1] H. Brookhuis: ASML and Dutch Physics: A History of the Advanced Research Center for Nanolithography (ARCNL), 2014-2024; Amsterdam University Press (AUP), 2025

Program

Thursday, September 10th, 2026

	Chair: ***Rebecca Ingle***
9:00 a.m.	**Francesca Calegari** Tracking electron charge migration in molecules using attosecond FEL pulses
10:00 a.m.	**Giuseppe Sansone** Three-path attosecond interferometry
10:30 a.m.	Coffee Break
11:00 a.m.	**Alicia Palacios** Attosecond non-linear dynamics in molecules: correlation, coherences and entanglement
11:30 a.m.	**Hugo Marroux** Attosecond spectroscopy of electronic decoherence in liquid water
11:50 a.m.	**Maria Richter** High-order harmonic generation in an organic molecular crystal
12:10 p.m.	**Karin Sarah Thalmann** Quantum dynamics of singlet fission, charge transfer, and triplet-triplet annihilation
12:30 p.m.	Lunch Break
	Chair: ***Toshinori Suzuki***
2:00 p.m.	**Daniel Rolles** Imaging Ultrafast Dynamics in Gas-Phase Molecules with Coulomb Explosion Imaging
2:30 p.m.	**Daniel Strasser** Ionization / neutralization induced Dynamics
3:00 p.m.	**Lorenzo Iori** Tracking Ultrafast Electron Dynamics in Acetylacetone with 3-fs-resolved UV/XUV Photoelectron Spectroscopy
3:20 p.m.	**Arnab Sen** Probing ultrafast molecular dynamics with few-fs VUV pulses
3:40 p.m.	Coffee Break
4:10 p.m.	**MOLEC Prize session**
5:10 p.m.	**Postersession 2** Entrance Hall KG I
7:00 p.m.	**Conference Dinner** at Dattlers Schlossberg Restaurant

Tracking electron charge migration in molecules using attosecond FEL pulses

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Electronic charge migration prompted by sudden molecular ionization/excitation forms the foundation of the rapidly growing field of attochemistry, which aims at controlling chemical reactivity via the coherent electronic motion [1]. Primarily, it is the quantum correlation between the electrons and the atomic nuclei that potentially affects the instantaneous force field and opens new reaction pathways via the mechanism of charge-directed reactivity [2].

The first experiments to detect charge migration were performed more than a decade ago with a table-top attosecond source in the aromatic amino acids phenylalanine [3] and tryptophan [4]. Despite being successful in identifying the signatures of coherent electron dynamics initiated by the attosecond pulses, these experiments lacked site selectivity and attosecond time resolution. Recently, advancements in the generation of attosecond soft X-ray light pulses at the Linac Coherent Light Source (LCLS) [5] enabled the investigation of charge migration with site-selectivity and unprecedented time resolution via attosecond time-resolved x-ray absorption spectroscopy (tr-XAS) [6]. Here I present a site-specific study of charge migration at both the oxygen and nitrogen K edges in the amino acids phenylalanine and tryptophan. The experiment has been conducted in a ω/2ω XLEAP configuration, exploiting the high data rate available from LCLSII. Preliminary results at the N K edge in Tryptophan indicate the presence of a 0.58 PHz frequency in the tr-XAS signal. A similar periodicity has been identified in the time dependent yield of the immonium dication, corroborating the XAS results.

These results indicate that attosecond tr-XAS based on FEL pulses is a perfect tool for tracking attosecond electron migration in molecules with site selectivity. However, attosecond FEL pulses are generated starting from a stochastic process (self-amplified spontaneous emission - SASE), and – contrary to attosecond table-top sources – often require single shot temporal characterization for sorting the collected data. I will here introduce a novel all-optical approach based on double blind holography (DBH) [7] for amplitude and phase retrieval of FEL pulses on a single-shot basis. The method has been implemented at the FEL FLASH II in Hamburg: By measuring the single-shot 2D interference of the XUV FEL pulse with an XUV HHG pulse, the reconstruction of sub-10 fs pulses and the simultaneous detection of the arrival time of the FEL pulses is demonstrated.

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Three-path attosecond interferometry

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Attosecond interferometry [1] is based on the interference of two quantum pathways leading to the same final state of a photoelectron wave packet emitted in the continuum. In this experimental technique, combining an attosecond pulse train consisting of odd harmonics of fundamental infrared radiation with a replica of the same field leads to the generation of photoelectron spectra characterised by main lines (due to absorption of a single extreme ultraviolet photon) and sidebands between them (due to exchange of one infrared photon by the outgoing photoelectron wave packet). This method is widely used to characterise the temporal structure of attosecond pulse trains [1] and to measure attosecond time delays in photoionisation [2]. In its typical implementation in atoms, the effect of the infrared radiation on the parent ion, which is created by the emission of the electron following the absorption of a single extreme ultraviolet photon, is usually neglected.
In this work, we report experimental evidence in two-colour photoionisation experiments in simple molecules, showing that an additional quantum path contributes to the final state of the ion-photoelectron bipartite system. This path is due to the absorption or emission of an infrared photon in the ion. We demonstrate how the additional pathway impact angle-resolved photoionisation time delays, and how its contribution depends on the entanglement between the ion and the photoelectron, as determined by the initial photoionisation event [3]. The ability to resolve the effect of infrared-induced ionic coupling is closely related to the ability to measure angle- and ion-state-resolved photoelectron spectra, making use of photoelectron-photoion coincidence spectroscopy [4]. By exploiting the unique capability of this approach, we show how the different interference terms contributing to the complex photoelectron spectra can be disentangled. Our results indicate that the effect of the infrared field on the ion plays a key role in attosecond inteferometry in molecules [5, 6].

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Attosecond non-linear dynamics in molecules: correlation, coherences and entanglement

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Attosecond science has rapidly progressed from observing fundamental electronic motion to manipulating complex, correlated electron-nuclear dynamics in single and multiple ionization processes. This talk presents recent theoretical developments describing ultrafast non-linear phenomena observed in both table-top set ups employing high-order harmonic generation (HHG) techniques and free electron laser (FEL) facilities. On the experimental side, seeded FELs like FERMI offer an unprecedented optical phase control in the XUV regime that enables the coherent control of electronic wave packet. This has allowed, e.g., the implementation of a self-referencing approach using combs of non-consecutive harmonics for the characterization of the photoionization phase, a sensitive probe of electronic structure and correlation that remains challenging to isolate due to measurement-induced contributions [1,2]. Recently, we have identified and evaluated these measurement-induced continuum-continuum phases, where breaking down long-standing asymptotic approximation was expected in XUV-IR photoionization [2]. Experiments realized also at FERMI demonstrated the usefulness of twocolor schemes using XUV frequencies (w/2w) to retrieve photoionization time delays in atoms [3,4]. In molecules, these transitions are further modulated by vibrational time scales [5]. These protocols complement standardized attosecond spectroscopic techniques such as RABBIT (reconstruction of attosecond beating by two-photon transitions) approaches realized at HHG laboratories, which can be still nowadays considered the flagship of attosecond science. Furthermore, HHG pulse synthesis has enabled the exploration of quantum entanglement as a control parameter in molecular photoionization [6]. Utilizing phase-locked pairs of isolated attosecond pulses, we track how entanglement between the photoelectron and parent ion influences electronic coherence in dissociative channels. Tuning inter-pulse and NIR-XUV delays allows us to preserve or erase the coherence required, e.g., for charge migration. These milestones represent a unified frontier in ultrafast science, where the interplay of electronic and nuclear degrees of freedom is not merely observed but controlled, paving the way for steering chemical reactivity at the attosecond level. In this regard, ongoing progress on on-the-fly molecular dynamics applied to large systems, where our grid-based accurate methods are prohibited, will be presented.

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Attosecond spectroscopy of electronic decoherence in liquid water

Gabriele Crippa[1,2], Geoffrey Carneiro[2], Jonathan Dubois[1], Rafael Menezes Ferreira[2], Nicolas Lericheux[2], Jérémie Caillat[1], Fabien Lepetit[2], Camille Lévêque[1], Olivier Tcherbakoff[2], Jean-François Hergott[2], Christophe Nicolas[3], Francis Penent[1], Rémi Dupuy[1], Marine Fournier[1], Richard Taïeb[1], Majed Chergui[4], Jérôme Palaudoux[1], Pascal Salières[2], Hugo Marroux[2]

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Electron scattering dynamics in liquid water play a central role in fields ranging from ultrafast chemistry to radiolysis [1]. Currently, comparisons of photoelectron angular distributions (PADs) measured in gas and liquid phases are the primary experimental approach for characterizing elastic and inelastic mean free paths in water [2]. Reported values are typically below 10 nm for photoelectrons with kinetic energies under 100 eV, corresponding to scattering times on the atto- to few-femtosecond scale. Attosecond spectroscopy therefore offers a promising complementary approach. Here, we perform reconstruction of attosecond beating by two-photon transitions (RABBIT) measurements on gas- and liquid-phase water over a kinetic energy range of 30–60 eV. [3,4] RABBIT is an electron interferometry technique based on two-photon transitions induced by an IR dressing field overlapped with an XUV attosecond pulse train, producing oscillatory photoelectron interferograms as a function of IR–XUV delay. The oscillation phase encodes photoionization dynamics, while the contrast reflects the coherence of the electronic wavepacket.

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

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High-order harmonic generation in an organic molecular crystal

F.-E. Wiechmann[1], S. Schöpa[1], L. Bielke[1], S. Rindelhardt[1], S. Patchkovskii[2], F. Morales[2], M. Richter[1,2], D. Bauer[1], and F. Fennel[1]

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We report on the first successful demonstration of high-harmonic generation (HHG) in a new class of materials: thin organic molecular crystals (OMCs) with perfectly aligned molecules. OMCs have attracted significant interest as promising candidates for organic electronics. They are distinguished from the previously studied (ionic or covalently bonded) solid-state targets by their weak van der Waals forces that bind the constituent molecules, thereby bridging the gap between gas-phase and solid-state physics. Their weak couplings prompt the question of whether high harmonics can be generated efficiently without damaging the crystals, and if so, whether the HHG spectra encode information about collective crystalline effects rather than about the response of nearly non-interacting molecules. Using linearly polarized 4 μm mid-IR laser pulses, we show that pentacene crystals endure laser intensities sufficient for efficient HHG up to order 17. Moreover, rotation of the driving polarization reveal maxima in harmonic yield for polarization directions aligned along axes connecting neighboring molecules, see Fig. 1, demonstrating the role of collective intermolecular effects in the HHG process.

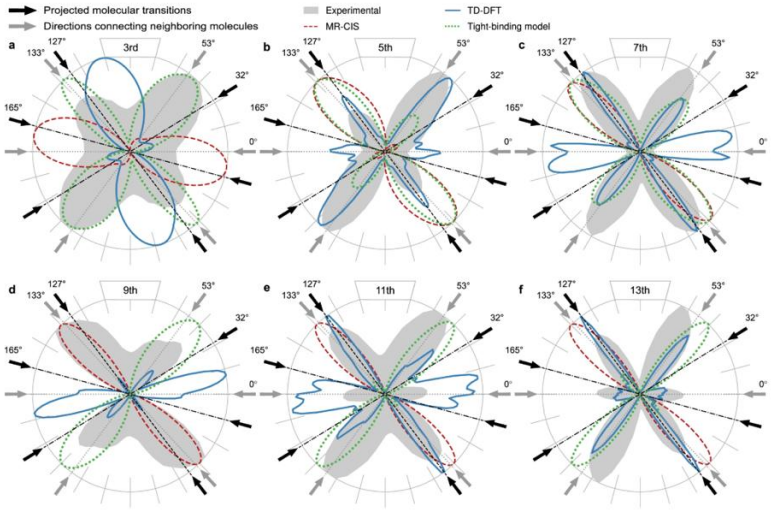

Figure 1: Experimental (grey shaded) and theoretical polarization-dependent harmonic yield in a pentacene crystal.

To uncover the underlying HHG mechanism in OMCs, we have combined our experimental observations with a detailed theoretical investigation that separates single-molecule from crystalstructure effects and accounts for variable intermolecular couplings. This involved simulating (i) the singlemolecule response using high-level MR-CIS electronic structure calculations (red), (ii) the response of the full periodic pentacene crystal using time-dependent density-functional theory (TD-DFT) (blue), and (iii) the response of a 2D tight-binding model crystal (green), see Fig. 1. Our results show that HHG spectra from weakly coupled OMCs carry clear signatures of intermolecular interactions, opening the door to HHG as a powerful all-optical sensitive probe of the electronic structure and intermolecular forces in complex organic materials.

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Quantum dynamics of singlet fission, charge transfer, and triplet-triplet annihilation

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Solar power is one of the renewable and environmentally sustainable energy sources. The efficiency of solar cells, however, is restricted by the Shockley-Queisser limit and thermalization losses, but can potentially be enhanced through photon up and down conversion using multiexciton processes [1]. In this contribution, we investigate two prominent examples of such processes. The first is the photoinduced process of singlet fission (SF) [2], which transforms an excited singlet state into two triplet states that can be harvested by introducing an acceptor molecule to a SF-active donor. The second is its reverse process triplet-triplet annihilation (TTA), which combines two low-energy triplet states to generate a high-energy excited singlet state, effectively enabling photon upconversion.
Using ab initio multireference perturbation theory and quantum dynamical simulations based on a vibronic model Hamiltonian, we investigate the dynamics of SF, charge transfer, and energy transfer from a bis(diazadiborine)-based chromophore as a donor to tetracyanoquinodimethane as acceptor [3]. Our findings reveal three competing transfer mechanisms: intermolecular SF, charge and energy transfer following intramolecular SF, and charge and energy transfer to low-lying states. In addition, we examine triplet-triplet annihilation from the multiexcitonic triplet state in covalently coupled acenes, which proceeds via a charge transfer state mediated mechanism. Overall, our results provide insights to guide the design of novel SF- and TTA-based materials for next-generation photovoltaic applications.

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Imaging Ultrafast Dynamics in Gas-Phase Molecules with Coulomb Explosion Imaging

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Despite significant progress in ultrafast imaging techniques, high-fidelity imaging of all nuclear positions of a gas-phase molecule remains a challenge even for relatively small molecular systems and, notably, regarding the positions of hydrogen atoms. Coulomb explosion imaging (CEI) can overcome this obstacle as its sensitivity does not depend on the mass of the imaged atoms [1]. Moreover, it often produces very intuitive images of the molecular structure [2] that are well suited to visualize ultra-fast structural changes [3,4] as well as the correlated nature of the nuclear wavefunctions [5].
I will show recent results demonstrating that CEI with both X-ray free-electron lasers and tabletop femtosecond lasers offers a powerful route to directly visualizing nuclear motions (e.g. isomerizations) in organic molecules on ultrafast timescales [1,3,4], especially when performed in a multi-ion coincidence mode. I will also show how machine learning tools can use correlations in the high-dimensional CEI data to identify and distinguish contributions from different photoproducts [6], and how neural-network-based reconstruction approaches can directly retrieve the molecular structure from the fragment ion momentum data [7].

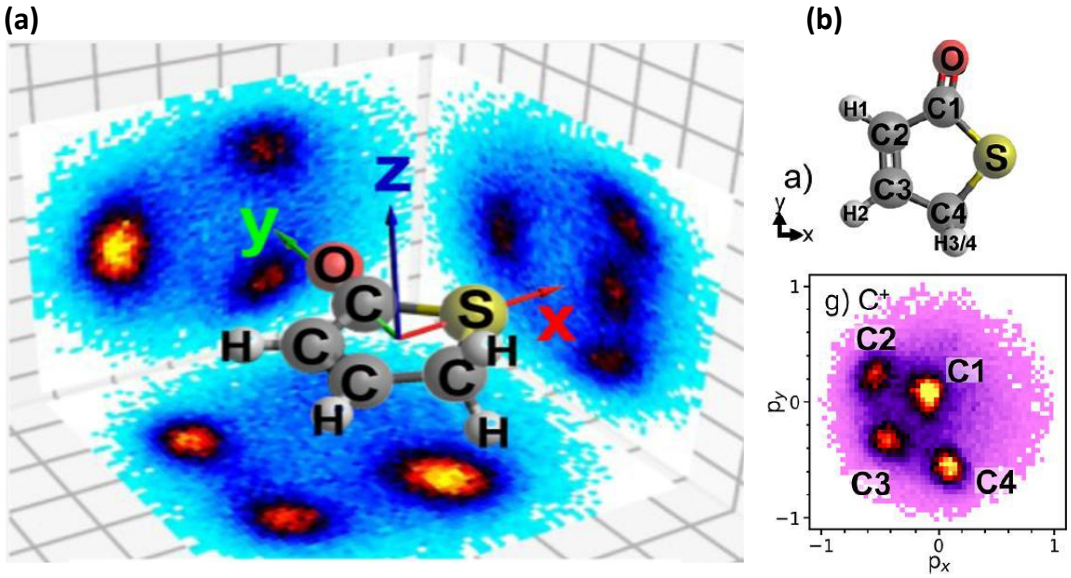

Fig. 1. Newton plots of the momentum distributions of (a) H+ and (b) C+ ions from the Coulomb explosion of thiophenone molecules (C4H4OS, see sketch) induced by an intense femtosecond X-ray pulse [1].

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Ionization / neutralization induced Dynamics

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Ionization and neutralization events can trigger intricate structural rearrangement dynamics in isolated molecular and cluster systems, thus, driving chemical evolution even under low temperature conditions. I will describe our experimental efforts of using 3D coincidence imaging for probing and visualizing molecular dynamics. I will show both ionization-induced dynamics that are initiated by ultrafast EUV pulses,[1,2] as well dynamics that are initiated by the mutual neutralization of molecular anions and cations in merged-beams experiments.[3,4] Furthermore, I will discuss our efforts to achieve direct comparison of experimental and theoretical studies towards a better understanding of time-evolving small quantum systems.
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Tracking Ultrafast Electron Dynamics in Acetylacetone with 3-fs-resolved UV/XUV Photoelectron Spectroscopy

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UV-induced electron dynamics in photoexcited molecules, typically mediated by transitions through conical intersections (CIs) on the few-fs timescale [1], are challenging to fully capture using standard time-resolved photoelectron spectroscopy (trPES). Conventional trPES relies on narrowband probe pulses, which limit the temporal resolution, and often lacks spectral tunability for few-fs pump pulses. To overcome these limitations, we developed a novel ultraviolet (UV) pump - extreme UV (XUV) probe beamline that achieves an unprecedented temporal resolution of 3 fs. Such performance is enabled by the combined interaction of attosecond XUV pulses, delivered by a semi-infinite gas cell [2], with tunable few-cycle deep UV pulses generated through resonant dispersive wave emission in a gas-filled hollow core fiber [3]. The overall instrumental response function, determined through in-situ UV-XUV cross-correlation in argon, is 3.2 ± 0.2 fs. We demonstrate the capabilities of this beamline by applying it to the study of photoexcited acetylacetone. While previous trPES measurements with a 20-fs resolution could resolve two kinetic components within the first 100 fs [4], the enhanced temporal resolution of this setup allowed us to disentangle three distinct population-dynamical channels, revealing two sequential passages through the $S2/S1$ CI. This observation is strongly supported by CASPT2 simulations, which accurately reproduce the experimental trace. More specifically, an ultrafast transit occurs after 8.8 ± 0.3 fs (theory: 8.1 fs), followed by a second passage at 15.4 ± 0.4 fs (theory: 17.2 fs) that drives the system into a long-lived state. By setting a new level of temporal precision, this beamline paves the way for the time-domain observation of coupled electronic-nuclear wavepacket evolution in molecular systems.

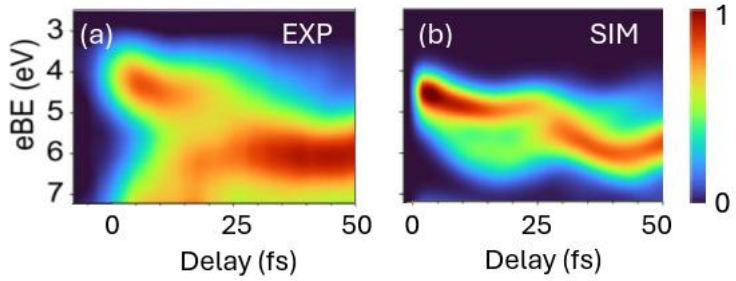

Figure 1. (a) 3-fs-resolved experimental trPES trace of acetylacetone, (b) simulated trPES trace.

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Probing ultrafast molecular dynamics with few-fs VUV pulses

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Recent advances based on the resonant dispersive-wave technique have enabled the generation of broadly tunable, few-femtosecond deep-ultraviolet (DUV) and vacuum-ultraviolet (VUV) laser pulses (100–300 nm) with high conversion efficiency [1,2]. These sources provide new opportunities for investigating ultrafast electronic and nuclear dynamics in photoexcited molecules. Here, we present applications of such ultrashort DUV/VUV pulses to benchmark molecular systems using time-resolved photoelectron spectroscopy (TRPES).

Ethylene, the prototypical molecule containing a C=C double bond, has served for decades as a model system for studying ultrafast dynamics following $\pi \rightarrow \pi^*$ excitation. Nevertheless, its extremely short excited-state lifetime has hindered a complete understanding of the fundamental processes governing the earliest stages of its relaxation dynamics [3,4]. Using sub-4-fs 158 nm pump–probe pulses, we directly resolve previously unobserved sub-10-fs dynamics in photoexcited ethylene. Supported by quantum-dynamics, our combined experimental and theoretical investigation reveals the crucial role of a previously overlooked $\sigma\pi^*$ state that is strongly coupled to the bright $\pi\pi^*$ state. This coupling drives ultrafast torsional motion and rapid electronic reorganization within the first 10 fs following excitation, leading to a revised picture of ethylene photochemistry [5].

Beyond ethylene, our approach is applicable to a broader class of molecules relevant to understanding ultraviolet photostability in biologically important chromophores. As an example, we investigated pyrrole, a simple nitrogen-containing heteroaromatic molecule that serves as a model system for understanding excited-state relaxation processes in more complex biomolecular chromophores, including nucleobases. Despite decades of experimental and theoretical investigation, the earliest wavepacket dynamics following excitation to the first absorption band (5.5–6.5 eV) have remained largely unresolved owing to the dense manifold of excited states and the ultrafast nonadiabatic relaxation pathways involved [6,7]. Using sub-4-fs 200 nm excitation pulses in combination with TRPES, we directly observed the early-time excited-state dynamics of pyrrole in real time. The experimental results are in excellent agreement with recent quantum-dynamics calculations [7].

These studies highlight the potential of combining time-resolved photoelectron spectroscopy with broadly tunable few-femtosecond DUV/VUV sources to resolve complex nonadiabatic dynamics in polyatomic molecules and to provide direct insight into the mechanisms governing ultrafast photochemical relaxation.

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Program

Friday, September 11th, 2026

	Chair: ***Alicia Palacios***
09:00 a.m.	**Christiane Koch** Quantum effects in cold and controlled molecular dynamics
10:00 a.m.	**Andrés Ordóñez** Theory of multi-photon excitation of chiral molecules with tailored light
10:30 a.m.	Coffee Break
11:00 a.m.	**Iain Wilkinson** High-Throughput Electron-Momentum Imaging from Liquids
11:30 a.m.	**Letizia Fede** Controlling Chiral Light-Matter Interactions with Tailored Multi-Color Laser Fields
11:50 a.m.	**Andrea Annunziata** High-order Harmonic Spectroscopy in Chiral Liquid Crystals
12:10 p.m.	**Nicolas Ladda** Real-Time Observation of a Controlled Femtosecond Enantiomeric Conversion
12:30 p.m.	**Concluding remarks**
12:40 p.m.	Lunch, Departure

Quantum effects in cold and controlled molecular dynamics

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The wave nature of molecules emerges at very low energy or very short timescales. In gas phase experiments carried out under these conditions, quantum effects may then completely govern the dynamics. In my talk I will present two such examples. Quantum resonances in low-energy collisions are a sensitive probe of the intermolecular forces. They dominate the final quantum state distribution even for strong and highly anisotropic interactions, as recently observed for Feshbach resonances populated by Penning ionization of dihydrogen colliding with a metastable rare gas atom [1]. For such a small collision complex, full quantum scattering calculations can be carried out [1]. The theoretical predictions for the cross section involve then only the approximations made when constructing the potential energy surface (PES). Changes in the shape of the PES thus translate directly into modifications of the cross sections. This can be used to to improve calculated PES, starting from the experimental data [2]. Conversely, one can also ask by how much the experimental resolution of measured cross sections must improve in order to unambiguously discriminate predictions derived from different levels of advanced ab initio electronic structure theory [3].
Moving from low energy to short time scales, I will discuss the quantum control of photoelectron circular dichroism (PECD) in the photoionization of chiral molecules [4]. Here, the control arises from the interference of various two-photon photoionization pathways that can be manipulated by suitably shaped ionization pulses [5]. PECD, remarkably, requires light-matter interaction only in the electric dipole approximation even for randomly oriented molecules. This results not only in a very large dichroic effect, but provides also a recipe for how to induce and subsequently probe chiral dynamics in initially achiral molecules [6]. The preparation of chiral superposition states with a preferred handedness may be useful in future experiments, e.g. on measuring parity violation with chiral molecules.

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Theory of multi-photon excitation of chiral molecules with tailored light

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The shape of light, as encoded in its polarization, has long been recognized as the key to its interaction with chiral molecules. While well-understood in the one-photon regime, the complexity of this interaction grows rapidly with the number of exchanged photons, often leading to fundamental phenomena challenging our intuition. Already the simplest variation to circular polarization, i.e. elliptical polarization, has revealed multiphoton enantiosensitive (different for opposite chiral molecules) signals that behave non-monotonously with the light's ellipticity [1], or which are completely insensitive to its sign [2,3]. Beyond this, sculpting light's polarization in three dimensions by combining several frequencies with different non-coplanar polarizations promises order-of-magnitude improvements in the enantioselective control over population transfer with respect to standard circular polarization [4]. In this talk, I will discuss the theoretical description of these chiral light-matter phenomena, starting with fundamental aspects related to their symmetry, the mechanisms by which they emerge, and the mathematical form of the coupling between light's polarization and molecular chirality in isotropic samples. I will then move on to numerical simulations exploring the effects of intensity fluctuations, variations of the polarization across the interaction region, variations in molecular geometry, and integration over final states, as typically found under experimental conditions.

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[3] Ordóñez et al., arXiv:2512.17840 (2025)
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High-Throughput Electron-Momentum Imaging from Liquids

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

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

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Controlling Chiral Light-Matter Interactions with Tailored Multi-Color Laser Fields

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We present a series of experiments combining multiple tailored laser fields to explore and control chiral light-matter interactions in gaseous molecular samples.

First, we use a strong elliptically polarized infrared field (1030 nm, ω) to produce photoelectrons that rescatter on the parent ion, inducing Laser-Induced Electron Diffraction (LIED) with sensitivity to molecular chirality [1]. Introducing a collinear perturbative second harmonic field 2ω, polarized parallel or perpendicular to the major axis of the ω ellipse, allows us to select the trajectories of recolliding electrons [2] and to modulate their recollision angle, controlling the chiroptical signal at the attosecond time scale.

When both the ω and 2ω fields are linearly and orthogonally polarized, the polarization of the combined field rotates switching handedness every half optical cycle. This produces an enantio-sensitive forward-backward asymmetry in the photoelectron angular distribution along the laser propagation direction, whose sign follows the ultrafast ellipticity reversal, giving a dichroic chiroptical response. Remarkably, when the detection geometry is appropriately chosen, the signal can be made insensitive to this periodic ellipticity switch, yielding a non-dichroic enantio-sensitive response. Such signals emerge in both multiphoton and strong-field chiral photoionization, and represent a new paradigm in chiroptical spectroscopy, which reflects symmetry protection [3].

Finally, when a third, non-collinear laser field is added to the interaction, the electric field oscillation is not confined to a plane and can follow a 3D-chiral shape. Such fields are expected to revolutionize chiral light-matter interaction [4], however, to date, no experimental investigations have been reported. We produce a 3D-chiral field made of two linearly polarized $2\omega/4\omega$ fields crossing orthogonally a circularly polarized ω field. The instantaneous shape and chirality can be finely controlled by tuning the $2\omega/4\omega$ phase. We observe a strong enantio-sensitive control of dissociative ionization of chiral molecules by these fields, opening new routes toward the optical control of chiral chemistry.

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High-order Harmonic Spectroscopy in Chiral Liquid Crystals

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When an intense mid-infrared (MIR) pulse interacts with matter, it can trigger the emission of high-energy photons at harmonic multiples of the driving frequency, a process known as high-order harmonic generation (HHG). In the three-step model, an electron is tunnel-ionised, accelerated by the strong electromagnetic field, and upon recombination with its parent ion, releases its acquired energy as harmonics of the driving field. This process inherently encodes information about the potential landscape experienced by the electron, which is directly reflected in the HHG spectra, making it a powerful platform for HHG spectroscopy in gases, solids, and, more recently, liquids. The exceptional sensitivity of HHG has been explored in both gas-phase molecules and solid-state systems [1]. In solids, intrinsic structural order naturally enhances sensitivity, whereas in gas-phase molecules, random orientational averaging limits chiral signal detection to beyond-dipole effects. Introducing orientational order in chiral molecules would therefore enable dipole-level contributions, significantly boosting enantiomeric sensitivity in HHG. Liquid crystals (LCs) offer an ideal platform to achieve this. These materials combine the ability to flow like a liquid with the orientational order characteristic of solids, making them well-suited to act as alignment matrices for embedded molecules. We have already demonstrated that orientational order in prototypical LCs survives under strong-field excitation [2], suggesting that LCs could serve as effective alignment layers for chiral molecules, opening new avenues for enantiomeric recognition in the liquid phase. In this contribution, we present experimental results on HHG from non-chiral liquid crystals, highlighting the key spectroscopic signatures observable in this medium, where only odd-order harmonics are detected (Fig. 1a). We then present the first results obtained from chiral liquid crystals. The presence of chiral molecules in our experimental geometry breaks inversion symmetry, giving rise to even-order harmonics (Fig. 1b). These findings represent an important step towards liquid-phase chiral recognition using strong-field methods. As LC alignment strategies are further optimised and the underlying strong-field dynamics in ordered molecular systems become better understood, HHG spectroscopy in LCs could establish itself as a viable approach for all-optical chiral recognition in the liquid phase, combining the structural sensitivity of strong-field methods with the orientational control provided by liquid crystals.

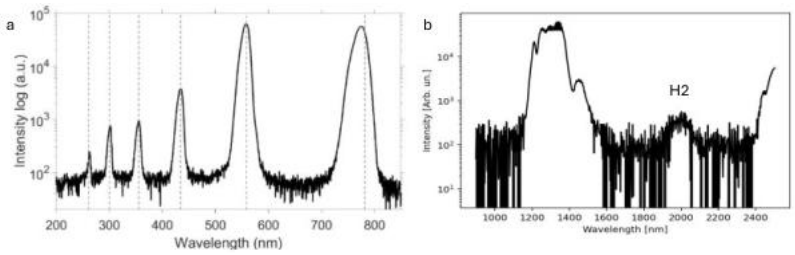

Figure 1 (a) High-order harmonic spectra from non-chiral liquid crystal (5CB) showing only odd harmonics. (b) spectra from the same liquid crystal doped with CB15 chiral dopant, showing the appearance of even harmonics

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Real-Time Observation of a Controlled Femtosecond Enantiomeric Conversion

Nicolas Ladda[1], Fabian Westmeier[1], Tonio Rosen[1], Sudheendran Vasudevan[1], Simon Ranecky[1], Sagnik Das[1], Krishna Kant Singh[1], Hendrike Braun[1], Jochen Mikosch[1], Thomas Baumert[1] and Arne Senftleben[1]

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We present the first observation of an enantiomeric conversion of an optically excited chiral molecule on the femtosecond timescale. Pumping the chiral molecule (methyl *p*-tolyl sulfoxide) into an electronically excited state with a deep-UV femtosecond laser pulse creates a vibrational wave packet, that can propagate to the other enantiomeric configuration due to a reduced inversion barrier [1]. By measuring time-resolved photoelectron circular dichroism (PECD), these molecular dynamics can be investigated in the gas phase, which provides an interaction-free environment. Advantageously, PECD, i.e., the forward/backward asymmetry of the photoelectron angular distribution with respect to the direction of propagation of ionizing circularly polarized light, is a strong (~10%) effect and can be studied in an energy-resolved manner using a velocity map imaging spectrometer [2].

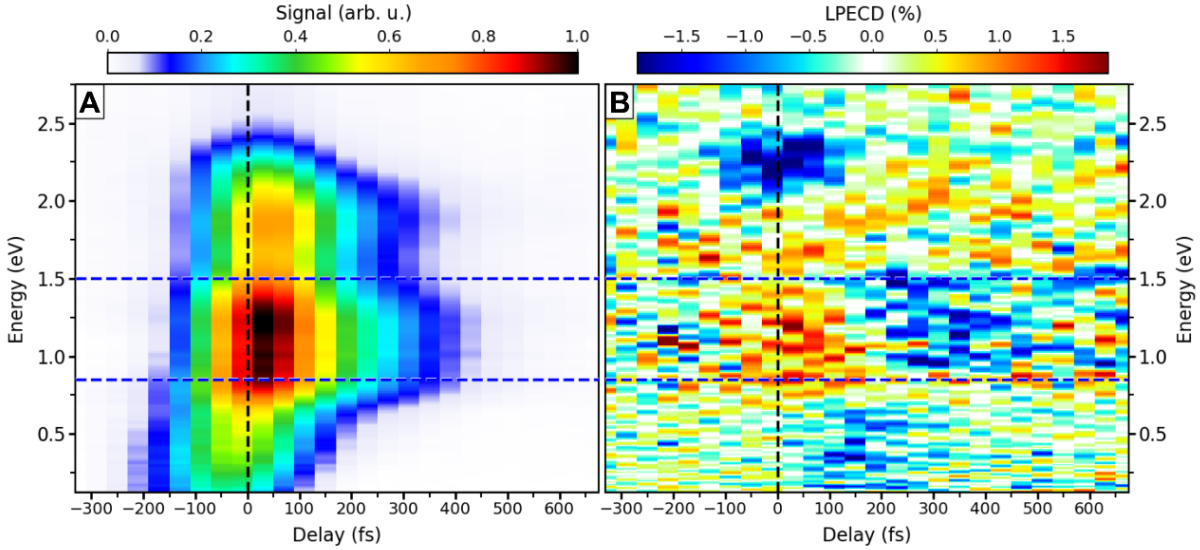

Figure 1: Time resolved photoelectron spectrum (A) and LPECD (B).

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POSTERSESSION 1

Tuesday, September 8, 2026

Poster Session I

Probing Ultrafast Charge-Transfer in Aqueous Sulfur-containing Biomolecules using Resonant X-ray Spectroscopy

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Sulfur-containing biomolecules occupy a central role in biological electron-transfer processes owing to sulfur's moderate electronegativity, high polarizability and multiple stable oxidation states. In proteins, sulfur functionalities stabilize the tertiary structure through covalent linkages, regulate redox activity and coordinate to transition metals to enable transcriptional and enzymatic functions. [1,2] While conventional X-ray spectroscopic methods have significantly advanced the identification [5] and speciation [3,4] of sulfur in biomolecular motifs, the ultrafast electron dynamics triggered by core-excitation in physiological conditions remain relatively unexplored.

Here, we employ Resonant Inelastic X-ray Scattering (RIXS) and Resonant Auger Electron Spectroscopy (RAES) to probe sub-femtosecond charge-transfer (CT) dynamics in aqueous sulfur-containing biomolecules. Combining spectroscopic measurements with molecular dynamics and *ab initio* quantum chemistry simulations, we investigate how chemical effects like protonation state, covalency and coordination influence ultrafast CT dynamics in aqueous solutions following core-shell excitation. Using aqueous L-cysteine as a model thiol system, we demonstrate that protonation strongly odulates the population and localization of transient charge-transfer-to-solvent (CTTS) states. Deprotonation of the thiol group enhances hydrogen-bonding between the solute and solvent molecules, leading to preferential CT towards solvent molecules which are strongly hydrogenbonded to the photoexcitation site. In contrast, the protonated form exhibits significantly weaker hydrogen-bonding network and a more secular CTTS. Extending this framework to increasingly complex molecular environments, we investigate disulfide bridged molecule –cystamine to observe experimental signatures of amine-assisted CTTS pathways which has previously only been predicted theoretically. Finally, using aqueous Zinc(II)-cysteine complexes as model zinc finger domains, we reveal how the electronic structure modifications caused by ligand coordination influences the CT signature of aqueous metallic ions.

These results combined establish resonant X-ray spectroscopy as a sensitive probe for ultrafast environment mediated charge-transfer processes in biologically relevant sulfur-containing molecules and complexes, and provide new insights into the coupling between local chemical structure and core-excited electron dynamics in aqueous environment.

References

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Mechanistic Insights into Nitric Oxide (NO) Release Following UV Excitation of Nitro Compounds

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Translational energy distribution profiles obtained using velocity map ion imaging combined with state-selected fragment detection provide insights into the mechanistic pathways leading to NO release from nitromethane (NM) in comparison with nitrobenzene (NB) following 213 and 225 nm excitation. NB exhibits bimodal translational energy distributions, indicating two distinct NO-release pathways with branching ratios close to unity. The fast component arises from dissociation via a three-membered-ring transition state, whereas the slow component originates predominantly from a non-trivial roaming pathway.1–6 In the words of Prof. Bowman, roaming occurs when “the energy from the sun was only just enough to break a chemical bond,” allowing the fragments to undergo an “intimate dance” before rearrangement and product formation. In contrast to nitrobenzene, where both pathways contribute comparably, NO release from nitroalkanes is dominated by the roaming channel, resulting in slow-to-fast branching ratios much greater than unity.7 To establish the generality of this behaviour, the investigation was extended to a series of linear and branched nitroalkanes, including 1-nitropropane, 2-methyl-2-nitropropane, and (nitromethyl)benzene, to assess the influence of molecular structure on NO-release dynamics.8 While α-substitution has little effect on the fundamental NO-release mechanism, variations in triplet-state yield and intramolecular energy redistribution significantly influence the relative contributions of competing pathways. These results provide a comprehensive mechanistic framework for understanding NO release in nitro compounds and highlight the central role of roaming in the excited-state photochemistry of nitroalkanes.

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Atomistic simulations of calcium carbonate crystallisation in water: mechanism and kinetics

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Calcium carbonate is one of the most abundant biominerals, yet its crystallisation pathways remain actively debated. Classical nucleation theory describes crystal growth as the successive addition of monomeric units overcoming a free energy barrier at the critical cluster size. In contrast, growing evidence supports nonclassical pathways involving multistep transformations through amorphous precursors [1].
We investigate the interplay between the ionic aggregation and organisation by probing the formation of the first coordination sphere in calcium carbonate. We applied two methods: infRETIS to evaluate reaction rates, and OPES to map the underlying free energy landscape. The effect of supersaturation was assessed by simulating different concentrations of calcium carbonate in water.

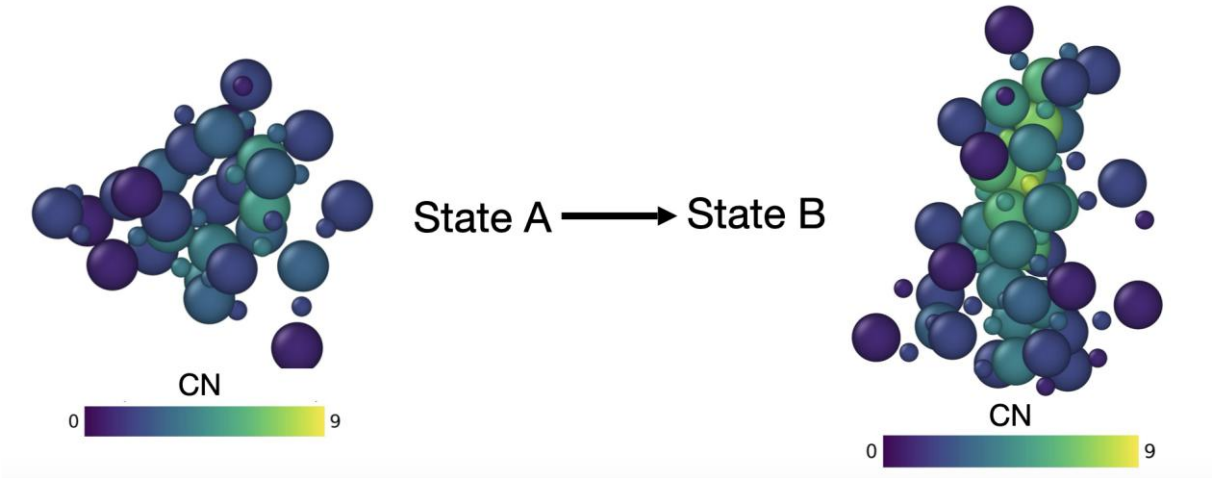

Figure 1: The larger spheres represent calcium atoms, while the smaller spheres represent

We find that ions first form an amorphous hydrated cluster, in which the formation of the first coordination sphere proceeds via dehydration and ionic reorganisation (shown in Figure 1). Such a complex multistep process is challenging to reconcile with classical nucleation theory. We also find the crystallisation pathway differs with concentration. At higher concentrations, ionic aggregation precedes formation of the coordination sphere, resulting in large, highly hydrated clusters. In contrast, at lower concentrations, the rates of ionic aggregation and organisation are comparable, enabling more controlled crystallisation and leading to different polymorphic outcomes.

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MAC: Experimental station for AMO science and Coherent Diffractive Imaging

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ELI Beamlines is an international large-scale research facility operating within the Extreme Light Infrastructure (ELI) ERIC framework, providing cutting-edge, high-power laser systems that generate secondary sources of photons and accelerated particles, including femtosecond XUV, NIR/Vis, and X-ray radiation, which are used for a wide range of user experiments.

Within this facility, the MAC end-station serves as a dedicated user platform for Atomic, Molecular and Optical (AMO) sciences and Coherent Diffractive Imaging (CDI). It is designed for experiments focused on ultrafast electron and ion dynamics in targets such as atoms, molecules, clusters, and Helium nanodroplets. Using femtosecond pump–probe techniques with synchronized XUV and NIR beams, MAC enables studies of key processes including multielectron dynamics, electron correlation, ionization, chirality and transient excited states. Recent work includes electron correlation dynamics in krypton, photoelectron angular distributions in the molecular frame, ultrafast processes in helium nanodroplets, with helium nanodroplets also used as model systems to study nanoscale ionization and relaxation phenomena. MAC is a user instrument offered in open calls to a wide scientific community.

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Two-sideband RABBITT

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Over recent years it has become possible to measure the phase shifts induced by photoionization of atoms and molecules with increasing precision. One of the most common methods to achieve this is RABBITT (reconstruction of attosecond beating by interference of two-photon transitions), which relies on ionization by an extreme ultraviolet (XUV) frequency comb and the interaction of the released electron with an infrared (IR) probe field. If the IR photon energy is half the comb spacing of the XUV frequencies, sidebands emerge in the photoelectron spectrum which oscillate with the XUV-IR delay. The phase of these oscillations gives access to the Wigner phase experienced during photoionization. However the IR interaction also has an influence on the resulting phase. In the asymptotic approximation one can view this as an additional continuum-continuum-Phase, which can mathematically be separated from the Wigner Phase [1].
In this contribution we will present a novel setup where the IR energy is shifted to a third of the XUV comb spacing using an Optical Parametric Amplifier (OPA) resulting in sideband pairs. Comparing the phases of two neighboring sidebands allows us to check for the limits of the asymptotic approximation.

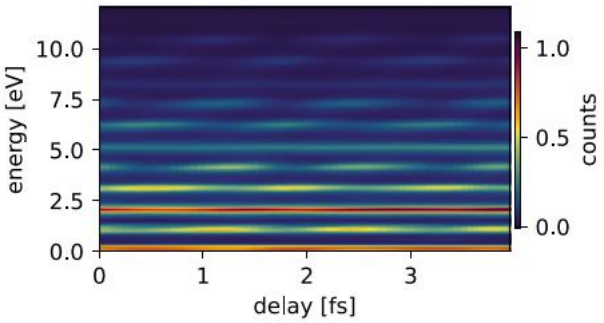

Figure 1: Two-sideband RABBITT spectrogram showing the photoelectron spectrum of Helium as a function of XUV-IR delay.

We will present the setup used to acquire these scans with a focus on the active delay stabilization between pump and probe reaching stability better than 50 as [2]. We will also show results in noble gases hinting at the breakdown of the asymptotic approximation.

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Spin-Chirality Coupling without Magnetic Fields

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Chirality underlies a wide range of phenomena in molecular physics, chemistry, and biology, giving rise to observables that reverse sign between enantiomers. In photoionization, the most prominent example is photoelectron circular dichroism (PECD), where circularly polarized light induces a forward-backward asymmetry in electron emission within the electric dipole approximation [1]. Beyond angular asymmetries, the photoelectrons can also be spin-polarized, opening an additional enantio-sensitive channel driven by spin-orbit coupling, and scattering dynamics. Recent discovery of chirality-induced spin selectivity (CISS) has revealed unexpectedly strong spin filtering in chiral systems [2], raising fundamental questions about the dynamical origins of spin-chirality coupling.
Here, we demonstrate that spin-resolved one-photon ionization of randomly oriented chiral molecules is governed by a universal geometric structure: all spin-polarized and enantio-sensitive observables are controlled by the same three pseudovectors. These pseudovectors generate the molecular pseudoscalars that determine enantio-sensitive signals and define the angular distribution of spin polarization, which we show to be enantio-sensitive even when the total spin-polarization is not [3]. This framework further reveals that the photoelectron spin and momentum are enantio-sensitively 'locked', forming spin-current correlations with a clear geometric origin [4]. Moreover, it predicts an enantio-sensitive 'molecular compass' which causes the photoelectron spin to orient differently for opposite enantiomers [5], thereby enabling a 'locking' between the photoelectron spin and the orientation of the molecular cation. Our results provide a unified picture of spin-chirality coupling in photoionization and establishes a direct conceptual link to the CISS effect, identifying the fundamental geometric quantitites responsible for enantio-sensitive spin-polarization across molecular systems.

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Study of dissociative single and double ionization of pyridine and thymine using coincidence spectroscopy

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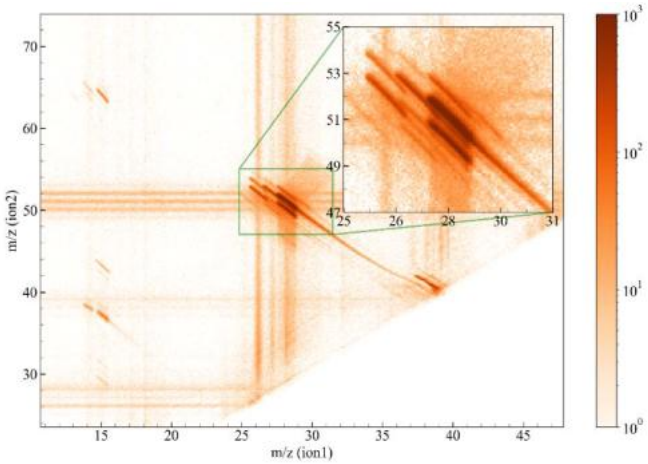
The formation of radiation damage in biological materials involves a multitude of different processes, ranging from direct interactions of energetic particles with molecules, over the formation of secondary electrons to chemical reactions between produced molecular fragments. The available molecular level understanding does not currently capture the full cascade of involved processes in the complex condensed phase environment. We aim to study the effect of XUV radiation on micro solvated biomolecules in gas phase, which provides a good model for fundamental processes considered to be important factors in the generation of secondary low energy electrons.

As a prerequisite for understanding the microsolvated case, we experimentally studied the dissociative single and double ionization induced by XUV radiation from DESIRS beamline at SOLEIL synchrotron on the nucleobase thymine and its simpler analogue pyridine. Electron-ion coincidence detection allows to obtain fragment-mass selected photoelectron signals to correlate populated electronic states to certain dissociation pathways. Electron-ion-ion triple coincidence detection enables us to distinguish double ionization channels from single ionization events. Our experimental results provide a detailed comparison between dissociative single and double ionization of pyridine and thymine. We find that doubly ionized pyridine undergoes predominantly two body dissociation reactions, while thymine fragments via much more complicated cascading dissociation reactions. The ion momentum resolution provided by the DELICIOUS III double imaging photoelectron photoion coincidence spectrometer provides detailed information to disentangle these complex dissociation cascades.



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Investigating the dissociative electron ionisation of polycyclic aromatic hydrocarbons

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Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous in interstellar space and are thought to account for approximately 10-15% of galactic carbon[1,2]. In the interstellar medium (ISM), PAHs are exposed to ionising radiation, including cosmic rays and secondary electrons[3]. Understanding their dissociative ionisation is crucial for assessing their stability and reactivity in the ISM.
We present a study into the gas-phase dissociative electron ionisation of triphenylene by velocity-map imaging (VMI), which records the scattering distributions of cationic products. Correlations between the scattering distributions of different product ions are elucidated by covariance analysis[4], providing a detailed understanding of the dissociation mechanisms of multiply-charged PAH parent cations. A notable dissociation pathway identified by this analysis involves the sequential ejection of neutral acetylene (C2H2) units after an initial dissociation forming two or more charged fragment ions[5]. This resembles the reverse of the HACA (hydrogen abstraction acetylene addition) mechanism, which is an important PAH growth pathway[6].

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Influence of the Bridging Length on the Ultrafast Isomerization Dynamics of Bridged Azobenzenes in a Molecular Beam

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Bridged azobenzenes have drawn considerable attention in the last decade due to their superior photochemical properties compared to conventional azobenzene (AB), providing for higher isomerization yields and bi-directional switching abilities upon irradiation in the visible region of the electromagnetic spectrum [1].
In diazocine (Dz), a -C2H4-bridged azobenzene, the *Z*-isomer becomes the thermodynamically stable isomer due to the induced ring strain by the bridge, albeit with improved switching capabilities [1]. However, the influence on the photophysical properties by different bridging lengths remains yet elusive. To approach this question, the -C2H2-bridged Dz and the -CH2-bridged diazepine (Dzp) were investigated under solvent-free conditions using time-resolved time-of-flight mass spectrometry, photoelectron imaging and photoionization-photofragmentation spectroscopy aided by quantum chemical calculations. In all experiments, the solid samples were heated to 130° C and expanded at 100 Hz repetition rate in a molecular beam into the high vacuum chamber of the setup using He carrier gas at 2 bar backing pressure. Two-color experiments use λ = 399 nm for one-photon excitation to the S1($n\pi^*$) state and λ = 798 nm for subsequent ionization.
After S1 ($n\pi^*$) excitation at λ_{pump} = 399 nm, two isomerization coordinates could be identified: Unfolding of the boat-like *Z*-isomer and CNNC torsional motion leading to the *E* form. While Dz isomerizes in a concerted fashion ($\tau_1 < 38 \pm 1$ fs), Dzp was found to unfold first and consecutively isomerize ($\tau_1 = 38 \pm 7$ fs, $\tau_2 = 680 \pm 96$ fs). In the single-color multi-photon photoelectron imaging experiments, strong thermal electron background was observed for both molecules. Careful evaluation of the spectra revealed bands originating from vertical as well as adiabatic ionization. In the multi-photon process (90 fs FWHM), absorption of the first photon resonantly excites the S1 state. This allows for an ultrafast structural rearrangement, i.e., unfolding, during the ionization enabling additional adiabatic transitions close to the D0 minimum. Surprisingly, the D0 minimum structures resembles an unfolded structure rather than the FC region.
In addition, we observed for both molecules that the ultrafast structural rearranging motion during the ionization is further conserved as a highly excited butterfly vibration in the freshly prepared ion. This excitation then manifests as a pronounced coherent oscillation of the depleted parent ion yield for several picoseconds in the photoionization-photofragmentation experiments matching the computed frequencies nicely.

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Electronic Spectra of Oxygen-containing Carbon Chains

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Carbon chains are reactive but can be stabilised by terminating the ends with, for example, H, O, or N. HC*n*O+ chains are of astrophysical interest as underscored by the detection of HC3O+ in the Taurus Molecular Cloud,1 and may be formed in the low-pressure interstellar environment by radiative association of C*n*H+ with CO,2 potentially contributing to the diffuse interstellar bands (DIBs). To identify HC*n*O+ chains as DIB carriers, the first gas-phase electronic spectra of HC2*n*O+ (*n*=3-6) chains are recorded in a cryogenically cooled quadrupole ion trap using resonant enhanced photodissociation (REPD) spectroscopy, monitoring C2*n*-1H+ photofragment yields as a function of the optical parametric oscillator (OPO) wavelength. HC2*n*O+ chains are formed via reactions of CO with C2*n*-1H+ generated by laser ablation of a graphite disk (with H likely sourced from trace water). These reactions are spin-forbidden as HC2*n*O+ chains possess X3Σ- ground states, whereas CO and C2*n*-1H+ possess X1Σ+ ground states, implying intersystem crossing along the reaction coordinate. Density functional theory calculations are conducted to interpret the formation and photodissociation of HC2*n*O+ chains, and the measured spectra. Each spectrum exhibits a sharp C3Σ←X3Σ- origin band accompanied by an intense vibronic band 1700-2000 cm-1 higher in energy, corresponding to the typical frequency for a CºC stretch vibrational mode. The origin band wavelength redshifts linearly by ≈100 nm per added C2 sub-unit, consistent with a common linear chain structure. Comparison with catalogued DIBs shows that the origin bands of HC6O+ and HC8O+ align with λ4762.2 and λ5828.6 DIBs, respectively, but are considerably broader, possibly due to lifetime broadening and/or vibronic couplings. Definitive determination requires absorption spectrum measurements as REPD may affect transition intensities and band profiles.

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Ultrafast spectroscopy of new near-IR transparent TiO2 dye-sensitized solar cells with solid-state electrolyte

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Dye-sensitized solar cells (DSSCs) are a promising low-cost complement to classical to Si-based solar cells, owing to their transparency, lightweight, and aesthetic features [1]. A key part of DSSCs is the dye, which absorbs the sunlight and injects an excited electron into the semi-conductor (SC) TiO2 conduction band. In solid-state DSSCs, the oxidized dye is regenerated by a solid-state hole-transporting material (HTM) instead of a liquid electrolyte. This approach enables a reduction in internal energy losses and higher photovoltages, and paves the way for fully printable device architectures with improved manufacturability [2].

In a search for a compromise between better transparency and performance, particular focus has been given to the design and study of near-IR absorbing dyes [3]. In such dyes, molecular aggregates form upon adsorption on the SC surface and it has been shown that monomer-to-aggregate resonant energy transfer (RET) competes with carrier injection from the monomer to the SC as they occur on the same time scale [4,5,6]. We report on the novel pyrrolopyrrole cyanine dye TB336. It has high absorption and good transparency in the visible (ε ~1.3x105 $M^{-1}cm^{-1}$ at 764 nm in solution), and bears a “Hagfeldt donor group” that introduces a push-pull electron character reducing charge recombination and possibly fostering electron injection [7].

Previous ultrafast spectroscopic studies in solution-based DSSCs show that TB336 achieves a record power conversion efficiency (PCE) of 4.2%, and reveal electron injection and RET (in the 1.6 to 7 ps range) faster than those observed in previous TB dyes [unpublished]. Despite faster RET, TB336 still displays the highest PCE, which raises the question of how much the excited aggregates contribute to the electron injection. In solid-state DSSCs, this sensitizer reaches a PCE of 2 % after optimization. Here, we present preliminary femtosecond transient absorption (TAS) and fluorescence up-conversion (FLUPS) results on electron injection dynamics of TB336 in solid-state DSSCs, with the aim of identifying the reason for lower short-circuit photo-current, and hence PCE, compared to solution-based DSSCs.

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Tomography of Feshbach resonance states in Ne+HD+ reaction

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Feshbach resonance in collisions is an interesting quantum effect, also plays a critical role in influencing the scattering cross section. However, this important phenomenon remains unclear to us due to the difficulty of experimental measurement. Two methods can be used to study Feshbach resonance in dynamics: 1. Measuring the energy-dependent cross section;[1] 2. Starting from an ion precursor, using the electron photo-detachment spectroscopy.[2]

Here, we developed a new method to investigate the Feshbach resonance based on ion-electron coincidence measurements.[3] It's similar to the second method, but starts with a cold collision that leads to Penning ionization. This new method was applied to research on Feshbach resonances in the Ne and HD+ collision. Assisted by the merged-beam technique, we lowered the collision energy to 22 mK and realized a p-wave (l=1) scattering. Combined with the high-resolution velocity map imaging technique, more substructures were observed and assigned to the Feshbach resonances arising from different vibrational modes of Ne-HD+ by high-accuracy quantum calculations. Furthermore, we obtained the product population information of all the channels from Ne + HD+ reaction, including the inelastic scattering Ne + HD+ channel, the reaction channels NeH+ + D, NeD+ + H, NeHD+. This work deepens our understanding of the Feshbach resonances in scattering.

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High-resolution mid-infrared spectroscopy of cold chiral molecules for precision measurements

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Quantum cascade lasers stabilized on optical frequency combs (QCL/OFC) with traceability to primary frequency standards represent a major advance for high-precision midinfrared spectroscopy. This capability has recently been demonstrated at the Laboratoire de Physique des Lasers [1], it provides an unprecedented level of frequency accuracy and spectral resolution in the mid-infrared molecular fingerprint region, enabling ultra-precise measurements of molecular transitions.
Such ultimate frequency control is particularly crucial for tests of fundamental physics and in particular molecular parity violation (PV) in chiral species. PV originates from the weak interaction, which breaks parity symmetry and induces an extremely small energy difference between left- and right-handed enantiomers of a chiral molecule. Measuring this enantiomer-dependent frequency shift would provide a direct observation of weak interaction effects in molecules [3]. These studies require extremely accurate and stable laboratory reference frequencies, as the expected parity-violating frequency shifts are exceedingly small, typically at or below the hertz level. Current experimental sensitivity is largely limited by the availability of suitable spectroscopic tools combining high resolution, tunability, and frequency traceability and stability, as well as by the difficulty of producing dense and cold samples of complex chiral molecules of interest for PV measurements.
We present our latest experimental efforts to overcome these limitations by extending the spectral coverage and tunability of QCL/OFC systems, while simultaneously developing approaches to prepare cold, dense molecular samples using buffer-gas cooling [2]. This combination aims to enable frequency-metrology-based spectroscopy of a broad range of complex chiral molecules [4, 5, 6].

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Shining Light on Intrinsic Fluorescence of Biochromophores

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Light emission in biological systems is both a fascinating natural phenomenon and a powerful and ubiquitous tool in the life sciences. Proteins such as GFP and luciferase, which give rise to captivating bioluminescence in jellyfish and fireflies, respectively, are widely used as fluorescent probes to visualize and quantify biological processes in real time. The emission from these proteins originates from small molecular chromophores embedded within the complex environments, making it difficult to disentangle intrinsic photophysics from environmental effects. Cryogenic ion fluorescence spectroscopy (CIFS) addresses this challenge by measuring excitation and emission spectra of isolated gas-phase ions, providing both intrinsic fluorescence properties and valuable benchmarks for theory. To demonstrate this approach, we present two recent studies from the LUNA2 setup in Aarhus.[1] In the first, we investigate the GFP chromophore HBDI, formed during protein folding and confined within the GFP barrel structure. Despite decades of study, fluorescence from the isolated chromophore had never been directly observed. By cooling ions below 150 K, we achieved the first gas-phase fluorescence measurements of HBDI. Combined with Franck–Condon simulations, the results confirm a planar emissive geometry and show that fluorescence is an intrinsic property of the chromophore itself.[2] In the second example, we study oxyluciferin, the emitter responsible for bioluminescence in fireflies and related insects. To understand how different species produce different emission colours using the same emitter, we examine the keto and enol tautomers of oxyluciferin. Cryogenic cooling narrows the absorption spectra, allowing selective excitation of each isomer from a co-trapped ion mixture. These measurements provide key experimental benchmarks for understanding biological colour tuning.[3]

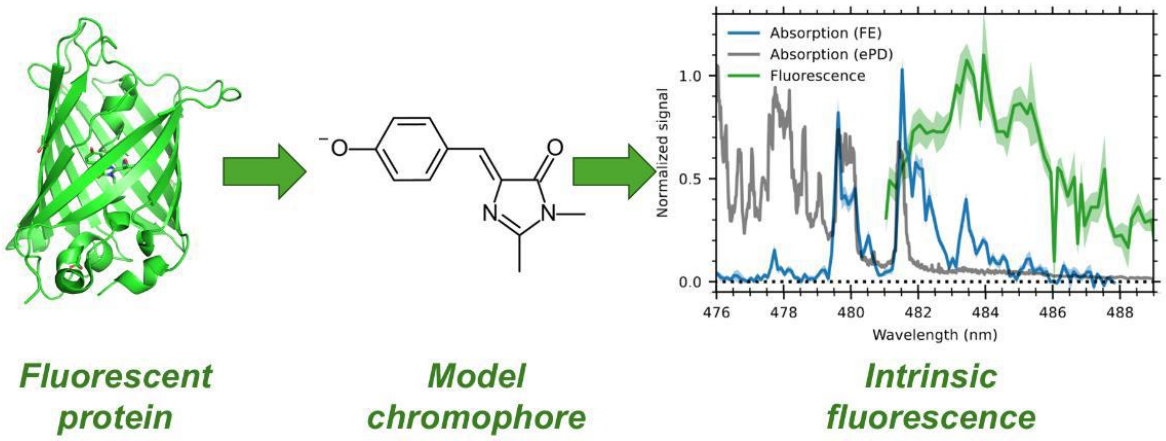

Figure 1: Gas-phase fluorescence spectra from cold model chromophore ions (HBDI) unveil the intrinsic photophysics of the green fluorescence protein

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Structure-Sensitive Photoelectron Elliptical Dichroism Enabled by Novel Tomographic Reconstruction

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Photoelectron dichroism has rapidly accelerated to the forefront of gas-phase chiral investigation and analysis, largely driven by significant enantiomeric sensitivities on the order of 1-10% [1] – up to two orders of magnitude greater than conventional chiroptical techniques. The molecular structure of the chiral species under investigation plays a crucial role in the magnitude and sign of the effect. Recent advances in tomographic data reconstruction techniques [2] now allow for the efficient extraction of the complete three-dimensional photoelectron angular distribution.

Building on this capability, combining these advances with photoelectron elliptical dichroism (PEELD) allows the full ellipticity-dependent evolution of the chiral response to be mapped. Here, we present a comprehensive set of PEELD measurements using 400 nm (2+1) resonance-enhanced multiphoton ionization. Alongside established chiral benchmarks, we report the first application of photoelectron dichroism to an extended, systematically varied series of six chiral aliphatic amines. These molecules share the favorable physical properties of conventional benchmark systems (e.g. volatility, rigidity) while additionally providing a highly controlled molecular testbed in which subtle structural modifications can be isolated and compared directly. Despite their structural similarities, each molecule exhibits a distinct dichroic response, with no predictive trends observed upon modification of functional groups or substitution positions. This pronounced variability reinforces the extreme sensitivity of photoelectron dichroism to subtle changes in molecular structure.

Ultimately, by exploiting full tomographic data acquisition, these findings highlight PEELD as a uniquely powerful and structure-sensitive probe, enabling its deployment in time-resolved studies tracking ultrafast structural dynamics. They further position chiral aliphatic amines as a versatile, benchmark-quality platform for probing dichroic photoionization phenomena in the gas phase.

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Observation of Scattering Resonances in Ion-Neutral Collisions

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The observation of quantum scattering resonances in ion–atom and ion–molecule collisions has remained a formidable challenge due to the stringent energy resolution required to resolve narrow scattering features and the difficulty of reaching the s-wave regime in heavy systems. To date, Ba+/Li is the only system in which Feshbach resonances have been successfully observed in a hybrid ion trap [1]. So far, no other experiment has succeeded in detecting quantum shape resonances in ion–neutral collisions and reactions.

Here, we report the first experimental observation of shape resonances in ion–neutral collisions, detected via charge-transfer reactions between helium isotopes. In the symmetric system of identical isotopes, the elastic and charge-exchange channels are indistinguishable, giving rise to additional interference terms in the scattering cross section.

Using highly excited helium Rydberg atoms merged with ground-state helium atoms, we observed shape resonances in the elastic scattering channel, reaching collision energies just below 1 K. By further reducing the accessible collision energies by a factor of 20, we reached 10 mK and detected a sharp shape resonance at 90 mK in the charge-transfer reaction between 4He+ and 3He. The introduction of a different isotope breaks the symmetry and requires a theoretical treatment that goes beyond the Born–Oppenheimer approximation. This system therefore provides a stringent test of state-of-the-art theory, and we demonstrate agreement without free parameters, representing the validation of beyond-Born–Oppenheimer quantum chemistry. Beyond this benchmark, we directly measure the ionization-energy difference between 4He and 3He as the energy release in the reaction. Our result is consistent with the only previous determination by Herzberg [2] and constitutes the first direct measurement using this method.

As an immediate extension, we move from ion–atom to ion–molecule systems, where we have also observed resonances in the elastic scattering channel of helium-ion collisions with H2 and HD.

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Characterising resonances in cold collisions between Rydberg He and HD/H2

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We have performed novel experiments to image elastic collisions between Rydberg He atoms and HD/H2 molecules which can stand in as a proxy for elusive ion- and neutral molecule scattering events. In particular, the He+-H2 system is of interest in the context of studying radiative charge-transfer processes[1]. Several peaks in the energy-dependent reaction rate, down to 1 K and below, were observed. These can be analysed and classified as either shape or Feshbach resonances using theoretical results which closely agree with the experimental observations. To this end, state-of-the-art ab-initio coupled channel calculations for collisions between He+ and HD/H2 have been performed. Our theoretical results sensitively depend on a new, strongly anisotropic, three dimensional CCSD(T) potential energy surface extrapolated from quin- and and hexatuple levels of theory and also includes FCI corrections. Agreement with the experiment is reached without the need for scaling the potential. By separating out resonant contributions to the reaction rate it becomes possible to pinpoint resonance energies and widths accurately. Further inspection of the wave function components at these energies reveals whether a given resonance possesses shape and/or Feshbach character.

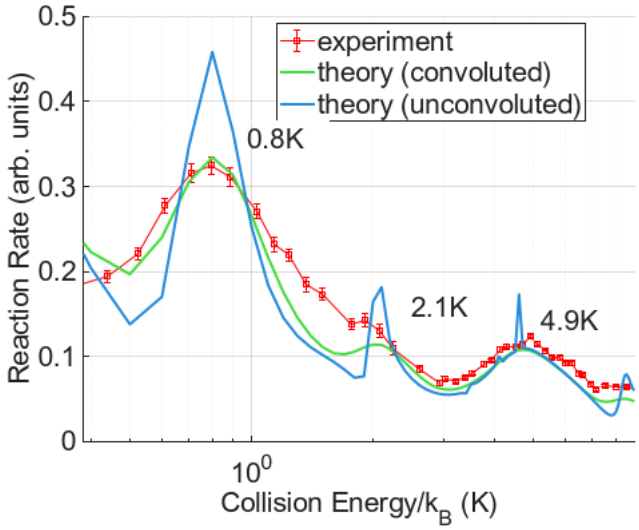

Figure 1: Energy-dependent reaction rate for He(Ryd)-HD (experiment) compared to He+-HD (theory) before and after convolution with the experimental resolution. Peaks in the reaction rate are found at approximately 0.8, 2.1 and 4.9 K respectively.

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Generation of broad-bandwidth deep ultraviolet pulses with achromatic second harmonic generation and interferometry via acousto-optic modulation

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The generation of deep ultraviolet optical pulses featuring broad spectral bandwidth and short pulse durations is a challenging task, especially when using high repetition rate (> 100kHz) laser systems that provide low pulse energies to drive the nonlinear conversion processes. We present a scheme based on second harmonic generation of the output of a non-collinear optical parametric amplifier. To increase the bandwidth and efficiency of the second harmonic generation we employ achromatic phase matching (APM) [1]. In order to achieve spectral resolution in pumpprobe scheme experiments up to the theoretical limit, we employ an interferometry approach automatically adapting to the optimal time-frequency resolution. The setup is used as pump source for extreme ultraviolet time-resolved photoelectron spectreoscopy (XUV TRPES).

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Isomer-resolved Ion-Molecule Reaction Kinetics of HCO+ and HOC+

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The [HCO+] / [HOC+] abundance ratio varies strongly across astrophysical environments [1, 2] and is therefore a promising diagnostic of the physical and chemical conditions of the interstellar medium. Its quantitative use, however, remains limited by uncertainties in key ion-molecule reaction rates and product branching ratios. We present new isomerresolved measurements obtained in a cryogenic 22-pole ion trap for some of the reactions controlling the HCO+/HOC+ balance, using chemical probing with 15N2 to distinguish the isomers.

We determine rate coefficients for the isomerization of HOC+ to HCO+ in collisions with H2 and CO, and for three formation channels yielding [H,C,O]+ products: CO+ + H2, H+3 + CO, and ArH+ + CO. None of the reactions studied produce the higher energy isomer efficiently, with only H+3 + CO resulting in a significant fraction (15%) of HOC+. Notably, our data show that CO+ + H2 forms predominantly HCO+, with only negligible (< 0.2%) HOC+ production, in contrast with earlier experimental results [3] but supported by more recent theoretical predictions [4]. We also find that HOC+ is efficiently converted to HCO+ by both H2 and CO under the explored conditions.

To assess the astrophysical implications, we implement the measured rates in a state-ofthe-art astrochemical model, evaluating the impact of the updated rates under typical conditions of cold molecular clouds and photon-dominated regions.

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Investigation of the reaction products resulting from C addition on PAHs

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Many individual polycyclic aromatic hydrocarbons (PAHs) have recently been detected through radio astronomy observations [1,2]. However, their observed abundances cannot yet be explained by current astrochemical models. Until recently, even the simplest aromatic precursors, such as C□H□ and C□H□, were underpredicted by several orders of magnitude [3,4]. We hypothesize that the growth of larger aromatic structures in dense molecular clouds proceeds primarily through carbon-atom addition reactions involving aromatic species. While reaction rates for these processes are expected to be rapid and can often be predicted theoretically with reasonable accuracy [5], determining the structures of the reaction products and their relative branching ratios remains highly challenging.
In our experimental setup, we will first investigate the branching ratios of the reaction products formed in reactions between atomic carbon and astronomically detected PAHs. In a second stage, we will aim to gain structural insight into these products using photoionization spectroscopy combined with a tunable vacuum ultraviolet (VUV) laser. A supersonic beam of carbon atoms is generated by an electric discharge of CBr□ diluted in Ar. The carbon atoms subsequently react with PAHs introduced upstream of the discharge region. Initially, a 118.3 nm (10.5 eV) VUV laser coupled to a reflectron mass spectrometer will be used to characterize the reaction products. In a later phase, we plan to install a tunable VUV laser to enable isomerselective detection schemes.

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Microsecond-resolved imaging of $CaCO_3$ formation in a free-flowing liquid flat-jet

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The early stages of calcium carbonate formation occur on timescales that remain largely inaccessible to conventional in situ methods such as stopped-flow scattering [1] or droplet-based microfluidics [2], which are limited to the millisecond range or slower. Here we use a free-flowing liquid flat-jet, formed by the impingement of two laminar aqueous cylindrical jets, to monitor $CaCO_3$ formation with microsecond time resolution. CaCO3 is formed within the liquid sheet by the metathesis reaction of CaCl2 and K2CO3, which are delivered separately through the two jets. The flow axis of the first laminar leaf is directly mapped onto the reaction time, converting a spatial coordinate into a kinetic one [3]. We characterize the flat-jet centerline velocity field using two independent, tracerfree methods: single-exposure streak imaging on the one hand and cross-correlation of the intrinsic sheet texture on the other hand. The two methods agree and confirm that the velocity scales linearly with flow rate, independent of solution chemistry.
Mapping the onset of optically visible CaCO3 formation across five solution conditions, we find that the visible onset time (22–110 μs) is independent of flow rate but varies systematically with reactant concentration and with the Ca2+:CO2− 3 ratio. The flow-rate independence indicates that the observed onset reflects intrinsic precipitation kinetics of the solution rather than mixing hydrodynamics. The flat-jet thus provides in situ optical access to the onset of CaCO3 formation on microsecond timescales and offers a promising platform for time-resolved studies of early-stage nucleation. This time window is central to the ongoing debate between classical [4] and nonclassical [5] descriptions of CaCO3 formation.

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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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Vacuum compatible temperature-controlled flat-jet for liquid crystal applications

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Recent developments in flat jet technology have enabled the characterisation of thin, flat films of flowing liquids for spectroscopic applications. The flow of liquid allows the sample to be continuously refreshed at the interaction region, while the flatness of the surface avoids unwanted defocusing effects that may lead to uncertainty in the measurements, making it an essential sample delivery system for extreme ultraviolet (XUV), photoelectron, and high-order harmonic generation (HHG) spectroscopies. The typical thickness achieved with the most common method for generating a liquid flat jet is based on the impinging geometry, where two streams of liquid collide with each other, and the momentum carried by each stream is transferred in the orthogonal direction, leading to the formation of a chain of flat liquid leaves. The typical sample thickness achievable with the impinging geometry is usually on the order of a few micrometres. All the spectroscopic techniques mentioned above would benefit from an even thinner liquid sheet by reducing reabsorption of the signal in HHG, minimising modifications of the low-energy photoelectron spectrum in photoelectron spectroscopy, and improving the signal-to-noise ratio in XUV measurements. Recently, Koralek et al. provided a novel scheme for the generation of ultrathin liquid films based on a single liquid channel that is squeezed down to the nanometer scale through the impingement of two lateral gas jets [1].
Thermotropic liquid crystals (LC), among other liquids, stand out for their peculiar mesophase nature, retaining a certain degree of positional and orientational order before phase transitioning in a common liquid. The implementation of such a sub-micron jet in combination with a dedicated temperature control system would enable several experimental investigations in the XUV to the soft-X-ray range, which remain largely unexplored.
In this contribution, the design and characterisation of a vacuum-compatible and temperature-controlled ultrathin flat jet for LC applications will be presented. In particular, thickness stability measurements based on an interferometric technique will be shown, as illustrated in Fig. 1b, together with temperature stability measurements based on a PID-controlled loop.

Figure 1: (a) microscope image of a thin liquid flat leaf produced by the gas-accelerated flat-jet described in [1]. (b) An interferometric image acquired with a monochromatic beam of the leaf produced by the same device.

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Chiral Selection in Rotational Quantum States

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Controlling the internal degrees of freedom of selected enantiomers of chiral molecules has a wide range of fundamental applications, from quantum information to precision spectroscopy. Enantiomer-Specific State Transfer (ESST) enables the separation of enantiomers in rotational quantum states of chiral molecules. In theory, full control over the population transfer of the enantiomers can be achieved. However, early experimental demonstrations reported only modest state-specific enantiomeric enrichment [1, 2]. This is due to the realistic limitations of thermal population and orientational degeneracy of the rotational states. In our work, we overcome the limitation due to thermal population by combining ultraviolet and microwave radiation [3]. Targeting a triad of rotational states including the absolute ground state, we thereby realized near-complete chiral selection in rotational quantum states [4]. In recent work, we address the limitation due to orientational degeneracy in a triad that does not include the absolute ground state. The M-state dependent Rabi frequencies impede the overall transfer efficiency when employing conventional pulse schemes. We incorporate theoretically tailored pulse schemes [5] and demonstrate enhanced control despite degeneracy.

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Modelling the Vibronic Structure of Cryogenic Gas-Phase Fluorescence Using a Python-Based Franck–Condon Framework

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Cryogenic gas-phase fluorescence spectroscopy, free from solvent and environmental effects, effectively probes ions' intrinsic photophysical properties through vibronic patterns in spectra.[1-3] However, spectral resolution in fluorescence emission is affected by excess internal energy from photoexcitation, excitation-dependent broadening and shifts in the emission maxima.[2,3] This energy alters vibrational populations in the emitting state, requiring accurate modelling of thermal populations in the vibronic transition.[2]

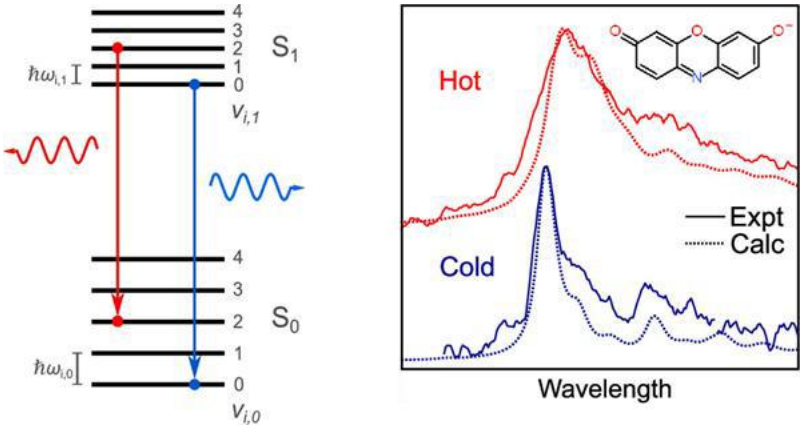

Figure 1: Room temperature (red line) and cryotemperature (blue line). Left panel, Jablonski diagram showing that the average energy of emitted photons from $\Delta v = 0$ transitions increases with cooling. Right panel, experimental and calculated emission spec

To address this, we developed a Python-based method for efficient Franck–Condon (FC) simulations under the harmonic and Born–Oppenheimer approximations. Assuming a unit Duschinsky matrix and direct Boltzmann sampling, accounting for thermal effects. [2,3] Benchmarking against conventional FC simulations at experimental temperatures (T > 100 K) shows excellent agreement, validating the approach for cryogenic gas-phase fluorescence spectroscopy of medium-to-large molecular systems. [1-3]

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Helium Nanodroplet Isolation Spectroscopy of Quinacridone and its Microsolvation Complexes

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Organic chromophores with conjugated π-electron systems, efficiently absorb light in a spectral region between near IR and UV, largely determined by the spatial extent of the electronic system. Besides playing a key role in nature, they are utilized in modern technology, such as organic solar cells, and have recently emerged as candidates for photocatalytic water splitting [1]. Among these materials, quinacridone is of particular interest for various reasons. Widely used as a printing pigment, it can form chiral surface structures despite being achiral as an isolated molecule [2]. In addition, quinacridone and its derivatives have attracted attention as potential photocatalysts for water splitting [3].
We use helium nanodroplet isolation spectroscopy to elucidate the vibronic structure of quinacridone molecules. The ultracold inert environment of the helium nanodroplets ensures cooling of the molecules to the vibrational ground state while not altering the vibronic structure significantly. This technique furthermore enables us to form and investigate cold molecular clusters and complexes under controlled conditions. In our experiments we combine these techniques with pulsed dye Lasers to obtain vibronic excitation spectra with a resolution below 1 cm-1.
The recorded excitation spectra exhibit an intriguing structure, pointing toward contributions from different tautomers. By varying the experimental doping conditions, different molecular clusters and complexes can be formed and investigated. These include for example hydrogen-bonded molecular dimers and quinacridone–water complexes. The latter are of particular interest for potential photon driven water splitting reactions. Various excitation energy shifts are observed and attributed to complexes. Surprisingly, peaks assigned to tautomers exhibit significantly different behavior upon water co-doping.
The potential formation of dark states and non-radiative relaxation pathways in these complexes will be investigated in future experiments using alternative detection schemes based on the photoionization of excited molecular complexes. A final assignment of the observed spectral features is expected through quantum chemical calculations.

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Thermodynamics of Confined Water in Swelling of Clays: Role of Competitive Cation Hydration

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The swelling capacity and stability of clay play a crucial role in various areas ranging from cosmetics to oil extraction; hence change in their swelling behaviour is important for their efficient utilisation. Here we focus on understanding the role of different hydration properties of cation on the thermodynamics of clay swelling by water adsorption. We have used mica as the reference clay, Na+, Li+, and H+ ions as the interstitial cations, and performed grand canonical Monte Carlo (GCMC) simulations of water adsorption in mica pores (of widths d = 4 − 40 Å). The disjoining pressure, swelling free energy, and several structural properties of confined water and ions were calculated. We expected higher water density in H-mica pores (ρH) due to the smaller size of H+ ions having higher hydration energy. However, the counter-intuitive trend of ρLi > ρNa > ρb (bulk density) > ρH was observed. The swelling free energy for Na-mica is characterised by global minima at d = 6 Å corresponding to crystalline swelling with significant and multiple barriers for crystalline swelling to osmotic swelling (d > 12 Å). A shift in the location of global minima of swelling free energy as well at it becoming more repulsive is observed in the increasing order of Na+, Li+, and H+ ions. We found that the competition between surface atoms and water molecules to hydrate the Na+ ions favour the non-swelling nature, whereas, it changes significantly in the Li + ions and H+ ions case thus favouring clay swelling.

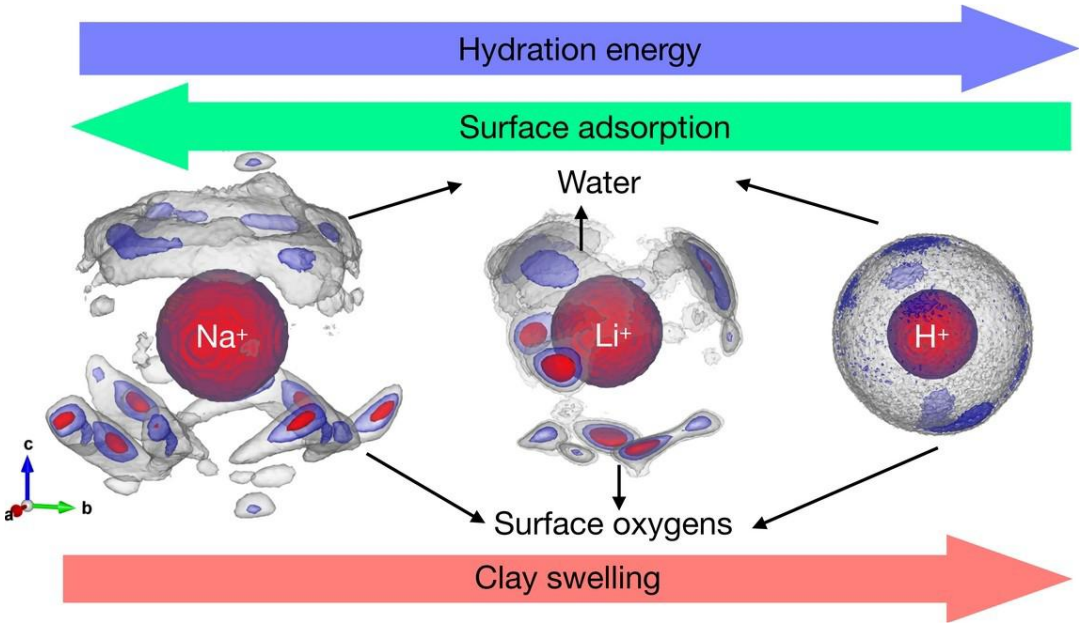

Figure : Three-dimensional pair-correlation function illustrating cation (central atom) hydration by oxygen of water molecules (top-side) and surfcae (bottom side) for various cations

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Non-Statistical Reaction Dynamics for Energized Criegee Intermediates

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Criegee intermediates (CIs) are important reactive species in atmospheric chemistry. One of their important decomposition products is the OH radical which drives a large number of bimolecular reactions. This contribution will describe the unimolecular decomposition dynamics into all molecular fragmentation channels for the smallest CI, H2COO. For this, a neural network-trained global potential energy surface at the CASPT2/aug-ccpVTZ level is used together with quasi-classical trajectory simulations. The simulations reveal pronounced channel-dependent deviations from RRKM kinetics. Lifetime distributions for decomposition through energized formic acid follow stretched or compressed exponentials instead of single-exponential decays. Formation of H2O+CO (β = 1.24 } 0.03) and HCO+OH (β = 1.28 } 0.21) exhibits compressed-exponential behavior, indicating non-statistical relaxation and non-equilibrium dynamics. In contrast, the CO2+H2 channel displays stretched-exponential kinetics (β = 0.90 } 0.03), consistent with a different exploration of phase space and relaxation mechanism. These findings demonstrate that the fate of a single internally excited intermediate can depend strongly on the product channel and cannot be captured by conventional RRKM-based unimolecular rate theories. Explicit molecular dynamics simulations are therefore essential for describing the decomposition of energized Criegee intermediates and uncovering the molecular origins of non-RRKM behavior in atmospheric reaction networks.

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How to deal with decoherence in trajectory surface hopping

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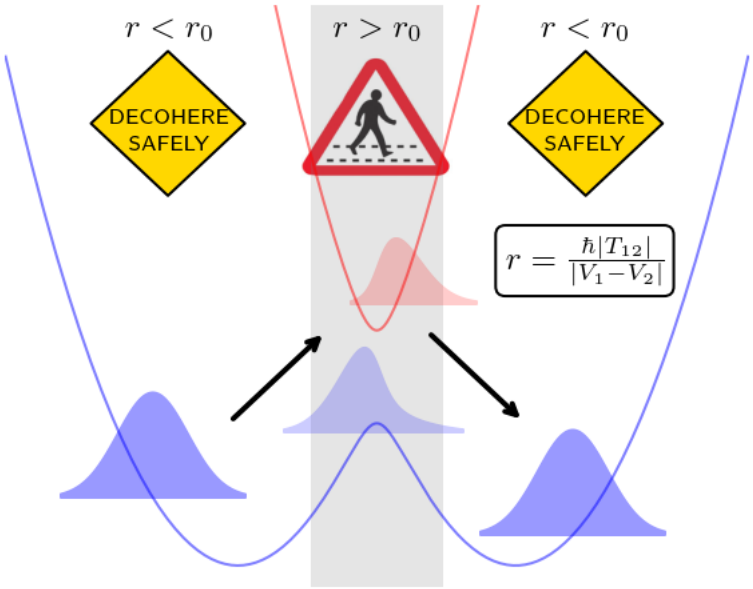
Tully's fewest switches surface hopping is a leading computational method for excitedstate dynamics in molecules and materials. It unfortunately lacks a proper description of decoherence, which has lead to numerous "decoherence correction" schemes based on more or less uncontrolled approximations. I have recently proposed a simple and general solution to this problem: to restrict decoherence to regions of low nonadiabaticity, as measured by the dimensionless Massey parameter [1]. When tested on a suite of benchmark systems, the same threshold values were found to be suitable for a variety of systems with vastly different size and absolute energy scales, whereas conventional decoherence corrections often suppress coherence too strongly. The results are relevant for any simulations of excited-state dynamics that allow for a natural separation in classical and quantum degrees of freedom.



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Design for a Monochromatic, High-Repetition-Rate XUV Beamline for Time-Resolved Photoelectron–Photoion Coincidence Spectroscopy

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Many molecular level processes, relevant in fundamental science and modern technology occur naturally in a condensed environments. The details of the molecular environment, while crucial for an exact description of the process poses challenges in the experimental and theoretical study of such processes. Molecular clusters and complexes can in some cases be used to study the effect of complex environments, while circumventing some of the challenges posed by larger condensed samples.
Photoelectron photoion coincidence spectroscopy has been demonstrated to provide detailed cluster-size resolved information on various molecular processes and properties. However, such cluster-size resolved experiments, do not routinely extend to ultrafast time-resolved techniques like time-resolved photoelectron spectroscopy. One bottleneck for such measurements is the existence of femtosecond, monochromatized VUV and XUV light sources operating at the high repetition rates necessary for coincidence detections.
We present our plans for an XUV beamline based on high-harmonic generation driven by a high-repetition-rate Yb laser, operating at up to 120 kHz. The beamline will be based on a high harmonic generation (HHG) scheme driven by an Yb laser. The NIR pulses will first be spectrally broadened by self-phase modulation in a gas-filled multipass cell and compressed to pulse durations of ~40 fs. The XUV radiation, generated by HHG of the fundamental (1030 nm) or second harmonic (515 nm) of the driving Laser [1] in a rare gas jet, will be coupled to a single-grating time-preserving monochromator [2]. With a plane diffraction grating in off-plane geometry, the monochromator will enable spectral selection of individual harmonics while minimizing temporal broadening to maintain pulse durations of tens of femtoseconds. In contrast to many existing HHG-based beamlines, we focus on the relatively low photon energy range of 10–20 eV. Using not only the fundamental but also the second harmonic to drive the HHG process provides several advantages. At these photon energies, conversion efficiency can be increased by driving with the second harmonic of the Yb laser while the shorter driving wavelength also simplifies the spectral isolation of individual harmonic orders. The latter allows the use of low-groove-density gratings, further reducing the temporal broadening introduced by the monochromator.
A home-built nonlinear optical parametric amplifier pumped by the same Yb Laser will supply frequency-tunable ultrashort pump pulses in the visible and UV spectral range. This beamline will be used in performing time-resolved XUV photoelectron–photoion coincidence spectroscopy in molecular complexes.

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Photofragment imaging of oriented alkyl bromides for evaluating their transition dipole moments

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Photofragment imaging of oriented methyl/ethyl bromide (CH3Br, C2H5Br) was performed at UV irradiation ~234 nm. Both bromides with large dipole moment 1.82/ 2.03 D were focused through our hexapole state-selector (12 kV/cm, 1 m length), oriented to the imaging TOF (time-of-flight) axis under the succeeding guiding fields (10 kV/cm). Intensity of methyl/ethyl bromide in the focused molecular beam increases seven/four times more than in the unfocused one, respectively. After UV photodissociation, the same light serving in [2+1] REMPI detection scheme, the spin-excited bromine atom fragment, Br [2P1/2] (as denoted Br*), was ionized at 234.021 nm (via 5p 2S1/2 ← 4p 2P1/2). The ion packet was slowly expanded through TOF acceleration region, extracted to TOF drift tube. Then its central segment (30 ns width) was observed with the slice imaging apparatus, which enables us to directly measure the speed and angular distributions of photofragment atoms. Fig. 1 exemplifies observed images of Br* fragment atom from isotropic (free-rotated/non-oriented) and oriented methyl bromide. The left image displays the nearly symmetrical arcs across the horizontal axis, in sharp contrast with asymmetrical intensity between upper and lower arcs on the right. Akin to methyl bromide, the kinetic energy release of Br* fragments from ethyl bromide reproduces the previous one [1]. The sliced image from oriented parents at the dissociation laser polarization angle 45° implies the vector correlation among the transition dipole moment □, its fragment velocity **v**, and the diploe moment **d** of parent bromide nearly along C-Br bond axis [2], which reveals the direction of the transition dipole moment □ of parent bromide to the first predissociation state. The detail of our examines will be shown in presentation.

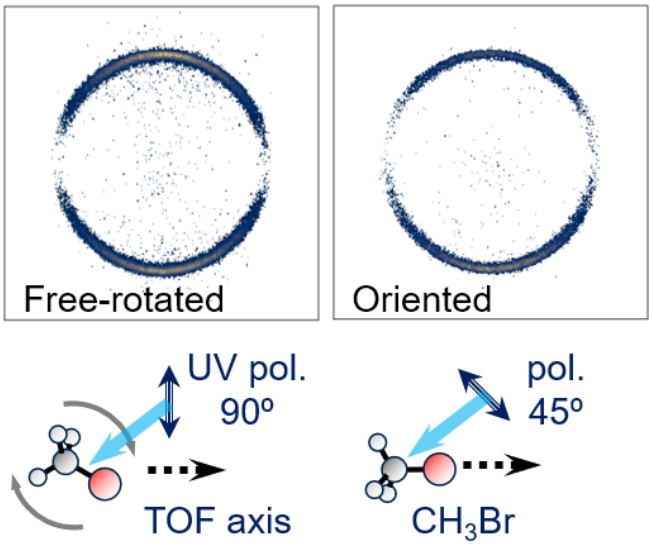

Figure 1 Sliced images of spin- excited Br (Br) fragment atom from free-rotated methyl bromide (left) and oriented one along TOF axis (right).*

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Dynamics of the activation of small molecules by a transition metal cation in the gas phase

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The use of well-defined model systems is an established method to investigate single reactive events at the atomic level. Probing the dynamics of the activation of small molecules e.g. methane by transition metal cations in the gas phase can be helpful to understand such processes. These reactions are endothermic and associated with high barriers on the ground state potential energy surface of transition metal cations like Ta+. Despite these barriers the reaction still takes place at room temperature due to an efficient crossing from the ground state surface over to the first excited-state surface. This multi-state reactivity is often observed for reactions involving open-shell transition metal centers, but their theoretical treatment is a challenge even today [1,2]. The rearrangement of atoms during a reaction, i.e. the atomistic dynamics can be investigated by measuring energy and angle differential cross sections [3-5].

The activation of small molecules by a transition metal cation were investigated by measuring experimental energy and angle differential cross sections at different relative collision energies via crossed beam velocity map imaging. The experimental results were supported by quantum chemical calculations by means of trajectory surface hopping studies on spin-specific full-dimensional potential energy surfaces [6].

At low relative collision energies, the activation of methane shows dominant signatures for indirect dynamics. For higher relative collision energies, the reaction suggests a trend toward more direct dynamics. Based on theoretical analysis it could be concluded that intersystem crossing presents a dynamic bottleneck that leads to the observed dynamics [6]. The reaction of carbon dioxide with the same transition metal cation shows indirect dynamics over all measured relative collision energies [4]. From a chemist's point of view the difference in dynamics seems counter intuitive because the seemingly more facile activation of methane requires elaborate bond rearrangement compared to a single oxygen atom being transferred in the case of carbon dioxide.

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Interferometry and Spectral Absorption Imaging in Liquid Flat Jets

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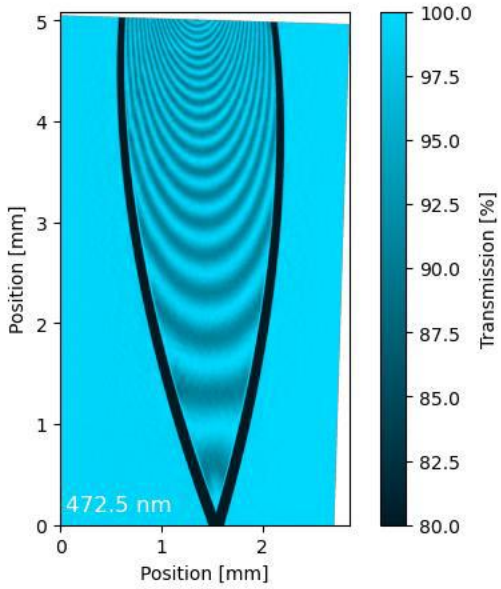
In order to study dynamics at liquid-liquid interfaces, we are developing a new approach to spectral absorption imaging, and here show how it can simultaneously be used to determine liquid flat jet sheet thickness with remarkable precision. Flat microjets are created by impinging microjets, resulting in optically flat thin sheets of two co-flowing liquids at speeds of around 10m/s.
Absorption imaging is used to record wavelength specific images or, in other words, to record the spatial dependence of the UV/VIS spectrum of the flat jet. Here we present the demonstration of this method by recording images of fat jets with methylene blue at different concentrations. As shown in the figure below, images recorded with light with a bandwidth of around 2 nm reveals interference fringes that originate from internal reflection at the two air-water interfaces. We demonstrate how these fringes can be used to determine the thickness profile of the flat jet.



Laser-induced alignment of nanoparticles and macromolecules: modeling and realization

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X-ray free-electron lasers (XFELs) promise the diffractive imaging of single molecules and nanoparticles [1]. This relies on recording a series of two-dimensional (2D) diffraction images from randomly oriented isolated particles, which are assembled in silico to a threedimensional (3D) diffraction volume so that the structure can finally be reconstructed. The orientational uncertainty is solved using advanced analysis algorithms. However, this can be very challenging at times and is a major bottleneck in achieving atomic spatial resolution [2]. Laser-induced alignment of nanoparticles and macromolecules can improve the achievable resolution by reducing the complexity of the diffraction volume search space and push it toward the atomic scale [3, 4].

We present quantitative modeling of nanoparticle alignment using classical mechanics and electrodynamics. Methods to predict molecular polarizability tensors were developed [5], and laser-induced rotational dynamics were simulated, demonstrating that strong alignment of biological macromolecules is generally feasible [6].

Based on these results, we experimentally demonstrate laser-induced alignment of tobacco mosaic virus (TMV). Strong alignment was detected through optical scattering in a setup compatible with XFEL experiments. Time- and intensity-dependent studies show a strong dependence of the scattering on the alignment laser polarization. Comparing computational and experimental results, we conclude that a very high degree of alignment of TMV was achieved in our experiments.

Beyond applications in XFEL imaging, laser-controlled rotational dynamics could provide a route toward observing quantum alignment revivals in massive nanoparticles, possibly testing the limits of quantum mechanics.

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Tetrasubstituted allenes: exploring axial chirality by time-resolved photoelectron circular dichroism spectroscopy

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Photoelectron circular dichroism (PECD) has emerged as a highly sensitive technique for investigating chiral molecules and offers unique opportunities for time-resolved studies of ultrafast chiral dynamics [1, 2]. Upon photoionization with circularly polarized light, chiral molecules exhibit a forward–backward asymmetry in the photoelectron angular distribution along the light propagation axis, giving rise to the PECD signal. While PECD has been applied to molecules with point chirality, axially chiral systems, to our knowledge, have remained unexplored despite their importance in drug design, asymmetric catalysis and biomolecular recognition.

Here, we present the **first PECD investigation of axial chirality** using a series of enantiopure tetrasubstituted allene derivatives as model systems, selected to systematically probe the effects of molecular structure and symmetry. Because these compounds are not commercially available, they were synthesized, enantioseparated, and fully characterized in our laboratory. Furthermore, we performed theoretical calculations of UV/VIS absorption and electronic circular dichroism spectra using TD-DFT, enabling interpretation of spectral features and assignment of absolute configurations.

Proposed static PECD measurements employing circularly polarized extreme ultraviolet radiation will allow ionization from multiple valence orbitals, providing detailed insight into how molecular geometry, substituents, symmetry, and electronic structure govern the chiral photoelectron response. Time-resolved PECD using a pump-probe scheme will then explore the temporal evolution of the chiral signal, thereby probing the dynamics of electronically excited states of the investigated allenes. Combined with theoretical modelling of photoelectron spectra and PECD signals, this work will establish the foundation for PECD studies of axially chiral molecules and open new perspectives on chiral photoelectron dynamics.

This work was supported by the Specific university research grant No. A2_FCHI_2026_017 and by The Czech Science Foundation, project No. 24-10298M. Computational resources were provided by the e-INFRA CZ project (ID:90254), supported by the Ministry of Education, Youth and Sports of the Czech Republic.

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QM/MM investigation of structure and reactivity of PSTK dependent on the protonation state of the Thiaminediphosphate cofactor

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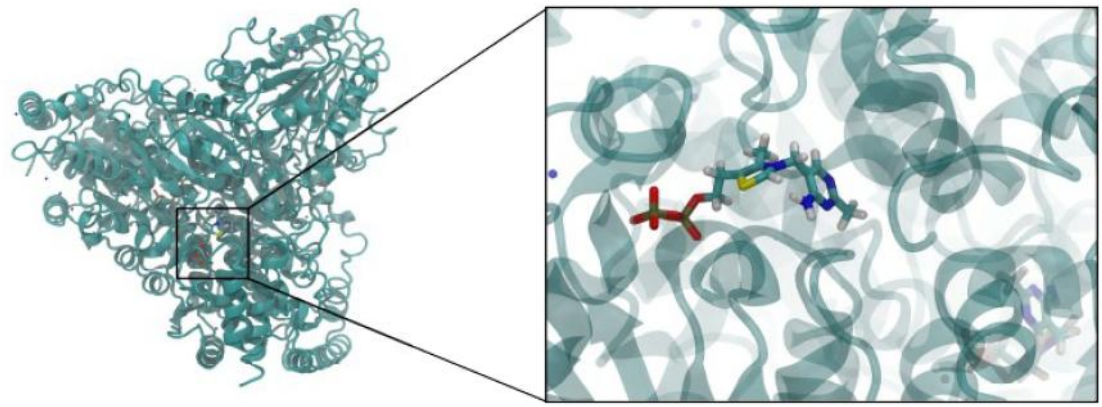
Thiamine diphosphate (ThDP), the active functional form of vitamin B1, is a common cofactor for a multitude of enzymatic systems. This ThDP cofactor is known to exhibit uncharacteristically low pKa values at key sites.[1] The low pKa values have been attributed to the protonation of the cofactor and nearby residues[1] both of which are central to the catalysis as well as regulation.[2] We are, therefore, investigating the ThDP cofactor using QM and combined QM/MM methods. Of interest is the behavior of both the isolated ThDP molecule as well as the assembly of the cofactor in the pocket of its host protein. Due to the dimeric structure of the protein, cooperativity between active sites needs to be taken into account in the investigation of the catalytic action.[1] Conformational analysis and the corresponding energies, pKa values, the electric fields acting upon the cofactor as well as the hydrophobicity of the surrounding cavity will be used in combination to provide quantitative insights into the forces acting on the cofactor and the protein environment. Our findings will shed light on the functionality of the protein and open avenues for biomimetic molecular design and catalysis.



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Dipolar Control of Molecular Complexation in Ultracold Environments

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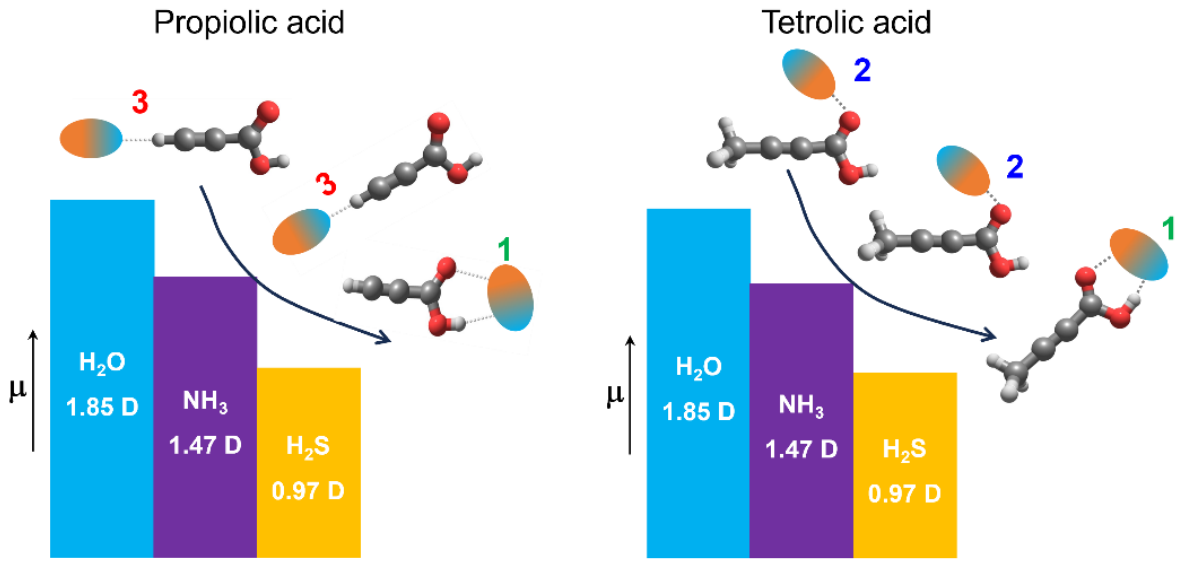
Selective production of desired species controlled by internal or external electric fields has attracted considerable interest because of its relevance to quantum computation and reaction dynamics.1 The approaching orientation of molecules during aggregation inside helium nanodroplets (0.4 K) is known to depend on the dipole moment of the interacting partners.2,3 To systematically map out this dipole-strength-dependent aggregation process, mass-selective IR spectroscopy in helium nanodroplets combined with quantum chemical calculations has been performed. Propiolic acid [HC≡C(C=O)OH, 1.59 D] and tetrolic acid [H3CC≡C(C=O)OH, 2.39 D], possessing substantial dipole moments, were individually complexed with H2O (1.85 D), NH3 (1.47 D), and H2S (0.97 D) in three separate sets of experiments inside helium droplets. The detected hydrogen-bonded dimer structures reveal a competition between long-range dipole-driven prealignment and local thermodynamic stabilization depending on the dipole strength of the interacting molecules. Concisely, long-range dipole–dipole interactions steer the geometry of the H2O and NH3 complexes with propiolic acid resulting in kinetically trapped local-minimum structures (site **3** or **2**) being prevalent.3 In contrast, complexes with weakly dipolar H2S populate the thermodynamically most stable binding motif (**1**), indicating that internal electric-field-induced alignment becomes less effective below a critical dipolar strength. To further examine this effect, the most preferred acetylenic (**3**) binding site in propiolic acid was blocked through methyl substitution in tetrolic acid. The resulting complexes further reinforce the earlier observations. Overall, this study provides a qualitative estimate of how dipole strength governs kinetic versus thermodynamic structure selection under ultracold conditions.



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Exactly solvable two-level model with time-dependent coupling, detuning, and loss: Application to strong-field resonance ionization

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Exactly solvable driven two-level models play a central role in understanding coherent quantum dynamics, from the Rabi solution to Landau–Zener-type transitions [1]. In this work we present an analytic extension of the Hioe–Carroll framework [3] that incorporates irreversible loss together with time-dependent coupling and detuning sharing a common pulse envelope [2]. This structure preserves integrability and yields closed-form expressions for the complex population amplitudes for any pulse whose intensity profile is analytically integrable, including Gaussian and sine-squared shapes.
We apply the method to the 2+1 photon resonance-enhanced multiphoton ionization of atomic lithium, where two-photon coupling, dynamic Stark shifts, and one-photon ionization rate naturally exhibit the same intensity dependence [4, 5]. The analytic bound-state solution enables an exact treatment of the continuum amplitudes and leads, for sine-squared pulses, to a closed-form expression for the photoelectron spectrum. This result provides direct physical insight into the formation of the Autler–Townes doublet, its multi-peak structure, and the role of decay in producing spectral asymmetry.
The presented model offers a compact analytic framework for strong-field dynamics including irreversible loss, complementing numerical approaches and providing a transparent tool for problems in multiphoton ionization, pulse-driven quantum control, and non-Hermitian quantum systems.

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Latest Results and Developments at the Ultrafast Dynamics AMO beamline FL26 at FLASH

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FLASH is an XUV and soft X-ray FEL offering femtosecond light pulses with high repetition rates. FL26 is a specialized beamline for time resolved AMO experiment with a reaction microscope and transient absorption setup as permanent endstations. The beamline is equipped with XUV split-and-delay units, synchronized pump probe lasers and a synchronized HHG source and thus offers great opportunities of time resolved experiments. Two experiment chambers are installed with a 1:1 focus imaging in between. The first focus is inside the reaction microscope chamber for coincident momentum spectroscopy, in the second focus a gas cell can be inserted for transient absorption experiments. At the end of the beamline is a VUV spectrometer for spectral diagnostic of the FEL and HHG photon beams.
We will give an overview of the FLASH facility and the FL26 endstation as well as current instrumentation developments. Furthermore we present highlights from recent publications that followed experiments conducted at the beamline.

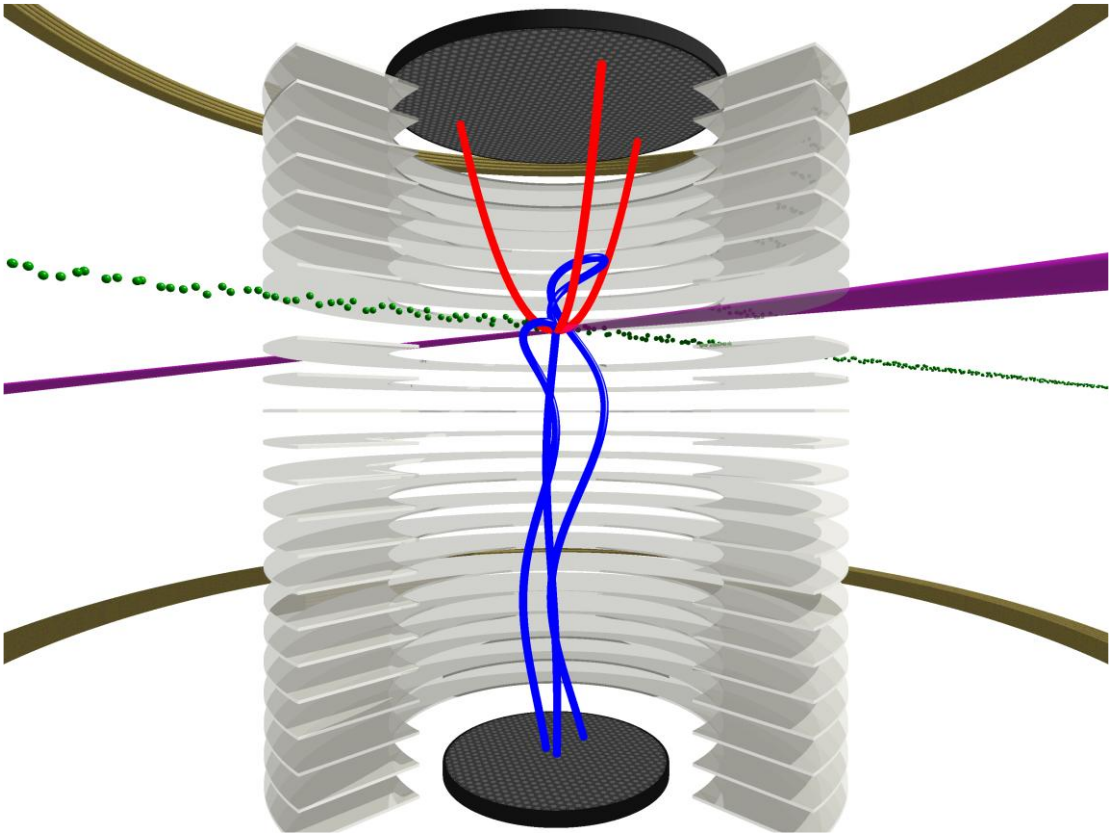

Figure 1: Rendering of an coincidence experiment with molecular fragmentation after ionization by XUV radiation in the FL26 reaction microscope. The XUV beam (purple) is focused into the gas jet (green particles). Electrons (blue trajectories) are guided to the bottom detector by homogeneous electric and magnetic fields. Ionic fragments are guided in the opposite direction to another detector.

Master Equation Modelling of the Ozonolysis of Green Leaf Volatile Aldehydes

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Green leaf volatiles are unsaturated organic C6 aldehydes released into the atmosphere by plants under environmental stress. These compounds subsequently react with atmospheric oxidants such as OH radicals or ozone, which are present in polluted environments. We report new results on the theoretical modelling of the ozonolysis reactions of trans-2-hexenal and 2-methyl-pentenal [1,2]. The reaction mechanisms were investigated at thelevel of M06-2X/aug-cc-pVTZ computations, the energy values of the stationary points were improved by single point calculations with the UCCSD(T)/aug-cc-pVTZ method. Ozonolysis reactions are very exothermic and difficult to model, as the sequential mechanism competes with the well-skipping mechanism. To take into account the two types of mechanisms, the system of kinetic equations was integrated with the Master Equation Solver for Multi-Energy Well Reactions (MESMER).

Both ozonolysis reactions have been investigated by several experimental groups, however the detailed mechanisms remained unclear because, in both cases, a carbon loss of up to 50% was observed. In other words, nearly half of the carbon contained in the aldehydes ended up in unidentified products. This long-standing problem is now resolved. The first steps of the ozonolysis reactions are according to the Criegee mechanism. Our results suggest that the formation of a secondary ozonide, resulting from the collisional stabilization of a Criegee intermediate with a carbonyl compound, can account for a large part of the experimental carbon loss, while a minor part is due to propylformate in the case of hexenal, or ethylformate in the case of methyl-pentenal, produced alongside (methyl)-glyoxal through the so-called hot ester channel. The computed rate constants are in excellent agreement with experimental measurements.

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Diabatic Representation of Molecular Property Operators Using Neural Networks: Application to Jahn–Teller Systems

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The accurate simulation of rovibronic spectra of Jahn-Teller systems requires not only the accurate potential energy surface (PES) but also an accurate representation of other molecular property operators, like dipole moment and electronic orbital angular momentum. While recent studies [1], successfully reproduced the position of the spectral lines for the ground state of NO3, significant discrepancies remained in the predicted line intensities. This highlights the need for improved representation of the dipole moment operator in addition to accurate energy levels.

We recently developed a general symmetry-based framework for deriving the diabatic representation of molecular property operators belonging to any irreducible representation in Cnv and Dnh [2]. The diabatic representation is, except for a very limited cases, not unique. As a consequence, when the diabatization of the potential and the one of molecular properties are performed separately, the resulting potential representation may fail to diabatize the molecular properties.

To overcome this challenge, we introduced simultaneous diabatization and fitting of both potential and molecular property operators to ensure that the resulting diabatic space is common for both. In recent years, the neural network-based diabatization of the potential energy matrix has achieved remarkable success [3-4]. Neural networks have also been applied to fitting dipole and spin-orbit couplings, mainly focusing on non-degenerate electronic states [5]. However, their application to molecular property operators in Jahn-Teller systems remains limited.

In our study, we perform simultaneous diabatization and neural network fitting of both potential and dipole moments for NH3+ in reduced dimensionality. The resulting potential model is then used in diabatizing the angular momentum operator, enabling us to validate the ability of the developed diabatic representation in diabatizing other molecular property operators.

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Influence of strong field ligands on the ultrafast photodynamics of square-planar nickel complexes

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Square-planar Ni(II) complexes with extended charge-transfer (CT) excited-state lifetimes represent attractive earth-abundant alternatives to the well-established isoelectronic Pt(II) photocatalysts. Previous studies have shown that Ni(II) complexes combining tridentate N-heterocyclic carbene (NHC) ligands with isocyanide coligands can generate sufficiently strong ligand fields to achieve triplet metal-to-ligand charge-transfer (^{3}MLCT) lifetimes on the order of several tens of picoseconds. In addition, torsional motions facilitating ^{3}MLCT → ^{3}MC relaxation as well as the influence of bulky isocyanide substituents providing enhanced axial shielding of the nickel center have been identified as key structure–dynamics relationships. [1,2]
To further investigate these design principles, we studied the ultrafast photodynamics of a new series of Ni(II) complexes with potentially improved structural and electronic properties. To obtain detailed insight into the structural changes governing their excited-state relaxation pathways, we employed polarization-resolved femtosecond visible-pump/mid-infrared-probe spectroscopy. Measurements were performed in the characteristic stretching region of cyano and isocyanide ligands (~2100 cm^{-1}), which serves as a sensitive probe of the monodentate ligand environment and is highly responsive to local electric fields and changes in the oxidation state of the nickel center. Complementary measurements in the mid-IR fingerprint region further provide information on the structural dynamics of the tridentate ligand framework.

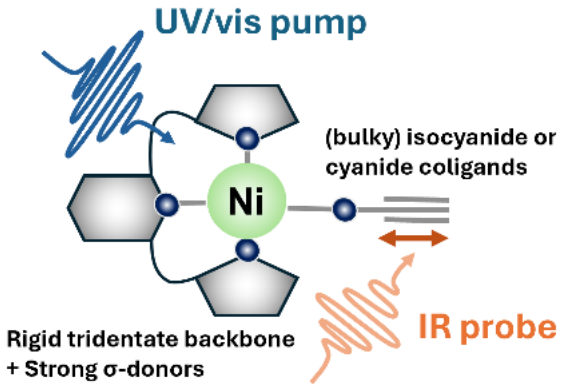

Figure 1. Design principle to achieve extended excited-state lifetimes in square-planar nickel complexes.

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[2] T. Ogawa and O. S. Wenger, Angew. Chem. Int. Ed. 62, e202312851 (2023).

Development of an instrument for isomer-selected ion-molecule reactivity studies

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The gas-phase chemistry of hydrocarbon ions is a key mechanism governing carbon growth in astrochemical environments. However, many fundamental species, including C3H+3 and C6H+5 [1, 2], exist as multiple structural isomers that cannot be distinguished by conventional mass spectrometry. As a result, measured reaction rates and product distributions typically represent ensemble averages over coexisting isomers, obscuring their intrinsic reactivities and limiting direct applicability to astrochemical models.

A representative case is C3H+3 , which exists as linear propargyl and cyclic cyclopropenyl isomers with markedly different reactivities [1]. The cyclic isomer is largely inert under typical conditions, whereas the linear form efficiently drives ion–molecule chemistry leading to larger hydrocarbons [1]. These differences underscore the need for isomer-specific information in reliable kinetic models.

To address this challenge, we are building on our expertise in isomer-selected ion–molecule kinetics using drift-tube ion mobility spectrometry [3]. We are developing a new instrument in which ions are mass- and shape-selected prior to reactivity studies. Reactions will be performed in a Thermo Fisher Scientific linear trap quadrupole (LTQ) operated with a homemade power supply and control software. In a later stage, we plan to replace the drift tube with a Structures for Lossless Ion Manipulations (SLIM) device to achieve state-of-the-art ion mobility resolution [4, 5].

[1] Loison, Jean-Christophe, et al. Astronomy and Astrophysics 709: A255 (2026)
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[3] Rossi, Corentin, et al.Chemistry-Methods 5.9: e202500013 (2025)
[4] Ibrahim, et al., Analyst 142, no. 7: 1010-1021 (2017)
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Progress on development of commercial table-top XUV beamlines and components

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Since 2009, UltraFast Innovations (UFI®) has provided a wide range of specialized and customized optics and components, as well as instrumentation for ultrafast optical science. Continuous development and extensive collaboration with Professor Krausz's research group (Nobel Prize in Physics, 2023) have allowed UFI to bring to market a series of complete solutions for pump-probe spectroscopy, XUV imaging, pulse compression, and the generation of coherent secondary radiation1,2. A prominent example of such a solution, encompassing most of the company's expertise, is an XUV beamline driven by a high-repetition-rate, industrial-grade laser. The beamline includes post-compression stages based on nonlinear spectral broadening and in-house-produced highdispersive mirrors (KILIMANJARO & SAVANNA), a beam stabilization system, a highharmonics generation chamber (NEPAL), a programmable IR-XUV delay and refocusing stage (K2), an XUV polarization converter (AURORA), and a VUV-XUV spectrometer (EVEREST). The performance of each module is optimized and tailored for specific applications in ultrafast optical science.
In this presentation, we will introduce a compact tabletop XUV beamline and discuss the parametric space of the KILIMANJARO, SAVANNA and NEPAL instruments.

[1] "XUV-beamline for photoelectron imaging spectroscopy with shaped pulses", M. Behrens, L. Englert, T. Bayer, and M. Wollenhaupt, Review of Scientific Instruments 95, 093101 (2024)
[2] Daniel Walke, Azize Koç, Florian Gores, Minjie Zhan, Nicolas Forget, Raman Maksimenka, and Iain Wilkinson, "High-average-power, few-cycle, 2.1 μm OPCPA laser driver for soft-X-ray high-harmonic generation," Opt. Express 33, 10006-10019 (2025)

Photo decomposition of dichlorine peroxide in the stratosphere

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As is well known, halogen compounds play a disastrous role in stratospheric chemistry where they participate in several catalytic ozone-depletion cycles. Dichlorine peroxide is formed in the stratosphere by recombination of two chlorine oxide radicals. It then absorbs solar UV radiation and decays subsequently, producing harmful radicals that destroy ozone. Surprisingly, it is not clear which excited electronic states of dichlorine peroxide are involved and what the quantum yields of the possible photo-decomposition products are. These questions are addressed in our poster. Photo absorption and nonadiabatic decay dynamics was investigated with help of the quantum-classical Newton-X code, coupled to the Gaussian G16 quantum chemistry package. The time-dependent density-functional (TDDFT) approach was used with the functional M05-2X and the aug-cc-pVTZ basis set. ClOOCl absorbs strongly near 250 nm, however only radiation with wavelengths larger than 300 nm are relevant for atmospheric chemistry, as the lower wavelength are absorbed by ozone. The quantum yields of the three product channels are given in Table 1.

Table 1: product channels and yields

initial state	ClO + ClO	2Cl + O_2	Cl + ClOO
S_1 ($1\,^1B$)	2%	26%	68%
S_2 ($1\,^1A$)	2%	11%	87%
S_3 ($2\,^1A$)	2%	8%	90%

However, ClOO is unstable and will decompose as ClOO → Cl + O_2. Hence the quantum yields are: 2ClO: 2% and 2Cl + O_2: 98%. All species are in their electronic ground states. The photolysis rate constant is obtained as, with *F* the actinic flux, *σ* the UV absorption cross section and neglecting the minor decay channel,

$$J_{calc} = \int F(\lambda)\sigma(\lambda)d\lambda = 9.87 \times 10^{-4}\,\mathrm{s}^{-1}$$

in excellent agreement with the experimental value, JPL evaluation 15 (2006)

$$J_{exp} = 9.17 \times 10^{-4}\,\mathrm{s}^{-1}$$

The detailed decay mechanism was investigated and will be presented at the meeting.

Attosecond time delays in the Ar dimer

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The time-resolved investigation of ultrafast processes such as electron dynamics in the valence shell of atoms or molecules [1-3] requires a time resolution ranging down to the attosecond domain. In this work, we are investigating the attosecond time delays in the argon dimer [4]. In the dimer, two Ar atoms are weakly bound together and since they are indistinguishable, the electron emitted in the photoionization from either atom shows an interference pattern [5]. This two-center interference affects the photoionization time delays which we are measuring relative to the monomer.

For the experiment, we first temporally compress an infrared (IR) Yb-based laser to around 20 fs and drive the high-order harmonic generation (HHG) process with these pulses, which then generates extreme ultraviolet (XUV) light. We then use together with the collinearly delayed IR photons to perform measurements using an XUV pump IR probe scheme in the attosecond coincidence spectrometer in Freiburg [6]. The Ar as the target is prepared in a supersonic expansion through a nozzle, where the dimer is formed by the cooling during the expansion. Utilizing the reconstruction of attosecond beating by interference of two-photon transitions (RABBIT) technique [7], we can extract phases and therefore time delays from these measurements.

The experimentally extracted phases and time delays of the Ar dimer with respect to the Ar monomer are compared to the theoretically calculated time delays. The calculations were performed by the multichannel single center method [8], as described in details in Ref.[9]. The experimental data and the theoretical calculations are in reasonable agreement.

[1] S. Kheifets, J. Phys. B: At. Mol. Opt. Phys 58, 072001 (2025)
[2] D. Ertel et al., Sci. Adv. 9, eadh7747 (2023)
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[5] H. D. Cohen, Phys. Rev. 150, 30 (1966)
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[7] P. M. Paul et al., Science 292, 1689 (2001)
[8] N. M. Novikovskiy et al., J. Phys. B 55, 175001 (2022)
[9] J. Rist et al., Nat. Commun. 12, 6657 (2021)

Surface collisions and thermalisation of a laser–coolable molecule aluminium monofluoride

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Until very recently, direct laser cooling of molecules has been restricted to reactive species with 2Σ electronic ground states. These molecules are challenging to produce and have only been laser–cooled in their first rotationally excited level. So far, molecular magnetooptical traps (MOT) have been loaded from pulsed, cryogenically cooled molecular beam sources, which are rather large, complex and difficult to bring outside of a research lab.
At the Fritz Haber Institute, we have now realised the first MOT of a spin-singlet molecule: aluminum monofluoride (AlF)[1]. AlF has a high chemical stability compared to 2Σ molecules, and can be made cheaply and efficiently at moderate temperatures (~900 K) in an oven. Remarkably, we even observe that AlF can survive collisions with, and therefore thermalise to, room temperature vacuum walls of our experiments.
Here, we study the outcomes of single AlF–surface collisions via Doppler–sensitive laser–induced fluorescence, and measure the angular, velocity and rotational level distributions of the outgoing molecules. We observe that AlF generally undergoes trapping–desorption at surfaces, with outgoing molecules having no memory of their incoming velocity, and with complete rovibrational and translational thermalisation to the surface. Our results open a pathway to molecular MOTs loaded from compact and inexpensive beam sources and suggest that the technology employed in atomic vapour cells may be applicable to a laser–coolable molecule.

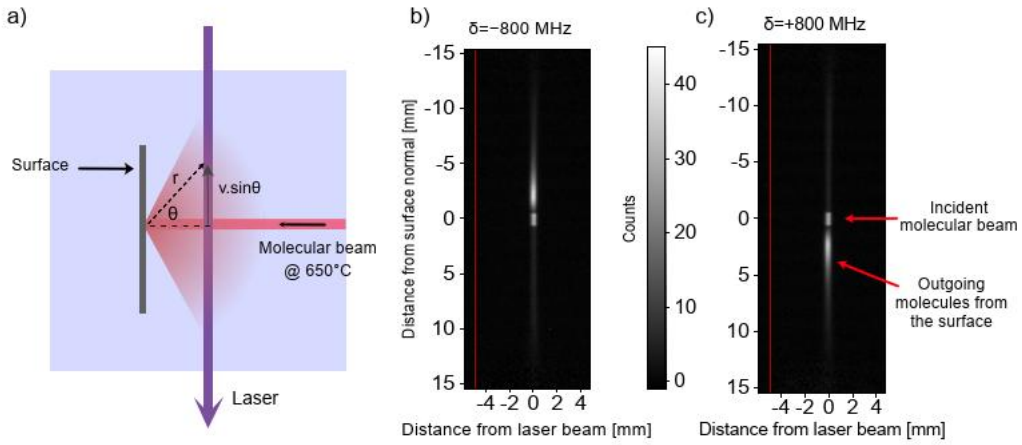

Figure 1: a) A schematic view of the experiment. The laser frequency can be scanned

[1] J.E. Padilla-Castillo et al., Phys. Rev. Lett. 135, 243401 (2025)

POSTERSESSION 2

Thursday, September 10, 2026

Poster Session II

Towards rovibrationally resolved photochemistry in H_2O-CO_2

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Water and CO_2 are the most important greenhouse gases in our atmosphere. The solvation of CO_2 is a decisive process in the chemistry of clouds and oceans. A precise characterization of the interaction of these two molecules is thus of prime importance. In the present work, we recorded a rotationally resolved spectrum of the triple excitation of the OH stretch in the H_2O-CO_2 molecular complex. This represents a further step in our longstanding effort to better characterize the dynamics of CO_2-H_2O interactions, notably through a systematic increase in vibrational excitation [1–4]. Increasing excitation will ultimately drive the isomerization of the complex into carbonic acid H_2CO_3. The complexes were formed from an 8 cm-long pulsed slit supersonic jet and probed by the CRDS technique in the spectral range of the second OH overtone of H_2O, using the FANTASIO setup [5,6]. A home-built external cavity diode laser (ECDL), stabilized to the frequency comb, was used as the light source. The recorded spectrum was vibrationally assigned to the $(v_1,v_2,v_3) \leftarrow (v_1',v_2',v_3') = (2,0,1) \leftarrow (0,0,0)$ and (2,0,1) + intermolecular mode ← (0,0,0) where v_1,v_2,v_3 are the vibrational quantum numbers of the isolated H_2O molecule are used to assign the involved vibrational states. In this talk, I will present the experimental spectrum and the improvements to the experimental setup that enabled the recording of this spectral signature. I am going to present our progress in the analysis of this spectrum using group theory and the effective Hamiltonian. Finally, perspectives on going across the isomerization barrier will be presented.

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[2] A.S. Bogomolov, A. Roucou, R. Bejjani, M. Herman, N. Moazzen-Ahmadi, and C. Lauzin, Chem. Phys. Lett. **774**, 138606 (2021).
[3] T. Gartner, C. Lauzin, A.R.W. McKellar, and N. Moazzen-Ahmadi, J. Phys. Chem. A 127, 3668 (2023).
[4] A.S. Bogomolov, S. Collignon, R. Glorieux, N. Moazzen-Ahmadi, M. Herman, C. Lauzin, Rotationally resolved triple vibrational excitation in D_2O-CO_2 van der Waals complex, in preparation (2026).
[5] M. Herman, K. Didriche, D. Hurtmans, B. Kizil, P. Macko, A. Rizopoulos, and P.V. Poucke, Mol. Phys. **105**, 815 (2007).
[6] A.S. Bogomolov, R. Glorieux, M. Herman, T. Corbo, S. Collignon, B.M. Hays, D. Lederer,
N. Moazzen-Ahmadi, A. Libert, B. Tomasetti, J. Fréreux, and C. Lauzin, Mol.Phys. **123**, e2413417 (2025).

Enantio-Sensitive Chern Numbers and Geometric Rotor Pumping in Chiral Molecules

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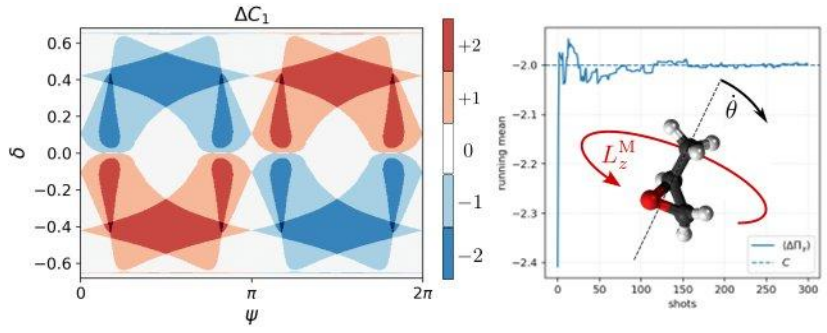
Detecting molecular handedness remains a central challenge in chiral spectroscopy. Synthetic chiral light, whose electric-field vector traces a chiral Lissajous figure in time, can induce strong enantio-sensitive electronic response already within the electric-dipole approximation [1]. Recent work has shown that such driving also imprints Berry curvature and geometric structure onto molecular dynamics [2, 3]. Here we show that this geometric structure can become topological, opening a route to robust and quantized enantio-sensitive observables.

Using a resonantly driven three-level model of a chiral molecule, we show that the laserdressed electronic states acquire Berry curvature on the molecular orientation sphere and integer Chern numbers. As shown in the figure, the phase diagram is controlled by the detuning δ and the laser phase ψ, which sets the handedness of the synthetic chiral field. It contains extended regions where opposite enantiomers carry different Chern numbers; these integer labels can change only when a dressed-state gap closes.



Left: enantio-sensitive Chern-number difference $\Delta C_1 = C_1^L - C_1^R$ for dressed state 1. Right: optical-centrifuge protocol and running ensemble mean of the angular momentum converging to the electronic Chern number.

Unlike earlier work where such topology arose in rotational dynamics [4], the topology here emerges directly in the electronic dressed states and feeds back onto molecular rotation through adiabatic geometric forces. In the proposed readout, a meridional sweep generates an angular momentum transfer which, after ensemble averaging over the remaining free angle, approaches the electronic Chern number. Thus the enantio-sensitive signal is not merely an enhanced chiral asymmetry, but is locked to an integer topological invariant, connecting chiral electron dynamics to a quantized rotational response.

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[3] A. Roos *et al.*, Phys. Rev. A **113**, 013111 (2026).
[4] K. Schwennicke and J. Yuen-Zhou, J. Phys. Chem. Lett. **13**, 2434–2441 (2022).

A Twist in the Fluorescence of Cold Molecular Ions in the Gas Phase

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The engineering of novel fluorescent proteins and markers requires fundamental understanding of the factors governing chromophore photophysics. Using our custom-built instrument, LUNA2 [1], we measure fluorescence from cold molecular ions in the gas phase. These measurements provide detailed information on intrinsic potential energy surfaces and Franck- Condon active modes and allow for direct benchmarking of computational models.

However, not all chromophores fluoresce outside their native environment. A common twistable motif, found in the green fluorescent protein (GFP) chromophore anion [2,3], and stains such as thioflavin T [4] and thiazole orange, facilitates excited-state deactivation via torsional motion. The isolated GFP chromophore anion is non-fluorescent at room temperature, but fluorescence is restored *in vacuo* upon cooling as reduced thermal motion mimics the steric hinderance of the protein barrel [2]. The chromophore is therefore intrinsically fluorescent. But not all twistable chromophores have intrinsically stable fluorescent states. In the case of thioflavin T, fluorescence is weak in the gas phase as well as solution phase. Spectra remain broad and unresolved with huge Stokes shifts whether at low or high temperature hinting to soft barrierless twisting on the excited-state potential energy surface [4].

Low-temperature measurements thus enable us to directly probe intrinsic excited-state twisting and chromophore photophysics, and in a bottom-up approach, the impact of the environment and small structural changes.

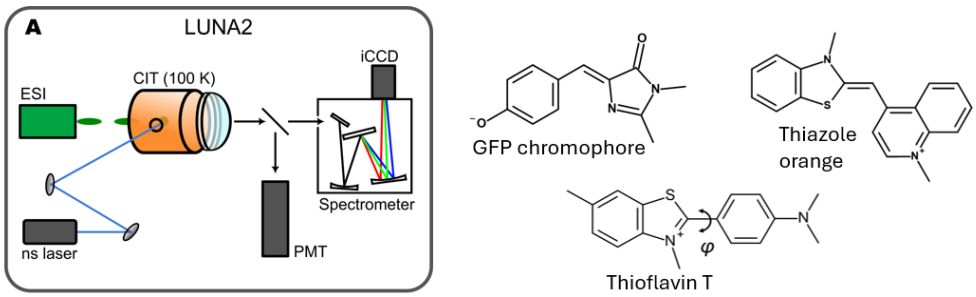

Figure 1: Schematic of the LUNA2 instrument together with three molecular ions that undergo twist motion upon photoexcitation.

[1] C Kjær, J Langeland, TT Lindkvist, ER Sørensen, MH Stockett, HG Kjaergaard, S Brøndsted Nielsen. *Rev. Sci. Instrum.* **2021**, *92*, 033105.
[2] TT Lindkvist, I Djavani-Tabrizi, LH Andersen, S Brøndsted Nielsen. *Phys. Rev. Lett.* **2025**, *134*, 093001.
[3] TT Lindkvist, AP Rasmussen, N Klinkby, LH Andersen, and S Brøndsted Nielsen. *J. Phys. Chem. Lett.* **2025** *16*, 13277-13283.
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Single-stage multipass spectral broadening and compression of 90 fs, 1 mJ laser down to 10 fs

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Spectral broadening and compression of ultrashort pulses is a widely employed technique. The applications range from ultrafast pump-probe spectroscopy to the development of X-ray and XUV sources. A fundamentally new approach for spectral broadening and pulse compression using a quasi-waveguide system, namely the Herriott-type multi-pass cell (MPC), was introduced recently [1]. So far, only a few demonstrations reached the sub-10 fs regime, mainly due to two challenges: The limited bandwidth of optics and the high demands on dispersion management inside the MPC. In this work, we report on our system breaking the 10 fs limit by employing custom-made dispersive mirrors covering the bandwidth from 850 to 1300 nm and Argon gas as a nonlinear medium.

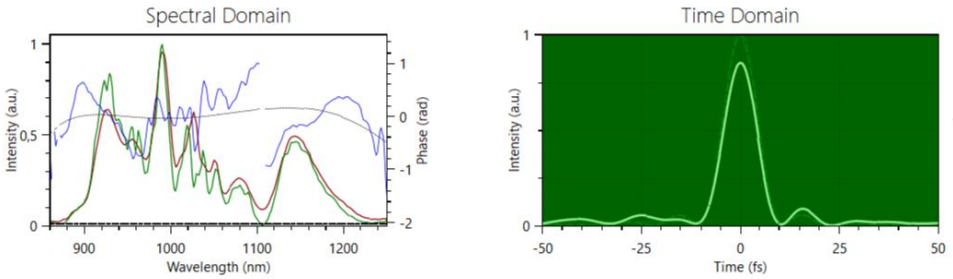

Figure 1: Compressed output spectrum and pulse duration measured with D-scan.

The industrial-grade driving laser (PHAROS-UP by Light Conversion) delivered 90 fs and 1 mJ pulses at 10 kHz, resulting in 10 W average- and 10.4 GW peak power. After coupling inside the MPC operating under absolute 600 mbars of Argon, the output pulses were broadened to cover the 850 to 1300 nm range. The compression was performed with dispersive mirrors compensating GDD and TOD. The compression was verified with a commercial D-scan device from Sphere Photonics (Fig.1). The output pulse duration was measured to be 10 fs, with the main peak containing 85% energy as compared to the Fourier-transform limit. This corresponds to a peak power boost of 5.5 x and peak power of 57 GW. The transmission of the cell and the dispersive mirror compressor remained over 71%. The long-term operation over 100 h is to be performed. The whole multipass compression unit (MIKS1 L) has a footprint of 1.5 x 0.24 m2. We plan to perform further energy scaling of this approach ultimately reaching the compression of 2 mJ, 90 fs pulses.

[1] Jan Schulte et al., Optics Letters 41, no. 19, 4511–14 (2016).

Ionization-induced dynamics in formic acid dimer

Saroj Barik[1], Ester Livshits[1,2], Roi Baer[1,2], and Daniel Strasser[1]
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Ionization of a dimer, composed of two identical molecular monomers, can initiate symmetry breaking dynamics.[1] I will present ultrafast EUV pump – near-IR probe studies of ionization induced dynamics in the formic acid (FA) dimer.[2,3] The experimental data are compared with ab initio molecular dynamics simulation providing detailed understanding of first 1000 fs after the ionization event. Figure 1 inset shows the ground-state geometry of the FA dimer, which similar to the 7 Azaindole dimer and DNA base pairs is held by two hydrogen bonds, making it an interesting benchmark model for the debated intermolecular proton-transfer mechanism.[4,5,6] Ionization of a single electron is shown to initiate symmetry-breaking proton-transfer dynamics resulting in a protonated FA ion (FAH^+).[2] Figure 1 shows the observed ~150 fs lifetime of the transiently enhanced FAH^+ yields that agrees with the simulated ultrafast proton-transfer, in concert with ring opening that forms a $(FA\text{-}H)(FA+H)^+$ complex. Double ionization on the other hand, exhibits rapid Coulomb explosion of the dimer that is followed by dissociation of one of the FA monomers and formation of H_2O^+ or OH products. Theoretical simulations that reproduce the measured three-body momentum correlations indicate that a rapid Coulomb explosion is followed by a roaming OH dynamics resulting in H_2O^+ + CO (or CHO^+ + OH). This, rather than proton migration or dissociation that could be naively inferred from the final products. Furthermore, I will show the experimental evidence for ultraslow dynamics of the $(FA\text{-}H)(FA+H)^+$ complex that yield FAH^+ on the μs time scale.

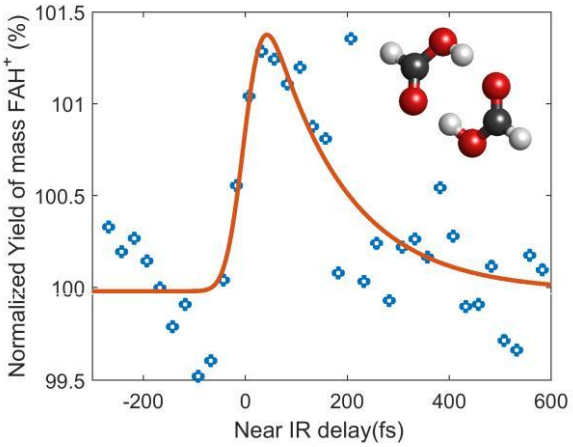

Figure 1: Transient enhancement of protonated formic acid cation signal as a function of the near-IR probe time-delay after ionization by an ultrafast EUV pump pulse

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[2] S. Barik et al., J. Phys. Chem. A. (2025)
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Collision-Energy Dependent Uptake of Hydroxyl Radicals at Atmospherically Relevant Surfaces

P. D. Lane[1], D. R. Moon[1], M. L. Costen[1], and K. G. McKendrick[1]

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We extend a recently developed[1-3] approach, planar laser-induced fluorescence (p-LIF), to study collisions of hydroxyl radicals with liquid surfaces. The technique detects ingoing OH radicals produced in a molecular beam as well as probing those which have scattered inelastically from the surface of a liquid. Recent improvements to the system, including modifications to the molecular-beam discharge source used to produce the OH radicals, has allowed scattering to be performed with a broader series of carrier gases (He, Ne, Ar and Kr), extending the incident-energy range to lower, more atmospherically relevant values than in previous work.

By performing comparative measurements with an inert sample of perfluoropolyether we were able to quantify the OH survival probability and hence its complement, the reactive uptake coefficient, as a function of collision energy. This was carried out for a wider range of atmospherically relevant systems, extending beyond saturated and unsaturated hydrocarbons studied previously to fatty acids and other liquids with more-complex oxygen-containing functionalities.

We find that for all liquids studied the OH radicals are more likely to survive collisions with the surface at *higher* collision energies; the mechanistic implications of this seemingly universal higher reactivity of OH radicals with lower collision energies will be discussed.

[1] R. H. Bianchini et al. J. Chem. Phys. **151**, 054201 (2019).

[2] M. J. Roman et al. J. Chem. Phys. **158**, 244704 (2023).

[3] M. J. Roman et al. J. Phys. Chem. A. **128**, 5166 (2024).

Strong-Field Response of Pentacene and Tetracene

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Organic molecular crystals (OMCs), such as pentacene, tetracene and their derivatives, exhibit unique electronic properties, attracting significant attention as an important material class for novel applications in optoelectronics and singlet-fission-based technologies. However, strong-field effects in OMCs have remained largely unexplored to date.

Despite their weak van der Waals bonding, recent experiments have demonstrated that pentacene [1] and tetracene crystals can withstand intense 4μm laser fields (up to 1V/˚A) and generate high harmonics (HH) up to order 17. Rotation of the driver polarization has further revealed a strong polarization dependence of the harmonic yield. To assess the importance of intramolecular effects of the individual molecules in the crystal for the HHG process, we calculated polarization-dependent HH spectra using two non-interacting pentacene molecules oriented as in the unit cell of the crystal, using high-level MR-CIS (multireference configuration interaction with all single excitations) electronic structure calculations of monomeric pentacene (Fig. 1a). While the measured polarization-dependent harmonic yield partially aligns with the characteristic molecular directions, the response of the non-interacting molecules is not sufficient to describe the full experimental HH spectra, demonstrating the importance of the weak intermolecular couplings. In addition, we present transient absorption spectra that reveal the modifications of the electronic structure and dynamics induced by intense MIR pulses. Fields in the range of 1V/˚A modify the electronic properties significantly, causing AC-Stark shifts of the bound states and new, light-dressed (Floquet) states to emerge (Fig. 1b).

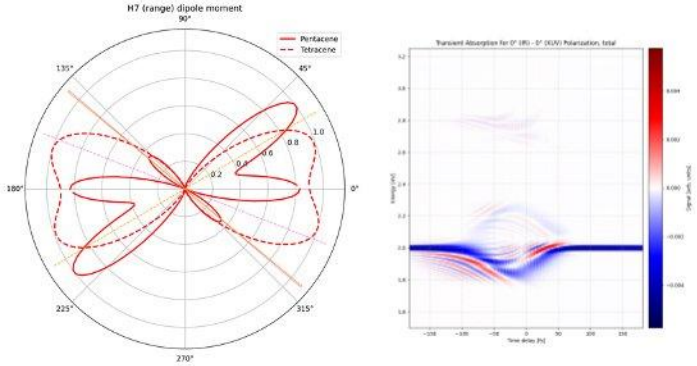

Figure 1: MR-CIS calculation of polarization-dependent yield for harmonic 7 in tetracene and pentacene (left) and transient absorption spectrum of pentacene (right).

Our results highlight the exciting opportunities for studying and tailoring the electronic properties of organic molecular materials by exploiting the ideas of strong-field engineering.

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Ultrafast Excited State Dynamics of Indolizine and Imidazopyridine

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The excited state photodynamics of aromatic heterocyclic molecules can be highly sensitive to the positioning of nitrogen atom centres within the ring system, regulating electronic coupling and non-radiative decay pathways. To further explore such processes, femtosecond time-resolved transient absorption spectroscopy was performed on indolizine, imidazo[1,2- a]pyridine and imidazo[1,5-a]pyridine in methanol and hexane solvents using a 267 nm pump and a broadband white light continuum probe (340-750 nm). Global fitting analysis was conducted to extract numerical time-constants and a series of decay associated spectra.

Thesedetail the various intramolecular pathways that mediate energy redistribution following photoexcitation. These data, along with supporting quantum chemistry calculations, indicate distinct photodynamics can depend on differences in nitrogen-positioning, influencing excess energy redistribution on the femtosecond and picosecond timescales. Developing a better understanding of such phenomena is an important step towards the future rational design of photoactive molecules for a range of applications including photodynamic therapy and optoelectronics.

Precision measurements in a cryogenic ion trap

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We report on several recent experimental results, pushing cryogenic multipole radiofrequency ion traps to new limits.

The dicarbon molecule C_2 and its anion C_2^- have been widely studied, due to their possible role in the interstellar medium and the anion's status as candidate for laser cooling. We have precisely measured the transition frequencies of the lowest three vibrational states, allowing for the precise determination of the C_2^- vibrational spacing [1-3].Additionally, we performed near-threshold photodetachment spectroscopy on two transi-tions, showing an s-wave and p-wave behavior, at different temperatures. We precisely determined the electron affinity of C_2, significantly improving previous measurements [4].

Three-body reactions are important chemical pathways in many areas of physics and chemistry. The number of reaction partners hinders a full quantum mechanical theoretical treatment in all but the simplest systems, which can be difficult to study experimentally. We have measured the termolecular reaction $Ar^+ + Ar + Ar \rightarrow Ar_2^+ + Ar$ in the range 80 - 160K and compare results to full quantum calculations [5].

In order to understand the chemical evolution of the interstellar medium, the chemical processes it undergoes must be verified experimentally. One of these is the reaction of anions with atomic hydrogen. We have measured the temperature-dependent reaction rate of several carbon anionic species with atomic hydrogen [6,7]. Another important process is mutual neutralization of oppositely charged ions, a non-trivial experimental task. We have successfully co-trapped positive and negative ions at 65K in an all-rf multipole trap, and present proof-of-concept measurements of the mutual neutralization rates.

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Collisional Shielding of Ultracold Polar Molecules: A Gateway to Quantum Degeneracy and Many-Body Quantum Physics

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Collisional shielding techniques based on static electric fields [1, 2, 3] and microwave fields [4, 5, 6] have become essential tools for the production of dense ultracold gases of polar molecules. Recently, the development of double-microwave shielding [7, 8] has played a pivotal role in the first realization of a molecular Bose–Einstein condensate (BEC). I will review the development of collisional shielding techniques for ultracold polar molecules, highlighting contributions from our work. We have demonstrated that microwave shielding, in contrast to static-field shielding, is universal [6]. In other words, the 2-body collision properties of different microwave-shielded molecules are very similar when expressed in suitable reduced units of length and energy. This applies to rate coefficients for inelastic scattering and loss, to scattering lengths, and to the properties of 2-molecule bound states. These insights provided practical guidance for selecting working-shielding parameters in experiments that led to the realization of a quantum-degenerate gas of NaRb molecules [9]. More recently, we have been among the first groups to propose tuning interactions between static-field-shielded molecules through the application of an additional circularly polarized microwave field [10, 11]. These pave the way for applications of ultracold polar molecules in quantum science [12].

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Spacecraft degradation in Low Earth Orbit : State Specific Reactivity of O^+ with Benzene and Production of Specific Population of Excited States from Dissociative Electron Ionization of CO_2 and H_2O Precursor Gases

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Spacecraft operating in low Earth orbit (LEO) are exposed to a highly reactive plasma originating from the ionosphere, which significantly affects the properties of spacecraft materials. O^+ ions represent the main ionic component, and due to their significantly higher reaction rate constants, ion–neutral reactions play a major role in material degradation[1].

O^+ ions can exist in ground state (^4S) and in long-lived metastable excited states (^2D and ^2P), which can persist long enough under LEO conditions to undergo chemical reactions[2]. These excited states are known to significantly influence reaction dynamics and product distributions in planetary ionospheres. Therefore, accounting for electronic-state populations is essential for accurately describing ion–molecule reactivity in space environments.

In this work, we investigate with the CERISES[3] instrument coupled to the DESIRS[4] beamline at SOLEIL synchrotron the state-specific reactivity of O^+ ions with benzene (C_6H_6), used as a molecular proxy for graphite materials in spacecraft. Collisions occur at energies around 5 eV, representative of the relative velocity between spacecraft and ions, enabling efficient processes such as charge transfer and bond dissociation. We report absolute cross sections as a function of collision energy and examine differences between ground and excited states. Additionally, we explore O^+ production via electron ionization of CO_2 and H_2O, enabling characterization of state distributions and validation of ion sources for state-resolved reaction studies. This work provides molecular-level insight into degradation mechanisms of spacecraft materials in the reactive and highly variable LEO environment.

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Simulating quantum dynamics of molecules at metal surfaces: A novelapproach combining the Hierarchical Equations of Motion (HEOM) and the Multi-Configurational Time-Dependent Hartree method (MCTDH)

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Simulating the quantum dynamics of molecules coupled to electrodes or metal surfaces is crucial for understanding a variety of physical, chemical, and biological processes. To do this, an open quantum system approach is typically used, whereby the electrodes or metal surfaces are treated as the environment of the molecule of interest. However, achieving numerically exact simulations of such open quantum systems across experimentally relevant parameter scales continues to be demanding, especially when the molecule itself poses a strongly coupled many-body problem.

Among the available approaches to open quantum systems, the Hierarchical Equations of Motion (HEOM) approach has emerged as a powerful and systematically improvable framework. Its high computational cost typically restricts it to small model systems, though. Over the past decade, several tensor-train- and tensor-network-based approaches have been suggested and realized to make the HEOM applicable to ever larger model systems [1,2]. In this work, we build upon the existing twin-space formulation of the HEOM [2] and introduce a novel approach employing the Multi-Configurational Time-Dependent Hartree method (MCTDH) [3,4] and its multi-layer extension [5] for the time propagation of the HEOM. We demonstrate the applicability of the resulting HEOM+MCTDH method by presenting electron transport calculations for a molecular nanojunction model with strong molecule-electrode coupling [6,7], for which fully quantum simulations have not been available previously.

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Disentangling Fragmentation and Conformational Structure in Heterogeneous Molecular Cluster Beams via Mass-Correlated Rotational Spectroscopy

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Characterizing complex chemical mixtures and weakly bound clusters within a molecular beam is often hindered by ubiquitous fragmentation, which obscures the structural origin of observed mass signals. Conventional mass spectrometry typically relies on prior assumptions to link fragment peaks to their neutral precursors. Here, we demonstrate the capability of masscorrelated Correlated Rotational Alignment Spectroscopy (CRASY) to unambiguously disentangle complex fragmentation pathways and resolve cluster geometries without interpretational ambiguity.

Using a high-resolution time-domain CRASY setup, a coherent rotational wave packet was excited in a heterogeneous carbon disulfide (CS_2) molecular beam using a 1-ps infrared pulse and subsequently probed via photoionization with a delayed 50-fs ultraviolet pulse. Fourier transformation of the delay-dependent signal modulations yielded high-resolution masscorrelated rotational Raman spectra spanning 22 distinct mass channels with an effective resolution of 17–18 MHz.

Through algorithmic Pearson correlation analysis of the complex-valued spectra, we successfully identified 12 distinct molecular and cluster species and assigned 33 distinct ionization and fragmentation pathways. Crucially, the extreme structural selectivity of this method allowed us to unambiguously assign the rotational lines of the weakly bound CS_2 dimer to its cross-shaped (D_{2d}) conformer as the dominant geometry, while fitting rotational constants for 9 distinct CS_2 isotopologues at natural abundances down to 10^{-5} without synthetic isotope labelling. Furthermore, we successfully utilized a 180∘ phase inversion in the complex spectra to systematically identify and filter out detector saturation artifacts in congested mass regions. These results demonstrate CRASY's unique capacity to directly correlate mass, geometry, and fragment kinematics, establishing a powerful experimental framework for probing the chemical dynamics of heterogeneous systems free from sample purity limitations.

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Attosecond UV/XUV pump-probe beamline for time-resolved spectroscopyin gases and liquids

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Transient absorption spectroscopy is a powerful technique for probing ultrafast electron dynamics in solids and gas-phase molecules and has only recently been extended to liquids with femtosecond resolution [1]. Extending attosecond transient absorption spectroscopy (ATAS) to solvated molecular systems requires light sources combining high stability, few-cycle pulse duration, high average power, and tunable ultrafast excitation in the UV range. Here, we present a newly developed ATAS beamline designed for pump-probe experiments on molecular systems in the gas and liquid phase. The setup is based on a CEP-stabilized Yb-doped laser system (Flint and Carbide, Light Conversion) delivering 2 mJ pulses with a duration of 330 fs at average powers up to 80 W. A two-stage hybrid nonlinear compression scheme [2] is employed to generate pulses as short as 5 fs, corresponding to approximately 1.5 optical cycles at 1030 nm, while maintaining a transmission efficiency of ~50% together with excellent longterm stability.
The beamline exhibits a measured temporal stability of ~150 as RMS over a 7 m interferometer arm length, providing the stability required for attosecond experiments. This performance is combined with a tunable few-femtosecond UV source based on resonant dispersive wave (RDW) emission in a gas-filled hollow-core fibre [3].

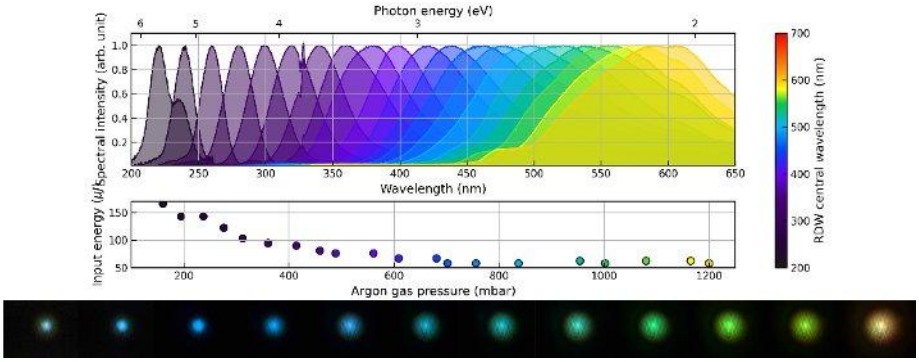

Figure 1: Top: RDW spectra for different phase-matching conditions. Bottom: filtered RDW beam profiles recorded on white paper.

The RDW stage consists of a gas-filled hollow-core fibre directly coupled to the vacuum chamber to preserve the pulse duration. Figure 1 shows representative spectra obtained at the fibre output, demonstrating continuous tunability over 4 eV across the 220-600 nm spectral range. Pulse energies in the microjoule range are routinely achieved, with a maximum measured energy of 5 µJ at 260 nm, on target.
The generated UV pulses are expected to support few-femtosecond pulse durations, enabling UV/XUV pump-probe measurements with high temporal resolution.

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The interaction of an organic chromophore with a rare-gas nanoparticle studied in the gas phase

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The dynamics of condensed-phase molecular systems are often highly complex due to the large number of coupled intra- and inter-molecular degrees of freedom. To develop a mechanistic understanding of the quantum dynamics governing molecular processes, complementary studies of simplified well-defined model systems are important. Rare-gas clusters provide a versatile platform for the controlled synthesis of such model systems, extending beyond isolated molecules to molecular complexes and solute–solvent complexes prepared in the gas phase. In our work, we developed two-dimensional electronic spectroscopy (2DES) to investigate the guest-host interactions and ultrafast dynamics of these systems[1-3]. Specifically, we will present the interaction of the organic chromophore 3,4,9,10-perylenetetracarboxylic dianhydride (PCTDA) with different cluster environments and present a systematic study of vibrational couplings. We find that the surface morphology of the clusters induces a Duschinsky coupling in the molecule which can be revealed with 2DES. Further, we compare systematically the vibrational relaxation of the molecule in different environments ranging from isolated gas phase to rare-gas clusters and bulk liquid solvents.

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Morphological transitions in heterogeneous flat jets

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Liquid flat jets formed by the collision of two microjets provide a continuously renewed optically accessible thin-sheet geometry for studies of interfacial dynamics in liquids [1-3]. While homogeneous flat jets have been widely used as model systems and liquid targets[4], less is known about modified sheet morphology, stability, and breakup of miscible liquids with different compositions. However the preparation of interfaces between two different solutions is a key element for studies of chemical and physical dynamics at liquid-liquid interfaces [5].

Here, we investigate heterogeneous flat jets formed from water/alcohol–water impinging microjets. These systems provide a controlled platform in which liquid composition changes the balance between inertia, capillarity, viscosity, diffusion, and interfacial transport. Using high-speed imaging combined with image-based morphological analysis, we identify reproducible transitions between smooth liquid sheets, surface-structured sheets, rimdominated states, and droplet-breakup regimes.

A central observation is the emergence of a textured region within the liquid sheet. This region appears as an intermediate morphological state between a smooth continuous sheet and downstream fragmentation, rather than as a simple final breakup product. Comparison between ethanol–water and isopropanol–water systems shows that similar global flow conditions can lead to different onset and development of these structures, indicating that the morphology of miscible heterogeneous flat jets cannot be described by Weber number alone.

These results suggest that composition-dependent interfacial and transport processes play an important role in the stability of multicomponent free liquid sheets. The study establishes miscible heterogeneous flat jets as a promising platform for probing coupled flow, mixing, and interfacial dynamics in thin liquid environments.

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Entanglement in Photoionization Reveals the Effect of Ionic Coupling in Attosecond Time Delays

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Attosecond photoelectron interferometry provides access to the photoionization dynamics of a quantum system by measuring the photoelectron spectra generated in a two-color field composed of extreme ultraviolet (XUV) harmonics and a synchronized infrared (IR) field. A widely used implementation of this approach is the reconstruction of attosecond beating by interference of two-photon transitions (RABBIT) technique [1], which has provided valuable insights into electron correlation effects and coupled electronic-nuclear dynamics [2,3]. Additionally, by combining two-color interferometric techniques with photoelectron-photoion coincidence spectroscopy, angle-resolved studies in the recoil frame can reveal information about the anisotropy of the molecular potential [4]. While such measurements typically access only the energy or momentum of the emitted photoelectron, they often leave the internal dynamics of the parent ion unexplored. In atoms, this is usually justified, as the ion remains in a single well-defined state or in states that are not efficiently coupled by the IR field, due to their large energy separation.

In molecules, however, the IR field can induce polarization of the ion. In CO_2, this corresponds to the dipole coupling between B $^2\Sigma^+_u$ and C $^2\Sigma^+_g$ cationic states. This extends the conventional two-path interference picture of the RABBIT technique, with an additional pathway arising [5, 6]. The interference between these three pathways introduces a measurable additional time delay in photoelectron emission associated with the B $^2\Sigma^+_u$ cationic state. The observed effect, consistent with theoretical predictions using a stationary multiphoton molecular R-matrix approach [5], is not mediated by the Coulomb interaction between the ion and the photoelectron but depends on the degree of entanglement of the reduced density matrix of the ionic subsystem conditioned on the energy absorbed from the harmonic 2q+1 [7]. Furthermore, looking into the dissociative channels and measuring in coincidence with O^+, the same ionic coupling leads to a pronounced phase jump, close to a π phase shift, in the photoelectron wavepacket [8].

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Cryo Activities of Transition Metal Clusters

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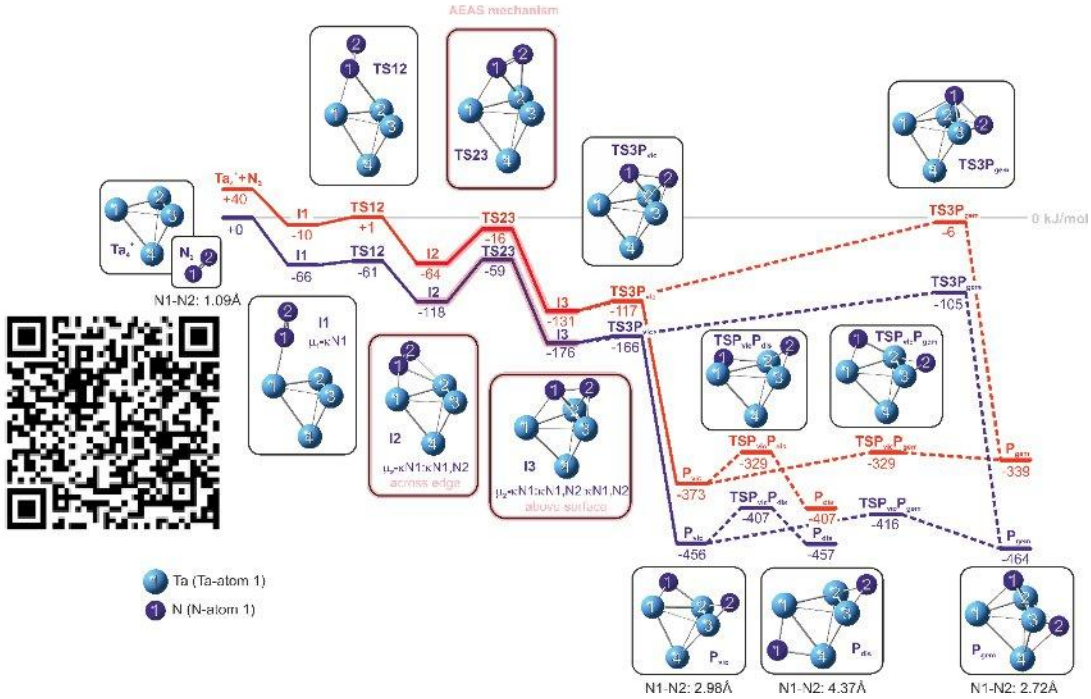
Cations and anions of size selected transition metal (TM) clusters attach N_2 molecules under single collision cryo conditions, and they may or may not subsequently activate the adsorbates. Cryo kinetics, infrared photon dissociation (IR-PD) spectra and DFT modelling reveal insights on the cluster morphologies and on likely or unlikely activation pathways. The analysis of spin states [1a,b] and molecular orbitals unveils the fluxional electronics of adsorbate cluster complexes. Our studies have so far covered clusters of Cobalt [2], Nickel [3,4,5], Rhodium [6,7], Iron [8,9], bimetallic Rhodium-Iron mixtures [10,11], Tantalum [12,13,14], and Ruthenium [15]. This presentation shall cover selected examples and outline routes to future work.



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[15] to be published

Quantum scattering calculations for the H_2CO–He collision probed by pressure broadening experiments at low temperature

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State-to-state collisional rate coefficients are often required for the proper interpretation of astronomical observations in non-local thermodynamic equilibrium conditions in interstellar space [1]. These can usually only be determined from molecular scattering calculations. In order to validate the quantum scattering methodology that is generally used for such calculations, we have experimentally measured low-temperature pressure-broadening cross-sections for the H2CO–He system. Since these data are determined as independent absolute quantities, a careful comparison provides an excellent basis for experimental validation of the quality of the potential energy surface (PES), which is the most common source of errors in quantum scattering calculations [2].

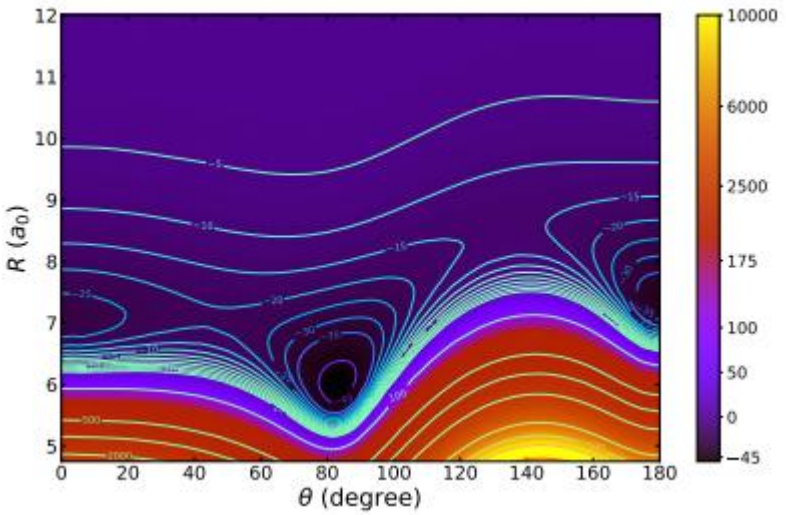

Figure 1: Contour plot of the H2CO–He potential energy surface as a function of R and θ coordinates at fixed azimuthal angle φ = 0◦.

The experiments employed the chirped-pulse in uniform supersonic flow method, generating H2CO in situ in cold He flows. High-level ab initio calculations were also performed to derive a new 3D rigid rotor PES for the H2CO–He system that used for quantum scattering calculations employing the close-coupling method to derive collisional rate coefficients and pressure-broadening cross-sections. The calculated values fall within the 95% confidence intervals of the experiments, demonstrating the high accuracy of the theoretical methodology, including the PES and state-to-state collisional data obtained.

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Accelerated Inter-Phase Energy Transfer in Alternating-Cation Layered Perovskites

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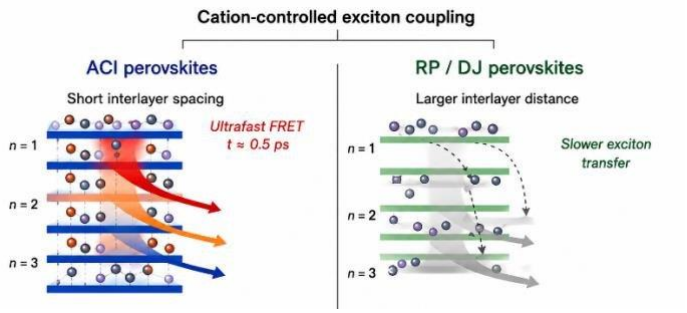
Efficient exciton transport across nanoscale heterogeneities is essential for optimizing the performance of low-dimensional semiconductor optoelectronics.[1] Layered metal halide perovskites provide a unique platform for engineering excitonic interactions through controlled structural design.[2] Here, we investigate exciton dynamics in mixed-phase two-dimensional perovskites with alternating-cation-in-interlayer (ACI) architecture and compare them with structurally related Ruddlesden-Popper (RP) and Dion-Jacobson (DJ) systems. Ultrafast transient absorption and time-resolved photoluminescence spectroscopy reveal highly efficient inter-phase exciton funneling from lower-n to higher-n quantum wells in ACI perovskites on sub-picosecond timescales. The observed transfer dynamics are consistent with Förster resonance energy transfer mediated by enhanced dipole-dipole coupling. We attribute the accelerated exciton migration to the reduced interlayer spacing and stronger electronic coupling induced by the alternating cation arrangement. In contrast, analogous RP and DJ perovskites exhibit significantly slower and less efficient inter-phase energy transfer under identical excitation conditions. These results highlight interlayer cation engineering as an effective strategy for controlling exciton coupling and directional energy flow in layered perovskite semiconductors, offering new design principles for high-performance excitonic and optoelectronic devices.



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Extending Chiral Analysis with Enantiomer-Specific State Transfer

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Enantiomer-specific state transfer (ESST) enables state-selective chiral analysis by exploiting coherent microwave control of rotational populations. In ESST, a sequence of rotational transitions is used to create enantiomer-dependent population transfer, enabling selective enrichment of one enantiomer in a chosen rotational state [1,2]. Recent developments in our group have demonstrated near-complete enantiomeric enrichment in individual rotational states through optimized coherent control schemes [3].

In this presentation, we show how ESST can be utilized to further extend chiral analysis. In particular, we introduce a strategy that combines ESST with circular dichroism (CD) spectroscopy, enabling chiral measurements in racemic molecular ensembles. We present experimental progress and promising initial data for this novel approach.

Beyond spectroscopy, ESST also provides a platform for the spatial separation of chiral molecules. We will discuss ongoing efforts toward enantiomer separation based on quantum-state-selective matter-wave diffraction, as well as state-selective ionization. Our work highlights the potential of enantiomeric excess control via ESST as a route toward both precision chiral spectroscopy and quantum-state-resolved enantiomer separation.

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Prospects for ultracold CsYb molecules: a theoretical study

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Ultracold polar molecules formed from an alkali-metal atom and a lanthanide atom offer a versatile platform for studying strongly interacting quantum systems, exotic phases of matter, and ultracold chemistry. CsYb is particularly attractive because it offers both electric and magnetic tunability, while the presence of multiple bosonic and fermionic Yb isotopes. Although ground-state CsYb has already been investigated[1], mixtures involving metastable Yb($6s6p\,^3P$) are expected to exhibit stronger magnetic Feshbach resonances, providing additional opportunities for efficient magnetoassociation. This motivates a detailed theoretical study of the excited electronic structure of CsYb, especially around the Cs($6s\,^2S$)+Yb($6s6p\,^3P$) dissociation limit.

Here we investigate the electronic structure of CsYb using quantum chemistry calculations based on large effective core and core polarization potentials, combined with an atomic spin-orbit coupling model. Compared with the previous *ab initio* study [2], our results include additional electronic states absent from earlier calculations, allowing for analysis of potentials above the Cs($6p\,^2P$)+Yb($6s^2\,^1S$) asymptote. Special attention is brought to the region between dissociation limits Cs($7s\,^2S_{1/2}$)+Yb($6s^2\,^1S_0$) and Cs($6s\,^2S_{1/2}$)+Yb($6s6p\,^3P_1$). The crossings arising in this region are modeled with local couplings and are shown to significantly affect weakly-bound rovibrational levels. Such effects may modify the character of magnetic Feshbach resonances and open pathways for electronic excitation transfer, providing useful guidance for future experimental and dynamical studies of CsYb.

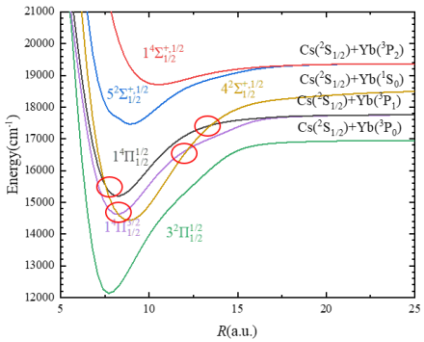

Figure 1: The PECs of CsYb around Cs($6s\,^2S$)+Yb($6s6p\,^3P$) with **Ω**=1/2.

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Homochiral Electronic Enantiomer Flip in 37 Attoseconds

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Photoexcitation of achiral molecules can prepare chiral electronic superposition states. They represent electronic enantiomers. Electronic chirality flips transform these enantiomers into their mirror images, i.e. into the opposite electronic enantiomers. Previous examples lead e.g. from the electronic R-enantiomer via an achiral intermediate to the opposite S-enantiomer, within few hundred attoseconds to few femtoseconds.[1-4] These flips can be monitored by means of time-resolved photoelectron circular dichroism (TR-PECD)[5] or by time-resolved electronic circular dichroism(TR-ECD).[6] We present a new type of photoinduced electronic enantiomer flip which takes only 37 attoseconds by a short-cut which avoids the "detour" via an achiral intermediate. As prototype, the process is demonstrated by quantum dynamics simulations for the model Mg-porphyrin. The previous[1-4] and new mechanisms are related to E. Ruch's 1968 distinction of two classes of chiral molecules with opposite enantiomers: "heterochiral enantiomers" are connected by paths via an achiral intermediate; "homochiral enantiomers" have connecting paths without achiral intermediate.[7]

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Electron Recollision-enhanced Coulomb Explosion of CH_2IBr

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We study electron recollision in the strong-field multiple ionization of the asymmetric polyatomic molecule CH2IBr using a reaction microscope. Correlated momentum conservation among three coincident fragments allows us to identify events in the CH+ 2 + I+ + Br+ channel. We show that electron recollision (occurs within an optical cycle) substantially enhances this multiple-ionization pathway. Three-body breakup by electron recoiled momentum is confirmed by the longitudinal momentum sum of the correlated fragments, measured along the time-of-flight direction, parallel to the laser polarization. It exhibits a sharp bimodal peak at zero, as required by momentum conservation. Recollision-driven non-sequential ionization is well established for atoms and simpler systems [1, 2]. Here we extend this picture to a complex polyatomic molecule. The high mass resolution of our measurement additionally resolves isotope-dependent structure in the parent-ion mass spectra. It cleanly separates the natural isotopologues 79Br+/ 81Br+ and 12C/13C. Our results show that electron-recollision-enhanced fragmentation of multiply charged molecular ions is a sensitive route to probe correlated electron dynamics in complex molecules. It also provides access to isotope-resolved structure, and the entire process could be studied in the near future using different colors of photons.

Figure 1. Strong-field multiple ionization and fragmentation of CH2IBr. (a) Overall time-offlight (ToF) mass spectrum (black) with fragment ions highlighted: CH+ 2 (12C, red), Br+ (79Br, green), I+ (127I, blue); the dashed box near 32 μs marks the parent-ion region. (b) Momentum sum of the three-body fragments, Pz(CH+ 2)+Pz(Br+)+Pz(I+). It peaks sharply at zero, demonstrating momentum conservation. Green dashed lines indicate a ±5 a.u. gate; the inset zooms to ±6 a.u. for the 79Br+ correlation. (c) Zoom of the parent-ion peaks. The isotopic structure of CH2IBr+ is resolved, clearly separating the 79Br+/ 81Br+ and 12C/13C contributions.

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Proton Transfer Dynamics in Photoactive Proton Crane Systems

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Photoactive molecular switches are most commonly based on bond isomerization or reversible bond breaking and formation. An alternative approach relies on proton transfer, in which tautomeric rearrangements combined with intramolecular motion induce reversible structural changes. Proton cranes belong to this class of systems and enable proton translocation across comparatively long molecular distances through coupled proton transfer and rotor rotation. In this work, we explore the switching dynamics of the 7-hydroxyquinoline-based proton crane 8-(benzo[d]thiazol-2-yl)quinolin-7-ol (HQBT) [1] using ultrafast time-resolved infrared (tr-IR) spectroscopy in combination with density functional theory calculations. Following photoexcitation, the enol tautomer representing the off-state undergoes an ultrafast excited-state intramolecular proton transfer, generating a transient intermediate. Rotation of the protonated rotor subsequently facilitates long-range proton migration within the molecule, while relaxation back to the electronic ground state produces keto-type structures associated with the switched on-state.

To further characterize the tautomeric equilibria and spectral signatures of the proton-crane states, complementary FTIR and UV–Vis spectroscopy were employed. In addition to HQBT, analogous derivatives containing oxygen and selenium heteroatoms were studied to assess how heteroatom substitution influences switching energetics and the stability of the keto tautomers. The combined experimental and computational results demonstrate that modification of the rotor unit offers an effective strategy for tuning proton-transfer dynamics and controlling the lifetime of the switched state, providing valuable guidelines for the development of proton-transfer-based molecular photoswitches.

This research is carried out and financed within the framework of the second Swiss Contribution SCIEX.

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Toward understanding of the ultrafast dynamics of uracil-water clusters

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Microsolvation of "isolated" biomolecules enables a bottom-up approach to understanding solvation effects on the ultrafast systems dynamics. For instance, the properties of ultravioletabsorbing chromophores are sensitive to their local solvation environment [1]. Mass discrimination, i.e., size selecting a particulate cluster of choice, of such neutral solvent-solute aggregates can be challenging. Our group specializes in the preparation of rotationally cold and pure neutral molecular-beam samples [2, 3] to investigate the ultrafast dynamics of size selected clusters on femto- to picosecond timescales.

We developed a versatile and transportable endstation for controlled-molecule experiments (eCOMO) [4], where we purify sample beams using the electric deflector [2] based on the molecules' rotational temperatures, rotational constants, and effective dipole moments. These purified samples are then probed in the ultrafast regime using a double-sided velocity-mapimaging spectrometer to record photoions and photoelectrons in coincidence. Here, we present our current progress on the ultrafast dynamics of the uracil cation, highlighting a metastable pathway of fragmentation into mass 69 cations. Further we plan to extent these studies to microsolvation in uracil-water cluster aggregates.

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Mutual neutralization of NO_x ions and pathway for HONO formation

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Atmospheric Nitrous acid (HONO) is an important source for OH radicals and therefore affects the oxidation capacity of the atmosphere. Nevertheless, its observed atmospheric concentrations remain unexplained, specially during day time when it is efficiently destroyed by photolysis.[1] It has been proposed that atmospheric HONO forms via heterogeneous hydrolysis and charge separation of NO_2 at water surfaces to form NO_x cations and anions. Subsequently, neutralization of the resulting NO_x ions (in the presence of water) was proposed to release HONO back to the gas phase.[2–4]

Recent merged-beams studies of isolated hydronium and hydroxide ions reactions in the DESIREE facility demonstrated how 3D coincidence imaging of the neutal MN products can provide detailed insights into the competing non-adiabatic pathways for OH radical formation.[5,6] Here we will present new results for $NO_3^- + NO^+$ as well as for $NO_2^- + H_3O^+$ reactions. One of the experimental challanges is due to the large gap between the ionization energy and electron affinity, which in the case of $NO_3^- + NO^+$ allows for 15 different neutral product channels. In contrast, our results show that the reaction proceeds via an exclusive non-adiabatic pathway yielding a single $NO + NO_2 + O$ product channel. Analysis of the kineticenergy-release distribution and three-body momentum correlations revealed a sequential dissociation mechanism initiated by long-range electron transfer at an ion–ion distance of ~6 Å that forms a vibrationally excited NO and an electronically excited NO_3 ($^2E'$) intermediate. Subsequent NO_3 dissociation involves an intricate non-adiabatic pathway that yields ground state $NO_2 + O$. The highly non-statistical dynamics enable the succesfull detailed analysis of the 3D coincidence imaging data, which would not be feasaible in the case of many actively competing channels. For $NO_2^- + H_3O^+$ neutralizaiton, preliminary analysis reveals evidence for competing electron-transfer and proton-transfer mechanisms, including evidence for HONO formation. These results provide a detailed mechanistic picture of molecular MN and demonstrate how merged-beams combined with 3D coincidence imaging allows to resolve complex non-adiabatic dynamics relevant to atmospheric ion chemistry.

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Development of an experimental setup for probing radiative cooling dynamics in cold molecular ions

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To understand the role of radiative cooling in astrochemical reactions and photo-processes, we are currently building a new experimental setup to perform state- and time-resolved fluorescence spectroscopy of cold molecular ions in a cryogenic ion trap. This setup will be used to investigate two primary processes that lead to radiative cooling, (i) recurrent fluorescence (RF) responsible for emission of Vis/NIR light and (ii) MIR fluorescence responsible for vibrational relaxation. During RF, a vibrationally hot molecule in the ground electronic state undergoes inverse internal conversion to populate an electronically excited state and then fluoresces [1]. RF is now thought to play a key role in radiative cooling of excited ions in the interstellar medium (ISM) [2], as it enables relaxation in a single step compared to IR fluorescence. Our current goal is to primarily investigate RF while MIR fluorescence will be investigated at a later stage of the project.

The setup, which will be presented, is broadly divided into two sections, (i) a pulsed ion source coupled with a time-of-flight (ToF) mass spectrometer and (ii) a cryogenic ion trap coupled with a grating spectrometer. In section (i), ions will first be generated, separated by mass, and prepared for injection into the cryogenic ion trap. The goal is to create a sufficiently dense ion cloud at the center of the ion trap, where it will interact with a pulsed excitation laser. The collected fluorescence light is coupled into the spectrometer equipped with a single-photon sensitive photomultiplier tube and an iCCD camera.

Ion optics were simulated using SIMION 8.2 [3] to optimize the various electrode parameters. Special attention was given to obtain a mass resolution of R=200, suitable for many astrochemically relevant molecules, at high ion throughput and efficient injection into the trap through a set of specifically designed decelerator ion optics. Additionally, the ion source will be operated in a 1 kHz burst mode to achieve the required ion density within a single measurement cycle.

After injection, a short pulse He/H_2 buffer gas pulse facilitates internal and translational cooling of the ions. The gas pressure, however, must decay on a short timescale (~10 ms) to ensure a collision-free environment during the fluorescence measurement to avoid vibrational relaxation of the highly excited ions and therefore quenching of the RF signal. For this purpose, both the ion trap and a surrounding 40 K shield will be equipped with specially designed gas outlets. The time-dependent pressure curves for each stage were modeled in the Molflow+ software [4] to optimize the gas outlet conductance while minimizing stray light.

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Fragmentation dynamics of multiply charged Diiodoacetylene

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We present a comprehensive experimental study of three-body and four-body fragmentation dynamics of diiodoacetylene (C_2I_2) following multiple ionization induced by low energy Ar^{8+} ion impact. Using a momentum imaging time-of-flight spectrometer with multihit coincidence detection, the complete three-dimensional momenta of all fragment ions were measured, enabling detailed reconstruction of breakup mechanisms in the molecular frame.

For the three-body fragmentation of $C_2I^{3+}{}_2$, the dissociation channel $C^+{}_2 + I^+ + I^+$ is found to be more dominant than $C^+ + I^+ + CI^+$ [1]. The observed branching ratios of the fragmentation channels are consistent with predictions from RRKM statistical theory. Momentum correlation analysis using Newton and Dalitz plots, together with kinetic energy release (KER) distributions, reveals the coexistence of concerted and sequential fragmentation pathways. Concerted breakup dominates and exhibits near-perpendicular emission of the lighter fragment relative to the heavier iodine ions, indicating dissociation from a slightly bent molecular geometry. Sequential fragmentation proceeds via metastable $C_2I_2{}^+$ and $CI_2{}^+$ intermediates, with clear signatures of intramolecular scattering arising from Coulomb-induced rotational motion prior to secondary bond rupture. Threebody fragmentation is observed up to $C_2I^{4+}{}_2$, whereas no four-body fragmentation channel is detected for this charge state.

In four-body fragmentation of highly charged $C_2I^{q+}{}_2$ (q = 5–10), correlated emission of two carbon and two iodine ions was observed [2]. The measured KER values are consistent with classical Coulomb explosion expectations, indicating predominantly Coulomb-driven breakup following rapid ionization. Momentum correlations reveal a pronounced asymmetry between heavy and light fragments: while the iodine ions dissociate predominantly in opposite directions, the carbon ions are strongly deflected, resulting in angular distributions peaked near perpendicular emission relative to the iodine recoil axis. Classical Coulomb explosion simulations incorporating small deviations from linear geometry successfully reproduce the observed angular correlations and momentum sharing.

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Stereodynamics of Ne($^3P_2$) + ND3 collisions

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We present our recent results from a study of Ne($^3P_2$) + ND_3 where we use aligned ammonia. The neon beam is created using an Even-Lavie valve with a discharge source[1], skimmed, and sent to the reaction region using a magnetic guide[2]. The ammonia beam is created in a General valve, skimmed, state selected, and sent to the reaction region using an electrostatic hexapole guide[3]. [2+1] REMPI with linearly polarized light allows us to determine the rotational temperature and the degree of alignment of the ammonia beam under different conditions. A vertical mass spectrometer, with integrated quadrupole alignment electrodes are used to maintain the alignment of ammonia during collisions and extract the ionic products. First results from collisions with aligned and nonaligned ammonia are shown and discussed.

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Development of a Split-and-Delay Unit for Long-Term Coincidence Attosecond Spectroscopy

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The generation of attosecond laser pulses through high-order harmonic generation (HHG) [1] has paved the way for a new field of ultrafast science. With these ultrafast pulses, electron dynamics in atoms and molecules can be resolved on attosecond timescales using techniques such as reconstruction of attosecond beating by interference of two-photon transitions (RABBIT) [2]. Since attosecond coincidence measurements often require long acquisition times to achieve sufficient statistics, sub-cycle stability of the pump-probe delay over the whole measuring time is essential. A split-and-delay unit was developed around a two-segment mirror [3] in combination with a piezo actuator, in order to realize precise, stable measurements over multiple days to weeks. The actuator provides a scan range of a few picoseconds with 15-attosecond steps. This combination enables studies of electron dynamics as well as vibrational and rotational motion in molecules. The pump-probe delay was actively stabilized to a level of around $\sigma = 30$ attoseconds, corresponding to only a small fraction of an optical cycle in the infrared regime, enabling the synchronization of pump and probe pulses with high precision over multiple days of acquisition. The split-and-delay unit will be implemented in a photoelectron–photoion coincidence spectrometer [4] to investigate correlated electron dynamics in atoms and molecules.

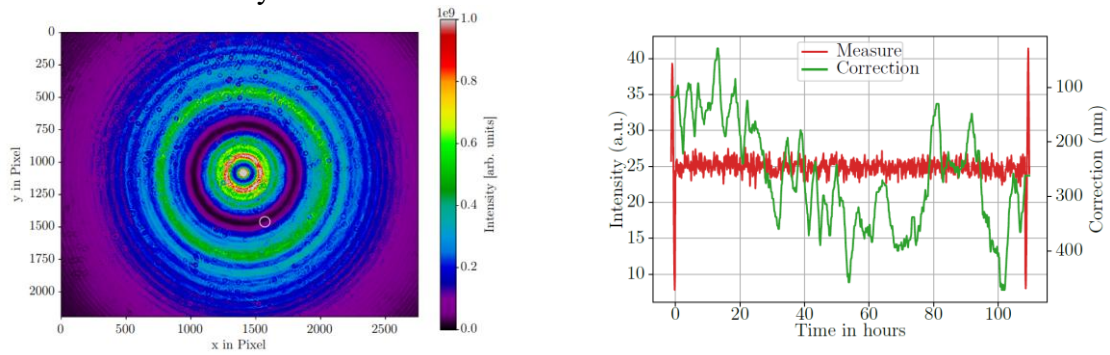

Figure 1: Left: The beam profile, split into inner and outer part after the delay unit. Right: Intensity (red) in the area of interest (white) in the beam profile where the spatial fringes are visible, taken during a long term stability measurement. The intensity is proportional to the $sin(\Delta t)$ of the delay between pump and probe. The corresponding correction of the actuator position responsible for the delay stabilization is shown in green.

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How do ions influence solvation dynamics at the water/air interface?

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The composition of ocean waters varies, however broadly contains 100 mM quantities of Na^+, Mg^{2+}, Cl^- and SO_4^{2-}.[1] Compared to the bulk, the water/air interface has lower water density, and charge permeates more easily. As a result, ions are enriched/depleted relative to their bulk concentrations.[2] Ions disrupt the structure of the interface: some ions are strongly solvated, ordering the water molecules, and others are more surface-active, creating disorder in the Hbonding network.[2] Water (dis)ordering changes the solubility of other species in the same solution. The Hoffmeister series orders ions according to their relative ability to "salt-out" or "salt-in" proteins.[3]
For example, SO_4^{2-} might drive a protein to the surface, whereas SCN^- might drive the protein into solution. Steady-state vibrational sum frequency generation experiments demonstrate that, for example, SO_4^{2-} drives co-solvated Cl^- to the interface, whereas Cl^- drives SCN^- to the interface.[2]

But the above focus on thermodynamic equilibria. What about the solvation dynamics at the interface? This poster explores how the notable change in equilibrium water structure effects the rate with which a hydrated electron generated at the interface becomes internalised to the bulk. Time-resolved electronic sum frequency generation demonstrates that an electron is "salted-in" faster when we add water-disordering salts and internalises slower when we add water-ordering salts, in accordance with the Hoffmeister order observed in steady state measurements.

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Femtosecond relaxation in Oxazole and its isomer

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Ring opening and ring puckering are key photochemical relaxation mechanisms in small heterocyclic molecules such as oxazole and its structural isomer isoxazole. Oxazole contains three carbon atoms, one oxygen atom, and one nitrogen atom, with the oxygen and nitrogen separated by a carbon atom, whereas isoxazole possesses a direct N–O bond. Despite their similar molecular structures, the two molecules exhibit markedly different ultrafast dynamics following vacuum-ultraviolet (VUV) excitation. Previous studies suggest that ring opening in oxazole occurs approximately twice as slowly as in isoxazole, with reported timescales of 85 fs and 45 fs, respectively [1]. However, direct experimental observation of the earliest stages of this process has remained challenging because of the difficulty of generating ultrashort VUV pulses.

Recent developments in the generation of few-femtosecond UV and VUV pulses through resonant dispersive-wave (RDW) emission in gas-filled hollow-capillary fibres [2,3] have enabled the investigation of ultrafast excited-state dynamics in gas-phase molecules with unprecedented temporal resolution. Here, we present time-resolved photoelectron spectroscopy measurements of oxazole and isoxazole using sub-3-fs VUV pump pulses generated by RDW emission.

In the experiment, a 190 nm pulse with an estimated duration of 2.4 fs is split into two replicas and focused into a velocity-map imaging (VMI) spectrometer coupled to a continuous molecular beam. One pulse initiates the excited-state dynamics, while the delayed replica probes the evolving wavepacket through photoionization. The measured photoelectron signal exhibits a rapid decay in both molecules, yielding characteristic lifetimes of 13.5 fs for isoxazole and 33.9 fs for oxazole.

Previous ab initio studies [1] attributed the relaxation dynamics of both molecules to ultrafast population transfer from the initially excited $\pi\pi^*$ state to dissociative $\pi\sigma^*$ states leading to ring opening. In isoxazole, a barrierless relaxation pathway was predicted to drive ring opening on a timescale below 30 fs, whereas in oxazole the presence of a small barrier along the $\pi\pi^*/\pi\sigma^*$ relaxation pathway was found to slow the process significantly. The substantially different decay times observed experimentally are consistent with this picture. To further elucidate the origin of the distinct relaxation dynamics, additional ab initio calculations are being performed. We will present here the first results of these calculations and discuss their implications for the interpretation of the measured ultrafast dynamics.

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Electronic Spectroscopy of PAHs Formed by the Reaction of Carbon with Atomic Hydrogen

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Individual polycyclic aromatic hydrocarbons (PAHs) have been identified in dense clouds[1, 2]. They play a key role in extinction, gas heating, charge balance, and the carbon cycle, and are possible carriers of the Diffuse Interstellar Bands (DIBs) [3]. Although PAH-related species are known to be identifed in dense clouds, no PAH has been confirmed as a DIBs carrier. Their possible role in the diffuse interstellar medium where DIBs are observed remains largely unknown. Laboratory studies of PAHs are therefore needed to determine which species can be formed and to provide electronic spectra for identifying possible species of diffuse interstellar clouds.

In this work, PAH cations are generated via laser ablation of graphite with atomic H introduced close to the ablation region. Drift-tube ion-mobility spectrometry coupled with mass spectrometry is then employed to determine isomer distributions. Electronic spectra of PAH cations are recorded using cryogenic-action spectroscopy and compared with quantumchemical calculations. By ablating a carbon target with a laser and allowing direct reaction with atomic hydrogen, a series of PAHs are generated under conditions that could be similar to those of their natural formation in space, making such PAHs more likely to exist in interstellar environments. The combination of this PAH generation method, isomer selection and cryogenic-action spectroscopy is used to obtain the electronic spectra of PAHs.

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Ultrafast intramolecular relaxation dynamics following electronic excitation of organic molecules in different environments

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Polycyclic aromatic hydrocarbons (PAHs) are currently viewed as promising materials in organic semiconductor technologies. Thus, gaining detailed insights into the electronic structure, relaxation dynamics, and the influence of the surrounding environment on these properties is essential. Employing time-resolved photoelectron spectroscopy, we are capable of probing ultrafast intramolecular relaxation dynamics in PAHs. In combination with a cluster isolation technique, this approach allows us to investigate how different cluster environments influence the relaxation dynamics. Time-resolved measurements of gas-phase tetracene molecules show the expected intramolecular relaxation dynamics to the first electronically excited state following the excitation of the bright singlet state [1]. When embedding the molecule in superfluid helium nanodroplets or attaching it to the surface of argon clusters, we can observe similar relaxation pathways. However, the relaxation time constants appear to be affected by the surrounding medium. In order to fully understand how different environments influence the relaxation dynamics, we plan to carry out a systematic study of acenes, ranging from anthracene to heptacene.

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Implementing a multi-color laser action spectroscopy setup to measure highly excited states of H_3^+ ions in the CSR

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The triatomic hydrogen ion H_3^+ is one of the primary drivers for astrochemistry in diffuse interstellar clouds, and it serves as a benchmark of molecular theory for polyatomic ions. Despite being extensively studied,its highly excited states above 16 500 cm^{-1} remain largely unexplored, as they are both experimentally and theoretically challenging to access. A multi-coloraction spectroscopy scheme was proposed to measure states above 20 000 cm^{-1} [1], providing a bridge to the unassigned pre-dissociation spectrum around 35 000 cm^{-1} [2]. In this approach, a versatile new spectroscopy setup is used to excite cold molecules stored in the Cryogenic Storage Ring (CSR) in two steps from their ground state into the region of interest, via a long lived meta-stable state. The ions are subsequently dissociated with a pulsed UV laser, allowing for coincident, quasi-background-free detection of the fragments on a single-particle detector. Since the recent successful demonstration of the first excitation step [3], a proof of principle for the dissociation step has been achieved, providing insight into cooling and photodissociation of highly excited HD^+ ions.

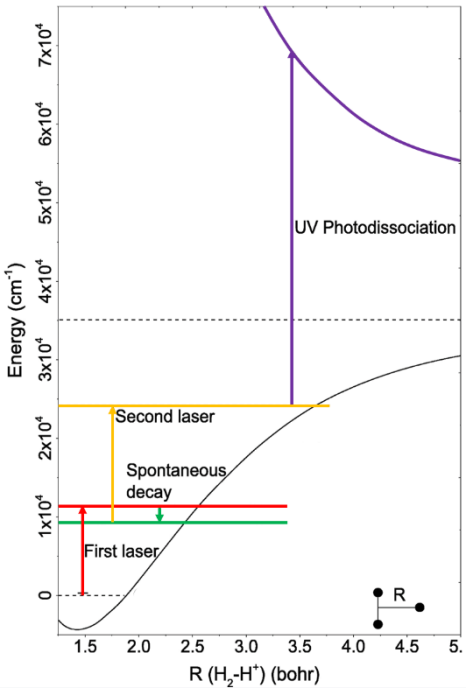

Figure 1 Schematic of the multi-color Spectroscopy scheme for stored H_3^+ ions

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Investigation of Solvent and Isotope Effects on Photostimulated Proton Transfer in 1,1′-bi-2-naphthol (BINOL)

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Photoinduced reactions in 1,1′-bi-2-naphthol (BINOL) have been linked to intramolecular proton transfer processes, with previous studies suggesting a strong influence of solventmediated mechanisms and hydrogen-bonding networks on the reaction pathways [1,2]. We investigated the solvent and isotope dependence of the photodynamics of BINOL using transient vibrational spectroscopy combined with density functional theory calculations.

Measurements were carried out in acetonitrile-d_3, methanol, and methanol-d_1, as well as in mixtures of controlled amounts of H_2O and D_2O. In pure methanol, following the subnanosecond decay of the fluorescent excited state, a long-lived intermediate is observed for approximately one third of the initially excited population. The fraction of molecules in this intermediate state grows with the addition of H_2O at concentrations > several 100 mM. Complete recovery of the ground state is observed within 100 ns.

In contrast, under identical conditions in methanol-d_1 an additional bleach feature in the OH bending region persists up to microseconds after the decay of the intermediate state. Addition of D_2O to methanol-d_1 enhances both the fraction of molecules in the intermediate state and the persistent bleach, indicating a common underlying process. In acetonitrile-d_3 both signals are observed but only after addition of D_2O in molar concentrations. We assign the intermediate state to (solvent-assisted) proton transfer from the alcohol to the naphthol moiety. In the deuterated solvents back-transfer may then result in a permanent partial deuteration of the aromatic ring.

While previous work proposed that proton or deuteron transfer in BINOL systems is strongly dependent on the presence of water to facilitate the process through hydrogen-bonded networks [1], our results indicate that H/D exchange can already occur in neat methanol. Moreover, the fraction of molecules undergoing transient proton transfer upon excited state decay is much larger that anticipated from steady state measurements.

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Evidence for Band-like Charge Transport in a 3D Metal-Organic Framework

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Metal-organic frameworks (MOFs) have attracted significant attention due to their highly tunable porosity and modular structures, which allow precise control over pore size, topology, and chemical functionality. [1] However, most MOFs are intrinsically electrically insulating, limiting their applicability in electronic and optoelectronic devices. Although a number of electroactive two-dimensional MOFs have recently demonstrated metallic or band-like transport [2], observing comparable transport behaviour in truly three-dimensional (3D), highly porous frameworks remains a challenge. In this work, we examine charge transport in a 3D Fe- HHTP MOF, constructed from hexahydroxytriphenylene (HHTP)-based supertetrahedral units interconnected by Fe(III) ions in a diamond-like topology. Van der Pauw (vdP) electrical measurements on bulk pellets reveal Arrhenius-type thermally activated transport. Terahertz time-domain spectroscopy (THz-TDS) is employed as a contact-free technique to determine the frequency-dependent complex conductivity. The terahertz conductivity spectra are well described by the Drude-Smith (DS) model, indicating the presence of band-like charge carriers subject to strong backscattering and hence localization. Analysis of the model parameters shows that the observed increase in conductivity is primarily driven by variations in carrier density, while the carrier scattering time remains nearly temperature independent, suggesting impuritylimited transport. A room-temperature DC conductivity of 6.5×10^{-3} S/cm is obtained from the terahertz measurements, in excellent agreement with vdP results. This consistency indicates that the same population of mobile carriers governs transport across both DC and highfrequency regimes. This study provides direct insight into the microscopic mechanisms of charge transport in conductive MOFs and underscores the potential of three-dimensional frameworks for future optoelectronic and photocatalytic applications.

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Title: Denoising velocity-map imaging datasets using data science and machine learning

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Velocity-map imaging (VMI) captures the scattering distributions of products resulting from photo-induced, electron-induced, or collision-induced chemical reactions enabling detailed analysis of underlying reaction mechanisms.[1] However, VMI data analysis has not yet reached its full potential and machine learning can address the limitations of conventional analysis methods.[2,3] This enables us to extract more detailed and accurate information from complex datasets, ultimately deepening our understanding of the underlying physical chemistry of gas-phase reactions and pushing the boundaries of what can be learned from experimental reactions.

An example of this is the application of machine learning to denoise VMI datasets, which can be prone to low signal-to-noise ratios in certain scenarios such as minor reaction channels. Effective denoising not only reduces the required acquisition time but also enables the investigation of these minor channels. We have developed a computationally efficient denoising algorithm which has been applied to experimental data from the electron-induced dissociation of trifluoroiodomethane (CF_3I) at electron energies of 20 eV and 200 eV. It has produced promising results in both experimental and simulated datasets, and further validation is underway to fully assess its performance.

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Electronic Spectra of Cyclocarbon Anions

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Carbon cluster anions are suspected to exist in space, supported by the detection of negatively charged hydrogen and nitrogen terminated carbon chains in the interstellar medium through their rotational transitions.[1] However, most bare carbon cluster isomers cannot be detected using the same method as they lack a permanent dipole moment. Carbon cluster anions may be detected through contributions to the unidentified infrared bands (UIRs) and/or the diffuse interstellar bands (DIBs) through their vibrational and electronic transitions, respectively.

The study of carbon cluster ions are complicated by their reactivity, difficulty in synthesising macroscopic quantities, and the presence of multiple naturally occurring isomers. To perform spectroscopic studies on these species, we employ a custom-built ion mobility mass spectrometer coupled with a cryogenic quadrupole ion trap and time-of-flight mass spectrometer.[2] Spectra were obtained through resonance enhanced photodissociation (REPD) with messenger tagging. At low temperature, the cyclocarbons can form a weakly bound Van de Waals complex with an N_2 molecule. The complex dissociates upon resonant excitation, and the photofragment yield is monitored as a function of the laser wavelength. Figure 1 presents the first gas-phase electronic spectra of monocyclic carbon cluster anions measured from 700-1800 nm for the C_{4n+2}^- series (left) and the C_{4n}^- series (right).

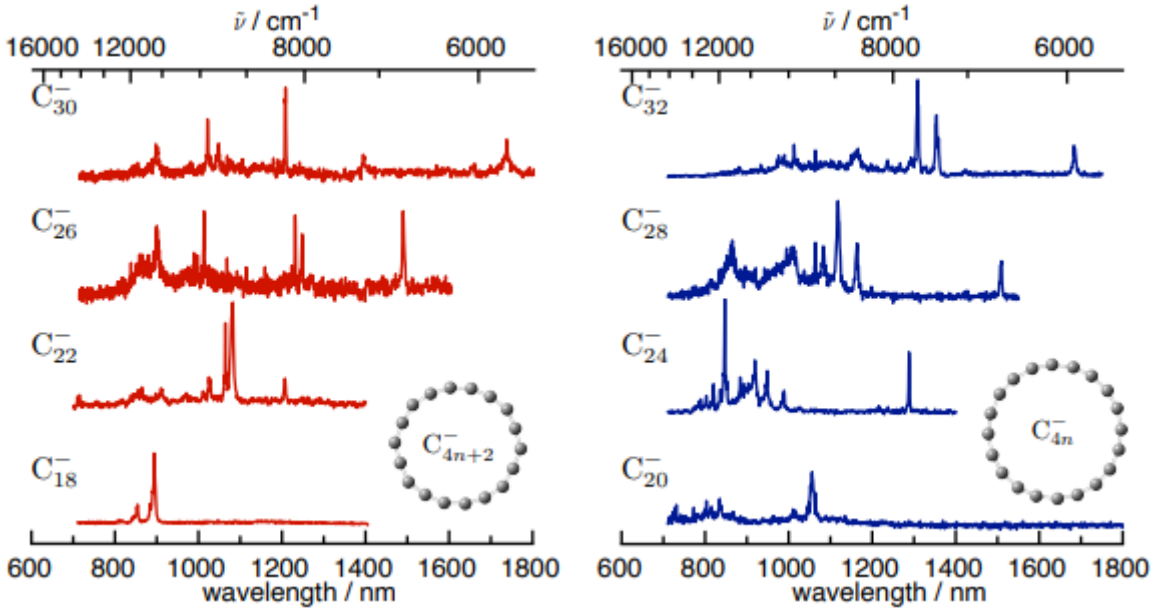

Figure 1. REPD spectra of monocyclic carbon cluster anions C_{4n+2}^- (left) and C_{4n}^- (right) series. Spectra were obtained by monitoring the growth of the C_{2n}^- parent following the dissociation of a C_{2n}^--N_2 complex as a function of wavelength of the tuneable laser.

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Modelling Quantum-Controlled Molecular Collisions of N_2^+ Ions with He Atoms

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The molecular ion N_2^+ plays a central role in both atmospheric and cold ion–neutral chemistry.[1, 2]. In cold and ultracold environments, helium (He) acts as a buffer gas to cool N_2^+ via elastic and inelastic collisions, controlling both translational and internal quantum states. Our group has recently demonstrated full quantum-state preparation and non-destructive quantum-logic spectroscopy of single trapped N_2^+ ions [3]. These advances open the door to probing molecular ion–neutral collisions at the single-particle level with exceptional sensitivity and state resolution. Leveraging this new experimental capability, we investigate the state-dependent collisional dynamics of N_2^+ with He under precisely controlled conditions.

At low collision energies, only non-reactive scattering is expected in the N_2^+ –He system, although rotational state-changing collisions may occur. To characterize these processes, we computed the N_2^+ potential energy surface (PES) at the UCCSD(T)/aug-cc-pVQZ level using MOLPRO, and subsequently constructed a three-dimensional N_2^+ –He PES via Reproducing Kernel Hilbert Space (RKHS) [4] interpolation. The potential well depth of this system is approximately 180 cm−1. All bound ro-vibrational levels of the complex were calculated, including detailed analyses of para- and ortho-N_2^+ states via wavefunction characterization.

Quasi-classical trajectory (QCT) and full quantum dynamical (QD) calculations were performed to obtain final rotational (j) distributions for ortho- and para- N_2^+, as well as the ratios of elastic to inelastic scattering events and the corresponding cross sections. In parallel, ongoing experiments are measuring the inelastic-to-elastic scattering ratio, providing key benchmarks for theoretical predictions.

Overall, this work provides a high-fidelity description of N_2^+ –He interactions and establishes a robust theoretical framework for understanding and ultimately controlling cold ion–neutral collisions, with implications quantum-controlled collision dynamics.

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SIMION-based optimization of ion optics for 3D surface-VMI studies of interstellar ice analogues

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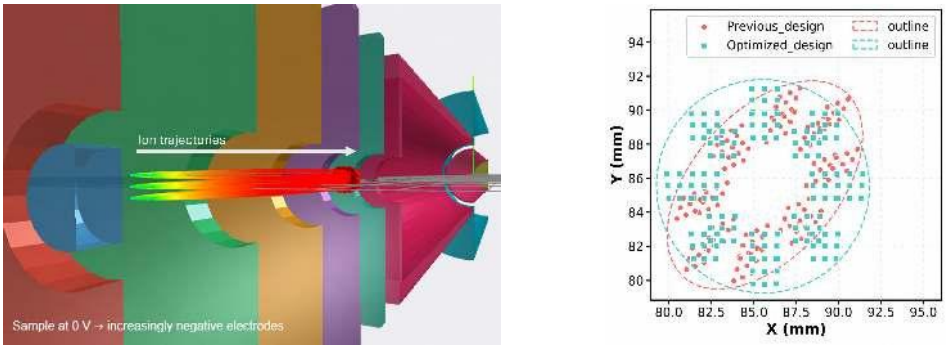
Photon-induced desorption from icy grain mantles is an important non-thermal process in cold astrophysical environments. To study its dynamics, a 3D surface-VMI setup is being developed for future angle- and velocity-resolved photodesorption experiments on interstellar ice analogues. [1] SIMION simulations were used to evaluate electrode and shield geometries in advance.
In the setup, the ice sample is kept at ground potential to reproduce the experimental conditions as realistically as possible. This results in a voltage scheme adapted to the experiment, differing from previous surface-VMI implementations by operating the following ion-optical elements at increasingly negative potentials.



(a) (b)

Figure 1: SIMION analysis: (a) 3D trajectories with electrode voltages; (b) YX detector impacts comparing oval previous (red) with circular optimized patterns (green).

The inverted voltage scheme of this setup causes the previous design used in surface-VMI implementations to produce oval-shaped detector patterns. Simulations of an optimized design restore circular ring patterns, demonstrating that adapted ion optics are required to achieve standard VMI imaging conditions under the present voltage scheme. To support this optimization, a dedicated program was developed for three-dimensional visualization and analysis of SIMION simulations. Together, the realistic SIMION simulations and 3D visualization provide a basis for targeted optimization and reliable imaging conditions in future velocity- and angular-resolved photodesorption measurements from interstellar ice analogues.

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Revolutionizing velocity map imaging with timepix3 technology

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Velocity map imaging (VMI) is a powerful technique for studying the dynamics of molecules and processes in the gas phase. However, conventional VMI detectors such as CMOS-based cameras or delay line detectors have limitations in terms of temporal and spatial resolution and the number of particles that can be detected. Timepix3 technology offers a revolutionary solution to these challenges, providing sub-nanosecond time resolution, excellent spatial resolution, and the ability to detect a large number of particles in real-time. With the help of Timepix3, it is possible to extract detailed information regarding particle dynamics, such as energy, velocity, and position.

I will discuss the advantages of Timepix3 technology for VMI experiments [1][2][3] and show how it has enabled us to gain insights into molecular dynamics. I will describe the design and implementation of different VMI setup, which uses Timepix3 detectors, and present experimental results demonstrating this technology. I will show how Timepix3 has enabled us to detect rare events that were previously difficult to observe and gain information about molecular dynamics.

Our results show how Timepix3 technology has the potential to revolutionize the VMI industry by enabling high-resolution and real-time imaging of atomic and molecular processes. Timepix3 technology will help us understand the underlying physical and chemical mechanisms that control these processes and will create new possibilities for the development of innovative applications in a wide range of scientific fields.

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Time-resolved photoelectron spectroscopy of biomimetic photoswitches

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Photoswitches are molecules, that absorb light and convert the photon energy into the energy of structural molecular deformation. Artificial photoswitches have been in the focus of scientific research for several decades, but their quantum efficiency typically remains low. Upon initial photoexcitation molecules relax along their potential energy surface towards a via conical intersections (CIs). These CIs must be located on the main path of relaxation to make the conversion process efficient. It has been suggested that dynamics throug CIs can be investigated by XUV time-resolved photoelectron spectroscopy (TRPES) in which the probe step is based on ionizing molecules with ultrashort XUV pulses[1]. In this contribution we report on the progress of application of the TRPES method to biomimetic photoswiches in connection with the recently establised European Docoral Network “LUMIERE”. We will report on the relaxation of the NHIP photoswitch and other molecules exhibiting C=C bond and N=N bond[2] isomerization.

Solvent environments often play a significant role in the relaxation dynamics by changing the energy landscape of the molecule via electrostatic interactions, interaction with ionic species often present in the molecular environment[3] or via hydration or protonation (in case of protic solvents). We aim at extending our investigation to several solvents polarities and proticities.

Results for several biomimetic molecules demonstrate, that ultrafast processes can be followed by TRPES with good time resolution, limited mostly by the duration of the pump pulse and that the detected signal bear information complementary to that obtained via alloptical methods, such as transient absorption spectroscopy (TAS). In case of NHIP the recorded signals indicate, that the excited state of the molecule relaxes very fast exhibiting the behavior akin to ballistic relaxation, rather than stochastic relaxation upon equlibriation in the excited state. Such behavior is expected for photoswitches with high quantum efficiency, which move towards key conical intersections directly and ballistically from the Frank-Condon regions. The TRPES results are generally compatible with the previous TAS investigation[5].

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Outer Valence Intermolecular Coulombic Decay and Fragmentation Dynamics of p-Xylene···Trimethylamine Complex

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Intermolecular Coulombic Decay (ICD) is a non-local, ultrafast electronic relaxation process that enables energy transfer in weakly bound systems, resulting in the ionization of a neighbouring molecule.1,2 While ICD has been extensively studied following core and inner-valence excitation, its occurrence via outer-valence excitation has only recently been recognized and remains relatively unexplored.3,4 Resonant two-color two-photon excitation of p-xylene at 8.33 eV, below its adiabatic ionization energy of 8.45 eV, results in ionization of TMA within the PX···TMA complex, with a pronounced enhancement in the TMA+ signal and a significant broadening of its translational energy distribution relative to isolated TMA, confirming an outer-valence ICD mechanism. Comparison of the experimental translational energy distributions of the TMA cation with those obtained from Born-Oppenheimer molecular dynamics (BOMD) simulations (Fig. 1) reveals that the {Ar}C–H···N hydrogen-bonded structure predominantly contributes to the observed fragmentation dynamics.

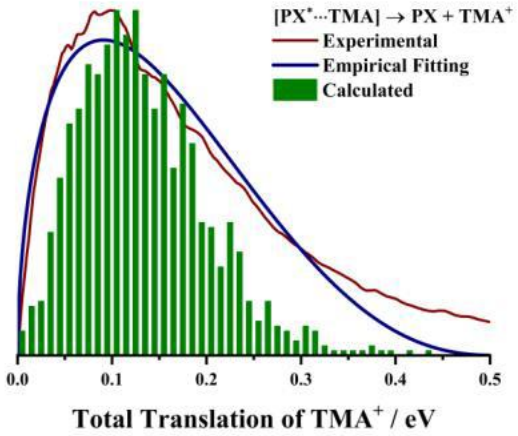

Figure 1. Experimental and calculated translational energy distributions of TMA^+ for the hydrogen-bonded PX···TMA cluster.

These findings demonstrate that fragment translational energy distributions following ICD serve as a sensitive probe for identifying preferred geometries in non-covalently bound complexes, establishing outer-valence ICD as a tool for structural characterization in weakly bound systems.

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From Rabi Dynamics to Dynamic Interference: Revisiting the Physical Origin of Multipeak Structures in Resonance-Enhanced Strong-Field Ionization

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We investigate the physical origin of multipeak structures appearing in resonance-enhanced strong-field ionization spectra, focusing on the transition between Rabi-driven dynamics and dynamic-interference-dominated emission. Using an accurate analytical–numerical treatment of near-resonant two-photon ionization, we demonstrate that the multipeak pattern of the Autler–Townes doublet cannot, in general, be attributed solely to dynamic interference, as often assumed in earlier interpretations. Instead, the spectral structure emerges from the interplay between temporally localized ionization bursts associated with Rabi cycling and the interference of electron wave packets released at different times during the laser pulse[1].

Our analysis shows that selective population of dynamically dressed states governs the gradual transition from Rabi oscillations to interference-dominated spectra, providing a unified picture of regimes previously treated separately[1]. In particular, we identify parameter domains where the spectral peaks originate from discrete ionization windows linked to maxima of the intermediatestate population, in contrast to the below-threshold dynamic-interference mechanism reported in earlier studies [3]. These results clarify the roles of detuning, pulse area, and ionization loss in shaping the Autler–Townes structure.

Beyond the specific hydrogen example considered here, the results connect naturally to recent analytic two-level models of resonance-enhanced multiphoton ionization, where closed-form solutions reveal how time-dependent coupling, detuning, and decay govern dressed-state dynamics and spectral formation [2]. Together, these perspectives contribute toward a more general theoretical framework for interpreting strong-field spectra in atoms and molecules driven by short coherent pulses.

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Nonadiabatic Tunnelling in Molecular Systems

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Nonadiabatic processes are central to chemical dynamics, especially in photochemistry, where structural motion and electronic transitions are intrinsically coupled. In such processes, nuclear tunnelling can strongly affect measured rates and mechanisms, but remains difficult to describe in realistic molecular systems because fully quantum-mechanical treatments are computationally prohibitive.

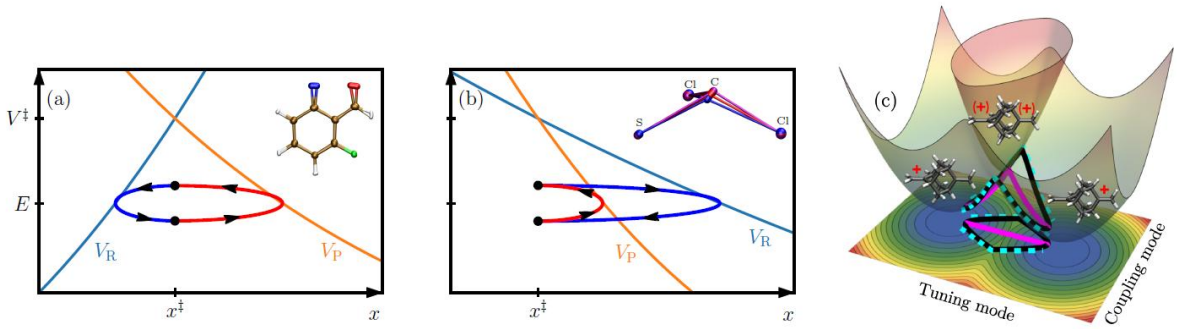

Figure 1: (a,b) Instantons (dark colours) for two spin crossovers, with insets showing the change of the molecular configuration due to tunnelling. (c) Conical intersection mediating a charge transfer, along with several competing instantons.

This contribution presents golden-rule instanton theory as a practical semiclassical method for predicting molecular nonadiabatic tunnelling [1]. The method generalizes the conventional transition state to an optimal tunnelling pathway, or instanton, connecting electronic states, and can be coupled to high-accuracy electronic-structure calculations. Applications to spin-crossover and charge-transfer reactions reproduce matrix-isolation and laser experiments quantitatively and reveal that nonadiabatic tunnelling can redirect reaction pathways and enhance rates by many orders of magnitude [2,3]. In these systems, even heavy atoms such as carbon, nitrogen and oxygen can tunnel at room temperature. These results suggest that heavy-atom tunnelling in nonadiabatic chemistry may be more widespread, and more experimentally relevant, than traditionally assumed.

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25th European Conference on the Dynamics of Molecular Systems

September 6th to 11th, 2026

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	Sunday, September 6th	Monday, September 7th	Tuesday, September 8th	Wednesday, September 9th	Thursday, September 10th	Friday, September 11th
Location	Instutute of Physics Hermann-Herder-Str. 3	Kollegiengebäude I Platz der Universität 3	Kollegiengebäude I Platz der Universität 3	Kollegiengebäude I Platz der Universität 3	Kollegiengebäude I Platz der Universität 3	Kollegiengebäude I Platz der Universität 3
9:00		**Takamasa Momose**	**Henrik Stapelfeldt**	**Daniel Neumark**	**Francesca Calegari**	**Christiane Koch**
9:30						
10:00		**Jennifer Noble**	**Stefanie Gräfe**	**Thomas Allison**	**Giuseppe Sansone**	**Andres Ordonez**
10:30		Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:00		**Evan Bieske**	**Andrew Orr-Ewing**	**Rebecca Ingle**	**Alicia Palacios**	**Iain Wilkinson**
11:30		**Jascha Lau** **Anthony Meijer** **Amit Debnath**	**Steen Bronsted Nielsen** **Brendan Wouterlood** **Sebastian Trippel**	**Jemma Gibbard** **Mathew Costen** **Wim van der Zande**	**Hugo Marroux** **Maria Richter** **Karin Sarah Thalmann**	**Letizia Fede** **Andrea Annunziata** **Nicolas Ladda**
12:00						
12:30		Lunch	Lunch	Lunch	Lunch	**Concluding remarks**
13:00						Lunch
13:30						
14:00		**Mischa Bonn**	**Bas van de Meerakker**		**Daniel Rolles**	Departure
14:30		**David Nesbit**	**Xingang Wang**		**Daniel Strasser**	
15:00		**Wutarath Chin** **Kim Lee Yeong**	**Andrea Orban** **Nanditha Sunil Kumar**	**Excursion**	**Lorenzo Iori** **Arnab Sen**	
15:40		Coffee Break	Coffee Break		Coffee Break	
16:10		**Kirsten Schnorr**	**Marcel Mudrich**		**MOLEC Prize session**	
16:40		**Daniela Rupp**	**Elisabeth Gruber**			
17:10	Arrival on site	**David Picconi** **Lok Yiu Wu** **Laura Pille**	**Poster**	**Lab visits**	**Poster**	
17:30	Registration					
17:50	**Welcome**					
18:00	**Toshinori Suzuki**					
18:30						
19:00	**Welcome Evening**				**Conference Dinner**	
19:30						
20:00						
20:30						