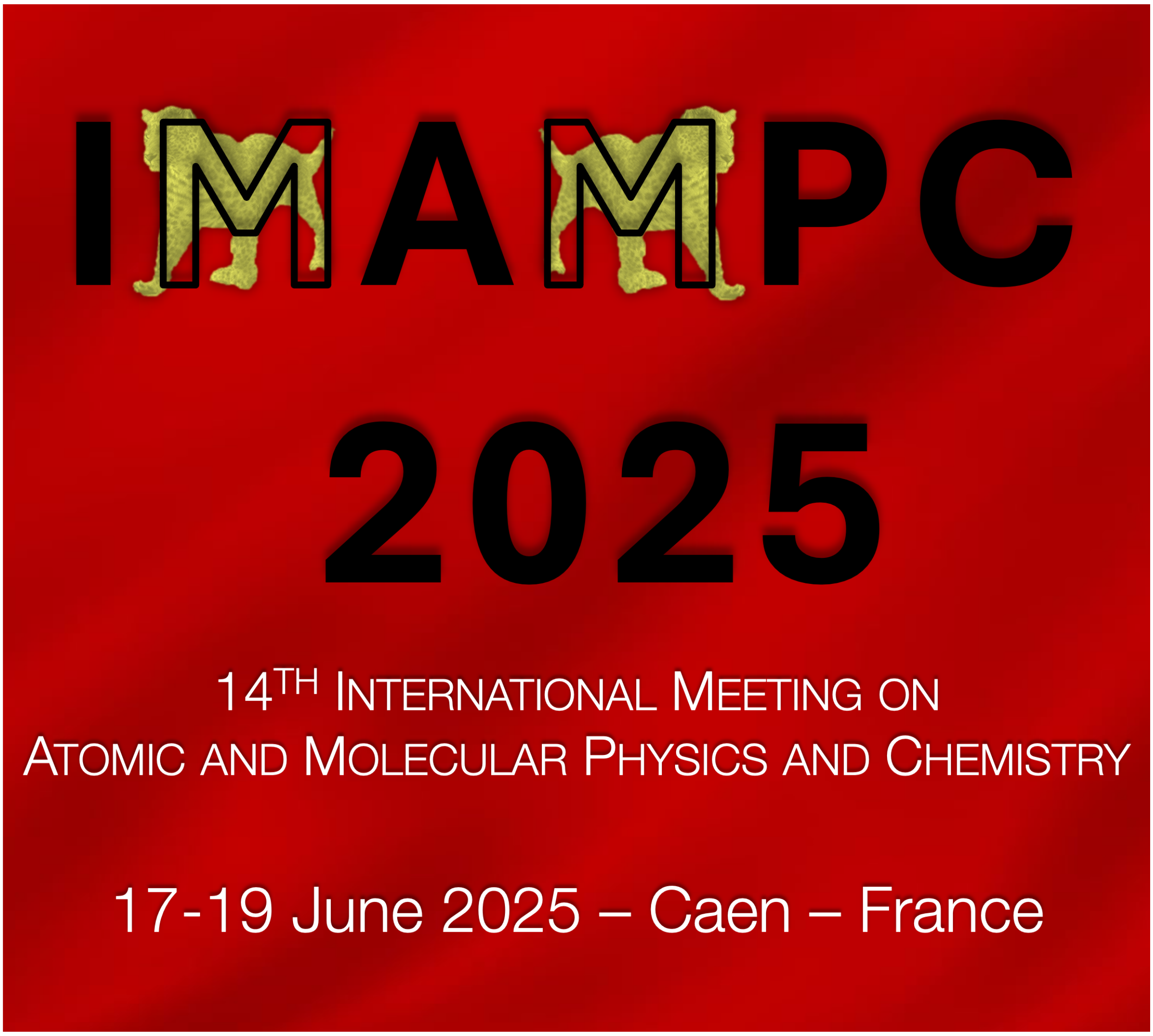


IMAMPC
2025

14th International Meeting on
Atomic and Molecular Physics and Chemistry

17-19 June 2025 – Caen – France

A few words

We are delighted to have you at the 14th International Meeting on Atomic and Molecular Physics and Chemistry, happening in Caen, France, from 17 to 19 June 2025.

This conference aims to support young researchers and foster interdisciplinary collaborations. Right from its inception (in 2010), IMAMPC has been organized by and for young researchers ($\leq$ 10 years after PhD completion).

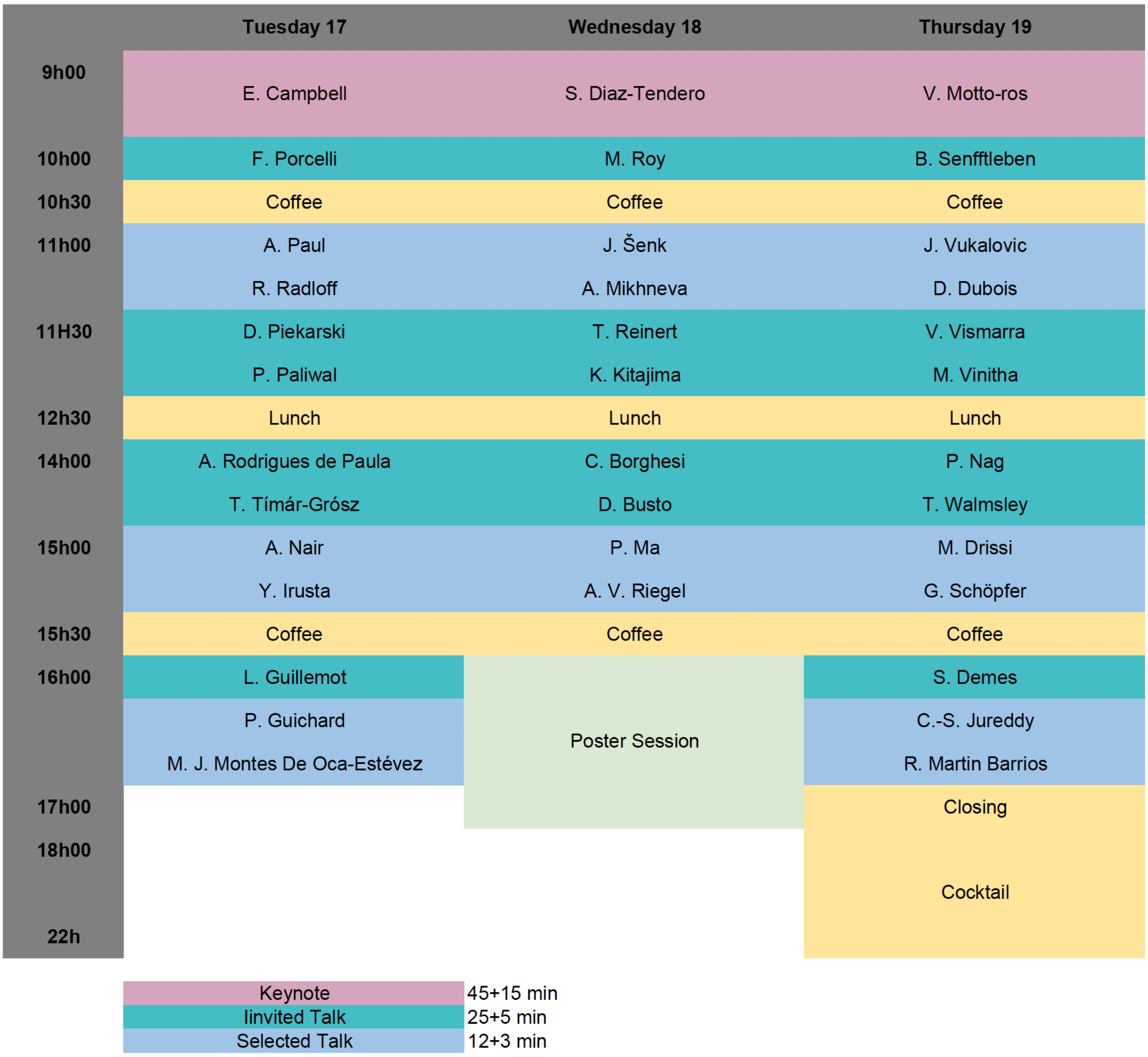
The event brings together researchers from both theory and experimentation in the broad field of atomic and molecular physics and chemistry, opening up new research directions and opportunities for collaboration.

We believe that the conference in Caen will create a pleasant environment for fruitful discussions and inspiration.

The local organizing committee is composed of CIMAP members:

- Sreeja Raghunandanan
- Sumit Srivastav
- Antonin Bourgeteau
- Patrick Rousseau
- Alicja Domaracka
- Sylvain Maclot

Program: overview



	Tuesday 17	Wednesday 18	Thursday 19
9h00	E. Campbell	S. Diaz-Tendero	V. Motto-ros
10h00	F. Porcelli	M. Roy	B. Senfftleben
10h30	Coffee	Coffee	Coffee
11h00	A. Paul	J. Šenk	J. Vukalovic
	R. Radloff	A. Mikhneva	D. Dubois
11H30	D. Piekarski	T. Reinert	V. Vismarra
	P. Paliwal	K. Kitajima	M. Vinitha
12h30	Lunch	Lunch	Lunch
14h00	A. Rodrigues de Paula	C. Borghesi	P. Nag
	T. Tímár-Grósz	D. Busto	T. Walmsley
15h00	A. Nair	P. Ma	M. Drissi
	Y. Irusta	A. V. Riegel	G. Schöpfer
15h30	Coffee	Coffee	Coffee
16h00	L. Guillemot	Poster Session	S. Demes
	P. Guichard		C.-S. Jureddy
	M. J. Montes De Oca-Estévez		R. Martin Barrios
17h00			Closing
18h00			Cocktail
22h			

Keynote	45+15 min
Iinvited Talk	25+5 min
Selected Talk	12+3 min

Sponsors

This conference was possible thanks to the financial support of:

UNICAEN
UNIVERSITÉ
CAEN
NORMANDIE

cnrs

cea iramis

ENSI
CAEN
ÉCOLE PUBLIQUE D'INGÉNIEURS
CENTRE DE RECHERCHE

Labex
Laboratoire d'Excellence
EMC3
ENERGY MATERIALS & CLEAN COMBUSTION CENTER

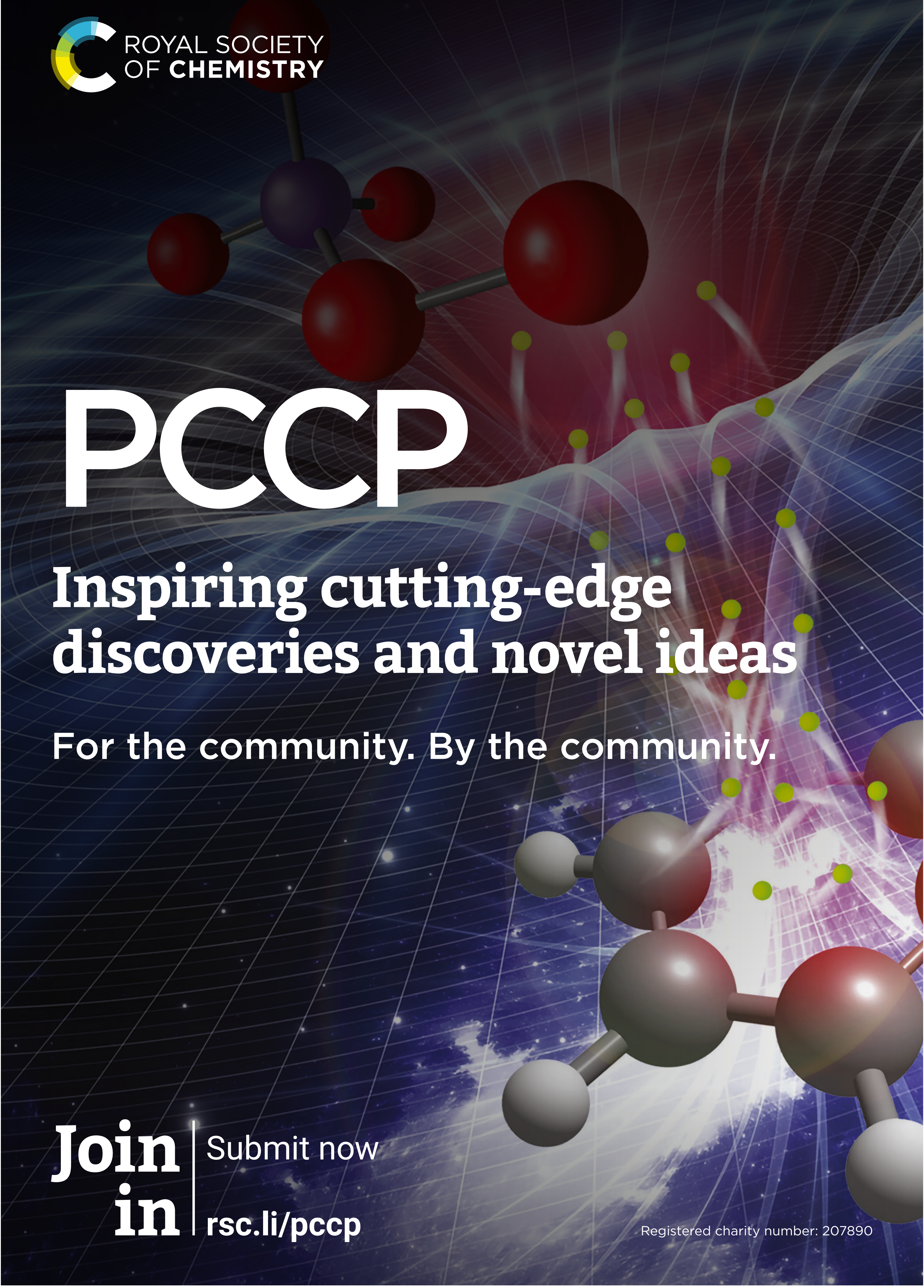
CIMAP

RoentDek
Handels GmbH
Supersonic Gas Jets
Detection Techniques
Data Acquisition Systems
Multifragment Imaging Systems

Caen la mer
NORMANDIE
COMMUNAUTÉ URBAINE

ROYAL SOCIETY
OF CHEMISTRY

PCCP



Uniquely positioned to support you, wherever you are in the world, with 19 national societies working together, we are advancing the frontiers of physical science on a global scale.

Physical Chemistry Chemical Physics (PCCP) represents cutting-edge research in the evolution of physical chemistry, chemical physics and biophysical chemistry. We span the breadth of experiment, theory, computation and data science, bringing you original work at the frontiers of physical science.

PCCP is committed to benefiting the whole scientific community – a mission supported by all 19 owner societies. Our expert professional editors and associate editors ensure that all the research published is innovative and insightful, and of significance to the community. That is why we are the largest journal in our field, publishing cutting-edge research and inspiring discovery across the breadth of physical science.

Editorial Board Chair
Anouk Rijs Vrije Universiteit Amsterdam, Netherlands

Impact factor 2023: 2.9, median time to first decision (peer reviewed articles only): 34 days.
Visit **rsc.li/metrics-explainer** for sources and a metrics explainer.

Indexed in MEDLINE and Web of Science.

Stay up to date: **rsc.li/alerts**

Contact us: **pccp-rsc@rsc.org**

𝕏 **@PCCP**

Join in | Submit now
rsc.li/pccp

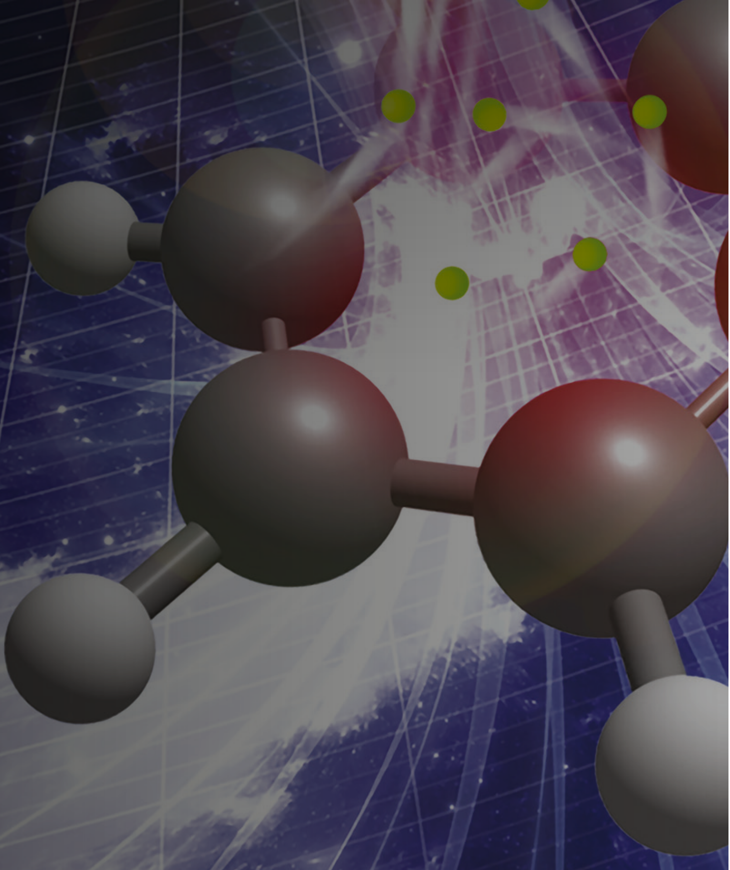


Table of contents

17 Jun 2025

Fundamental Studies of Fullerenes: the Astrochemical Revival

Eleanor Campbell * [1]

[1] School of Chemistry, University of Edinburgh – United Kingdom

Since their discovery in 1985, fullerenes have been very fruitful model systems for applying the techniques of atomic and molecular physics to the study of more complex molecular and cluster systems. C_{60} in particular has been well studied and can be considered to truly "bridge the gap" between molecular and solid state systems, showing both molecular characteristics and statistical behaviour more akin to small metal particles or even looking like a large hydrogen atom, depending on the particular experiment. Since the discovery of C_{60} and C_{70} in space 10-15 years ago there has been an increased awareness of the importance of these molecules in an astrochemical context. This coincides with the development of exciting new experimental facilities to probe their properties in unprecedented detail and the wealth of spectroscopic data being produced by the James Webb space telescope. I will trace out these developments, many of which are currently occurring within the COST Nanospace network, and give my perspective on the role of atomic and molecular physics in solving the puzzles concerning the role of nanocarbons in space.

---

*Speaker

Photoemission Spectroscopy of Organic Molecules Using Plane-Wave/Pseudopotential Density Functional Theory and Machine Learning: A Comprehensive and Predictive Computational Protocol for Isolated Molecules, Molecular Aggregates and Organic Thin Films

Francesco Porcelli *† [1], Francesco Filippone [1], Emanuela Colasante [1], Giuseppe Mattioli [1]

[1] National Research Council, Institute of structure of matter (CNR-ISM) – Italy

Photoemission measurements performed in gas phase at low pressure opened the exploration at the scale of single molecules of the complex relationship between electronic and structural properties of the matter. Experimental results collected on molecules isolated from interaction with other species provided, in turn, an ideal breeding ground for developing ab initio simulations capable of interpreting and predicting photoemission spectra. Regarding the atom- and site-specific core ionization binding energies (BEs), accurate methods facilitate the interpretation of experimental data, also helping to assign the contributions of all non-equivalent atoms of the same species even in unresolved features arising from a molecular structure. In this context, we have developed, extensively tested and made available to a broad readership a computational protocol rooted on plane-wave/pseudopotential density functional theory (1)(hereafter referred to as PW-DFT), based on a ΔSCF approach, to predict X-ray photoemission spectra (XPS) in molecules, molecular aggregates and molecular thin films deposited on inorganic substrates. Calculations have been performed using a representative set of semilocal and global/range-separated hybrid density functionals, containing increasing fractions of Hartree-Fock exact exchange (EXX). Specifically, PBE, B3LYP (20 % EXX), HSE (range separated with 25 % EXX at short range) and BH&HLYP (50 % EXX) have been used for the assessment of the computational protocol. Equation-of-motion coupled-cluster with single and double excitations (EOM-CCSD) has been employed as reference theoretical method for comparison. The computational protocol has been tested against a wide set of molecular classes encompassing aromatic, heteroaromatic and aliphatic compounds as well as drugs and biomolecules, demonstrating to be generally accurate and robust even using semilocal DFT. Moreover, valence photoemission measurements represent a complementary tool to core photoemission, particularly useful to investigate the properties of delocalized and π- conjugated molecular orbitals, and sensitive to chemical modifications which involves large molecules through non covalent interactions. We have used the same set of density functionals to assess their capability to predict valence-shell ionization spectra for different molecular classes using Kohn-Sham

---

[*] Speaker

[†] Corresponding author: francesco.porcelli@mlib.ism.cnr.it

eigenvalues as estimators. Finally, our PW-DFT data-set of C1s, N1s and O1s BEs have been used to train machine learning (ML) models finalized to the prediction of XPS spectra in isolated organic molecules from their structure. To ensure the reproducibility of our results and foster the use of our protocol, we have made available at https://doi.org/10.5281/zenodo.14905828 through a public repository, a library of pseudopotentials and input files for ab initio calculations, together with the data sets employed to train the ML models.

References:

(1) **Porcelli F,** Colasante E, Filippone F, Mattioli G. Photoemission Spectroscopy of Organic Molecules Using Plane-Wave/Pseudopotential Density Functional Theory and Machine Learning: A Comprehensive and Predictive Computational Protocol for Isolated Molecules, Molecular Aggregates and Organic Thin Films. ChemRxiv. **2025**; doi:10.26434/chemrxiv-2024-h0g2d-v3

Structural rearrangements and fragmentation pathways induced by low-energy electron attachment to trifluorotoluene ($C_6H_5CF_3$)

Anirban Paul * [1], Samrat Saha [1], Dipayan Chakraborty [2], Sylwia Ptasinska [2], Juraj Fedor [1], Pamir Nag† [1]

[1] Heyrovský Institute of Physical Chemistry of the Czech Academy of Sciences – Czech Republic
[2] University of Notre Dame [Indiana] – United States

Dissociative electron attachment (DEA) is a fundamental interaction in electron-molecule collisions, where a low-energy electron is temporarily captured by a molecule, forming a temporary negative ion (TNI). This unstable intermediate then dissociates, leading to the formation of one or more anionic fragments along with neutral counterparts. DEA plays a crucial role in various physical, chemical, and biological processes, particularly in radiation chemistry, atmospheric chemistry, and plasma-assisted reactions. In biological systems, low-energy secondary electrons produced from ionizing radiation mainly induce molecular damage through DEA, leading to single- and double-strand DNA breaks. Similarly, in environmental and industrial applications, DEA contributes to the degradation and transformation of halogenated and fluorinated organic compounds, making its study essential for understanding pollutant behavior and designing targeted decomposition strategies.

Trifluorotoluene ($C_6H_5CF_3$), also known as benzotrifluoride, is widely used as a solvent and intermediate in the production of pharmaceuticals and agrochemicals. The presence of the trifluoromethyl (CF_3) group significantly alters the electronic properties of the benzene ring, leading to high chemical and thermal stability. However, its degradation pathways, particularly under electron-rich environments such as plasmas and high-radiation conditions, remain poorly understood. In plasma processing, understanding the complete dissociation mechanism of such molecules is crucial for optimizing reaction conditions and controlling byproduct formation. A key aspect of DEA studies is the measurement of absolute DEA cross sections, which quantify the probability of anion formation as a function of the incident electron energy. These measurements are essential not only for modeling electron-driven processes in plasma reactors but also for understanding the molecular degradation pathways in various environments, including interstellar space, planetary atmospheres, and radiation-induced chemical transformations.

In the present work, we have investigated the DEA dynamics of trifluorotoluene using velocity slice imaging and measured the absolute DEA cross-sections for different fragment anions using the well-established relative flow technique (RFT). The absolute dissociative electron attachment cross sections as a function of incident electron energy (0–12 eV) reveal three major resonance peaks at approximately 5.2, 8.5, and 11.8 eV, corresponding to different dissociation pathways.

---

[*] Speaker

[†] Corresponding author: pamir.nag@jh-inst.cas.cz

The dominant fragment observed is F^-, along with other anionic species such as HF_2^- and C_2H^-, indicating complex structural rearrangements. Kinetic energy and angular distributions of the F^- ions suggest multiple bond-breaking mechanisms, including both two-body and three-body dissociation pathways. The experimental findings are further supported by quantum chemical calculations performed using density functional theory (DFT) to determine threshold dissociation energies.

Enhancement of X-ray scattering cross-sections by transient resonances in metal foils and nanoparticles

Robert Radloff * [1], Rasmus Buchin [1], Nils Muthreich [2], Jan Leutloff [2], Felix Zimmerman [3], Slawomir Skruszewicz [1], Yanwen Sun [4], Taito Osaka [5], Gota Yamaguchi [5], Jumpei Yamada [5,6], Ichiro Inoue [5], Anatoli Ulmer [1], Phay Ho [7], Florian Schulz [1], Juan Barrios [1], Xin Liu [1], Samuel Sahel-Schackis [8], Sandra Mous [4], Andrew Aquila [4], Sebastien Boutet [4], Stephan Kuschel [2], Tais Gorkhover [1]

[1] Universität Hamburg – Germany
[2] Darmstadt University of Technology [Darmstadt] – Germany
[3] Physikalisch-Technische Bundesanstalt [Berlin] – Germany
[4] SLAC National Accelerator Laboratory – United States
[5] RIKEN SPring-8 Center – Japan
[6] Osaka University – Japan
[7] Argonne National Laboratory [Lemont] – United States
[8] Stanford University – United States

Diffraction with intense, ultrashort, hard X-ray pulses generated by free-electron lasers (FELs) permits the acquisition of images with high spatial and temporal resolution.
At high X-ray intensities, like the ones provided by FELs, further increasing the intensity of the X-ray pulse does not necessarily lead to an increase in the brightness of the diffraction pattern to the same extent. Instead, the absorption of multiple high-energy photons during X-ray exposure leads to electronic on a femtosecond timescale.

The removal of bound electrons by photoionization and subsequent relaxation processes such as the Auger-Meitner process typically leads to a decrease in the scattering cross-section and then, on longer time scales, to structural changes due to the high charge states generated in the first step. However, Hartree-Fock Monte-Carlo simulations and recent experimental results in the soft X-ray regime(1) suggest that this is not always the case and electronic damage is not necessarily detrimental for diffraction experiments.

Given the right pulse and photon energy, as well as length of the X-ray exposure, atoms can be driven into electron configurations with increased orbital overlap and, hence, enhanced absorption and scattering cross-sections. As these resonances are short-lived, they are referred to as transient resonances.

In this contribution, we show recent experimental results obtained at SACLA (Japan) and LCLS (USA), trying to leverage the effects of transient resonances in the hard X-ray regime and dis-

---

*Speaker

cuss the energy dependence of the absorption and scattering cross-sections in thin iron and gold foils. Furthermore, we present evidence of sub-nanometer resolutions obtained by Bragg coherent diffractive imaging of gold nanoparticles with diameters $<$ 10 nm at photon energies close to the gold Lα lines.

Reference:
(1) S. Kuschel *et al.*, "Non-linear enhancement of ultrafast X-ray diffraction through transient resonances," *Nat. Commun.*, vol. 16, no. 1, p. 847, Jan. 2025, doi: 10.1038/s41467-025-56046-y.

Long live the anionic triazole king

Dariusz G. Piekarski *† [1], Smith Pataraprasitpon [1], Thomas F.m. Luxford [2], Roman Čurík [2], Jaroslav Kočišek [2]

[1] Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, 01-224 – Poland
[2] J. Heyrovský Institute of Physical Chemistry v.v.i., The Czech Academy of Sciences, Dolejškova 3, 18223 Prague – Czech Republic

Our study of anionic triazole derivatives' reactivity reveals how hydrogen position affects reaction dynamics. Low electron energy-dependent ion yields shows significant differences for two very similar molecules. Quantum chemical calculations reveal that bromine atom migration is responsible for long life of anionic state. Moreover, movement of the heavy atom is energetically more favored than hydrogen atom migration for triazole derivative with H atom adjacent to Br. This is enabled by the favorable formation of a non-covalent complex of Br- around the triazole ring. The interplay between Br and H is driven by light atom moderator, while heavy singly negatively charged atom is traveling around 4H-1,2,4-triazole ring.
Triazole derivatives are widely used bioisosteres and chiral organocatalysts that mimic various functional groups while maintaining high resistance to external conditions. In particular cases such as removing azole-based antifungal reagents from wastewater, their extra stability is an unwanted property. Low-energy electrons can be used to change the stability of this special class of organic molecules.

We show that two very similar target molecules, 3-bromo-1H-1,2,4-triazole (1HBrT) and 3-bromo-4H-1,2,4-triazole (4HBrT), differ only by the position of one hydrogen atom but exhibit different reactivity after low-energy electron attachment. The origin of such discrepancy is explained as the ability of 4HBrT anion to facilitate straightforward negative bromine roaming. This reaction mechanism is reflected in different intensities and fragments in dissociative electron attachment experiments, mainly Br^- vs. HBr releases. Potential energy surfaces, molecular dynamics, and analytic continuation calculation demonstrate that the position of hydrogen on the ring is crucial and determines the character of the lowest-lying resonant state. Consequently, it affects the exothermic motion of the Br^- around the triazole ring. A picosecond long resonance lifetime allows such roaming dynamics, particularly a high propensity of neutral HBr release. This work was supported by the National Science Centre, Poland, grant no. 2022/47/D/ST4/03286.

---

[*] Speaker

[†] Corresponding author: dpiekarski@ichf.edu.pl

Investigating and manipulating chemical systems through quantum logic

Prerna Paliwal * [1]

[1] University of Basel – Switzerland

In recent years, there has been an increasing interest in the coherent control of isolated quantum systems-such as atoms, ions, superconducting circuits, and quantum dots-which has led to significant advancements in quantum metrology, sensing, and computing. The current focus in the quantum physics community is to extend these quantum technologies to molecules. However, molecules pose a unique challenge due to their complex internal structures and the absence of cycling transitions, making them hard to cool, control, and manipulate. In our laboratory, we address this challenge by co-trapping a single molecular ion with an atomic ion. The atomic ion serves dual purposes: it cools the molecule translationally and acts as a messenger for the molecule's internal state without destroying it. Essentially, we transfer the information of the complex molecular ion onto an easily controllable atomic ion, from which we can read it out (1-3). I will explain our method for quantum-non-demolition detection of the rovibrational state of single nitrogen ions which is a crucial step towards their coherent manipulation. This approach not only pushes beyond current capabilities of molecular state readout but also allows us to projectively prepare molecular ions in well-defined hyperfine-Zeeman states (4). Additionally, I will discuss how we are adapting this technique for polyatomic ions, laying the groundwork for detailed exploration of their spectroscopy and molecular dynamics (5).

References:

(1) Schmidt P O et al., Science 309, 749 (2005).
(2) Sinhal M et al., Science 367, 1213 (2020).
(3) Najafian K et al., Nat. Commun. 11, 4470 (2020).
(4) Shlykov A et al., Advanced Quantum Technologies 8, 2300268 (2025).
(5) Paliwal P et al., Chimia, 78, 654 (2024).

---

[*] Speaker

Ultrafast imaging techniques

Alisson Rodrigues De Paula * [1,2], Thomas Godin† [1,2], Saïd Idlahcen [2],
Denis Lebrun [2], Ammar Hideur [2], Pierre-Henry Hanzard [1,2]

[1] Complexe de recherche interprofessionnel en aérothermochimie – CNRS, Université de Rouen - Normandie et INSA de Rouen - Normandie – France
[2] CORIA – CNRS : UMR6614, Université de Rouen, Institut National des Sciences Appliquées (INSA) - Rouen – France

Many physical, chemical, and biological phenomena occur on ultrafast (sub-nanosecond) timescales and microscopic spatial scales, making them inaccessible to conventional technologies like high-speed cameras, which are fundamentally limited by the relatively long response times of electronics and their bandwidth. To address this challenge, optical methods have proven exceptionally effective across various fields, offering ultrahigh temporal resolutions in the femtosecond-to-attosecond range. Different techniques play a crucial role in advancing this field of acquisition. For instance, simple and repeatable events are best captured using pump-probe techniques, while unique or hard-to-reproduce events require single-shot approaches. Furthermore, the technology used differs significantly depending on whether the event is self-luminescent (passive detection) or requires external illumination (active detection). Other important parameters include the number of sequential frames available (sequence depth), frame rate (measured in frames per second), image size in pixels (pixel resolution), as well as spatial and temporal resolution. In this talk, I will present state-of-the-art techniques and highlight the most relevant factors to help the audience choose the best-fitting approach.

---

*Speaker

†Corresponding author: thomas.godin@coria.fr

Recent Experiments and Developments at the 100-kHz HR Condensed Beamline of ELI ALPS

Tímea Tímár-Grósz * [1]

[1] ELI ALPS Laser Research Institute – Hungary

Time-resolved studies of electron motion requiring high statistics or high signal-to-noise ratio necessitate the development of attosecond-pulse sources operating at high repetition-rates. When analyzing solid chemical or biological samples, where multi-electron processes are strongly contributing to the observed phenomena, these tools are essential.

The High-repetition-rate laser-driven Gas-based High-order Harmonic Generation (HR Gas and HR Condensed) beamlines of the Extreme Light Infrastructure Attosecond Light Pulse Source (ELI ALPS) have been operating and serving users for multiple years by now. The two beamlines are both driven by the state-of-the-art high-repetition-rate (HR-1) laser system, supplying sub-7 fs pulses at 100-kHz repetition-rate and 1 mJ energy centered around 1030 nm. One of the beamlines is specifically designed for condensed samples – the HR Condensed beamline – which provides high-flux extreme ultraviolet (XUV) radiation with near-infrared (IR)-XUV pump-probe possibility at a high (100 kHz) repetition rate. In addition, this beamline is equipped with a time-delay-compensated XUV monochromator, that provides the possibility of selecting different XUV photon energy regions of the generated high-order harmonic radiation down to the 100 meV spectral bandwidth, while preserving the few (tens of) femtosecond duration of the XUV pulses. The beamline is connected to the NanoESCA end-station, incorporating a photoemission electron microscope (PEEM), a double hemispherical electrostatic energy analyzer, a time-of-flight energy analyzer, a unique spin filter and a sample preparation chamber for real and k-space band structure mapping. These devices enable spin diagnostics, magnetic imaging, plasmonics and angle-resolved photoemission spectroscopy (ARPES) with few tens of meV energy, nanometer spatial and femtosecond-attosecond temporal resolution.

In this work, the aim is to give an overview on the capabilities and recent experiments carried out with the HR Condensed beamline available to researcher from around the globe.

---

*Speaker

Radiation damage of nucleotides-the story revealed by X-ray action spectroscopy

Aarathi Nair *† 1, Rebecca Boll 2,3, Tobias Lau 4,5, Juliette Leroux 1, Rebecka Lindblad 6,7,8, Carlos Mahecha 9, Bart Oostenrijk 1,2, Laura Pille 2, Lucas Schwob 10, Vicente Zamudio-Bayer 11, Sadia Bari 12,13

1 The Hamburg Centre for Ultrafast Imaging – Germany
2 Deutsches Elektronen-Synchrotron [Hamburg] – Germany
3 European X-Ray Free-Electron Laser – Germany
4 Abteilung für Hochempfindliche Röntgenspektroskopie, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany – Germany
5 Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany – Germany
6 Abteilung für Hochempfindliche Röntgenspektroskopie, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany – Germany
7 Department of Physics, Lund University, Lund, Sweden – Sweden
8 Inorganic Chemistry, Department of Chemistry – Ångstrom Laboratory, Uppsala University, SE-75121 Uppsala, Sweden – Sweden
9 Technical University Hamburg Harburg [Hamburg] – Germany
10 Deutsches Elektronen-Synchrotron [Hamburg] (DESY) – Notkestraße 85 D-22607 Hamburg, Germany
11 Abteilung für Hochempfindliche Röntgenspektroskopie, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany – Germany
12 Deutsches Elektronen-Synchrotron [Hamburg] (DESY) – Notkestraße 85 D-22607 Hamburg, Germany
13 Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands – Netherlands

The combination of soft-ionisation techniques, such as electrospray ionisation, with radio-mass spectrometric techniques, including radiofrequency ion filtering and trapping, is a powerful tool for studying biomolecules like proteins and DNA in the gas phase, free from solvent interference. Activating these isolated biomolecules with UV, VUV or X-rays from synchrotron sources helps us to gain more insight into their intrinsic properties.
A detailed understanding of DNA nucleotides, and the different dissociation mechanisms involved in radiation damage can help explain the photoprotection mechanisms in DNA. In this context, soft X-ray absorption being element specific makes it particularly ideal to explore the resonant photo-absorption at the C, N, O and P inner-shell edges. Moreover, to obtain a full picture, it is crucial to investigate the role of the sugar and phosphate moieties and whether their presence near the nucleobases affects the photoabsorption and the stability of the system. In this study, near-edge X-ray absorption mass spectrometry experiments were performed at UE52_PGM Ion Trap end station at the BESSY II synchrotron on a protonated oligonucleotide containing all four DNA bases-guanine, cytosine, adenine and thymine-linked via a sugar- phosphate backbone. Measurements were taken at the C, N, O K-edges and the P L-edge. The resulting data offer insights into

---

[*] Speaker

[†] Corresponding author: aarathi.nair@desy.de

fragmentation mechanisms and resonant electronic transitions within the nucleotides, contributing to a deeper understanding of DNA's radiation response at the molecular level.

Modeling and design of materials and surfaces for the improvement of their catalytic activity

Yako Irusta *† [1], Héctor Lozano [2], Guillermo Revilla [2], Manuel Alcamí [1,3,4], Fernando Aguilar-Galindo [1,3], Sergio Díaz-Tendero [1,3,5]

[1] Universidad Autonoma de Madrid – Spain
[2] Repsol Technology Lab, Móstoles, 29935 Madrid – Spain
[3] Institute of Advanced Research in Chemical Sciences (IAdChem) – Spain
[4] Instituto Madrileño de Estudios Avanzados en Nanociencias (IMDEA-Nanociencia) – Spain
[5] Condensed Matter Physics Center (IFIMAC) – Spain

One of the most trending topics in renewable energy sources has been green energy production and storage, as well as the sustainable production of related chemicals. To achieve efficient energy production, it is necessary to investigate alternative materials with improved properties. Understanding the structure and electronic properties of materials and surfaces is key to enhancing their catalytic activity. In this context, numerous investigations are being carried out to find new materials that can produce high catalytic activity. From surface stability to nanoparticle modeling, we have deeply studied the properties of various catalytic candidates for industrial purposes using Density Functional Theory methods. We have performed several analysis such as charge density distribution, electronic density of states and adsorption energies for a variety of reactants and materials. We have determined surface stability and nanoparticle structure for further adsorption studies. Reaction pathways and coordinates were also investigated to obtain transition states of certain reactions. In this communication we will show promising recent results of surfaces activity and in-depth understanding of their properties to enhance the catalytic activity of these materials. We will unveil relevant conclusions for their applications in industrial processes.

---

[*] Speaker

[†] Corresponding author: yako.irusta@inv.uam.es

Recent progress on solid-state mid infrared lasers in the 2-3 μm range

Lauren Guillemot * [1], Pavel Loiko [1], Rémi Soulard [1], Ji Eun Bae [1], Simone Normani [1], Liza Basyrova [1], Kirill Eremeev [1], Alain Braud [1], Jean-Louis Doualan [1], Patrice Camy [1]

[1] Centre de recherche sur les Ions, les MAtériaux et la Photonique – Université de Caen Normandie, Ecole Nationale Supérieure d'Ingénieurs de Caen, Commissariat à l'énergie atomique et aux énergies alternatives, Centre National de la Recherche Scientifique – France

Abstract: This communication reviews the latest advances in thulium and erbium ion-doped solid-state lasers emitting in the mid-infrared in the 2-3 μm region. Such lasers emitting in the near mid-infrared domain are in high demand nowadays because of their applications in molecules sensing, especially pollutants or biological molecules. Two transitions are presented, the 3H4→3H5 thulium ions around 2.3 μm and the 4I11/2→4I13/2 of erbium ions around 2.8 μm. In thulium ions, a better understanding of the interaction mechanisms between ions and original pumping schemes and cavity design have enabled record efficiencies. At 2.8μm, a study on the host matrix for erbium ions have paved the way for ultrafast efficient lasers.

1. Efficient lasing around 2.3 μm enabled by better understanding of the 3H4→3H5 transition of thulium ions

Ultrafast laser sources emitting in the "molecular fingerprint" near-mid-infrared spectral range of 2-3 μm are attractive for molecular spectroscopy, environmental sensing, medicine, multi-photon imaging and pumping of nonlinear frequency converters accessing emission wavelengths up to 20 μm (1). In particular, the emission around 2.3 μm falls into the atmospheric transparency window and spectrally overlaps with absorption lines of carbon monoxide (CO), formaldehyde (H_2CO), methane (CH_4) and glucose ($C_6H_{12}O_6$) molecules. A well-known approach to generate laser emission at such wavelengths is to employ Cr2+-doped II-VI chalcogenides (ZnS, ZnSe). However, the fabrication of these crystals of good optical quality is complicated. Recently, another type of laser based on the 3H4 → 3H5 transition (2) of thulium ions have been investigated. The main difficulty for achieving ~2.3 μm emission from Tm3+-doped materials is that the lifetime of the upper laser level (3H4) is much shorter than that of the lower-lying meta stable 3F4 terminal state. The 3H4 lifetime is strongly quenched by the cross-relaxation (CR) process for adjacent Tm3+ ions, 3H4+3H6 →3F4+3F4, and the CR is enhanced with increasing of the Tm3+ doping level (3). Thus, in terms of Tm3+ concentration, there exists a trade-off between a long upper laser level lifetime and strong pump absorption. Under the conventional pumping scheme (λP ~ 0.8 μm; see Fig. 1(a)), the 2.3 μm laser emission suffers from a strong competition with the high-gain 1.9 μm (3F4 → 3H6) emission transition, especially at high Tm3+ doping levels.

Recently, our group proposed novel pump schemes for 2.3 μm Thulium lasers which can help to overcome these limitations. This pump scheme is relying on a photon avalanche mechanism (4)

---

[*] Speaker

populating the intermediate (3F4) metastable level by the combination of a resonant ESA (3F4 → 3F2,3 or 3F4 → 3H4) and a very efficient CR, so that the 3F4 terminal level further acts as an "effective" ground-state. The physical advantage over conventional pumping is the suppression of the unwanted 1.9 μm (3F4 → 3H6) laser transition because of the resonant ESA from the 3F4 state; it also leads to lower thermal loading. Technically, pumping at 1-1.1 μm is easier because of the availability of high-brightness and powerful pump sources (e.g., Yb fiber lasers), which is a clear advantage for waveguide lasers. The proposed approach of UC pumping has allowed to demonstrate record power at 2.3 μm in fiber (5), in continuous wave and in mode-locked regime (6) and enables original cavity designs (7).

Moreover, we demonstrated that solid-state lasers based on Tm3+-doped materials and operating on the 3H4 → 3H5 transition are excellent candidates for compact, simple, highly efficient and wavelength tunable coherent light sources in the short-wave infrared spectral range. Contrary to the well-established considerations, they are rather tolerant to such key parameters of the gain media as their phonon spectra (8) and Tm doping levels. This is because of a relatively complex physical nature of the 3H4 → 3H5 laser scheme affected by both cross-relaxation and energy-transfer upconversion between neighboring Tm3+ ions (9). We proved that highly-efficient lasing at 2.3 μm (with a slope efficiency exceeding the Stokes limit) can be achieved even in high-phonon energy Tm3+-doped crystals at moderate doping levels leading to a notable self-quenching of the upper laser level by CR. The evidence of one-to-two pump process associated with the energy-transfer upconversion refilling the upper laser level and probably with the gain at the vibronic sideband of the 3F4 → 3H6 transition is shown.

2. Ultrabroad emission around 2.8 μm thanks to new laser gain media for erbium ions

Further in the mid-infrared, around 2.8 μm, transition of erbium ions have raised interest due to their vast application potential in medicine (10), molecular spectroscopy, and frequency down-conversion toward mid-infrared spectral range. The aforementioned Er3+ laser transition has a self-terminating nature, as the luminescence lifetime of the terminal laser manifold is usually longer than that of the upper laser level (with the latter being subject to a significant multiphonon non-radiative relaxation). In low-phonon media, energy-transfer upconversion (ETU) process, 4I13/2 + 4I13/2 → 4I9/2+4I15/2, recycling the energy of electronic excitation and mitigating the bottle-neck effect, enables the true continuous-wave 2.8-μm laser operation Er ions. An in-depth study on the possible host matrices has revealed promising materials for ultrafast laser operation. In particular, crystals with ion clustering such as CaF2 enhance the energy-transfer processes among the activator ions (11), crystals with a disordered structure (12) allow to access to broad band gain, and first result have been obtained in mode locked regime with fiber lasers (13).

3. Conclusion

To conclude, we report on the recent advances in 2.3 μm Thulium lasers and 2.8 μm Erbium lasers. In thulium, a better understanding of interaction mechanisms between ions and with the matrix, and original pumping schemes and cavity designs have enabled record efficiencies from various fluoride and oxide materials. In erbium, an in-depth study of the possible host matrixes have paved the way for ultrafast laser operation.

References:

(1) A. Garnache, A. Liu, L. Cerutti, and A. Campargue, "Intracavity laser absorption spectroscopy with a vertical external cavity surface emitting laser at 2.3 μm: Application to water and carbon dioxide," Chem. Phys. Lett. **416**(1-3), 22–27 (2005).
(2) J. F. Pinto, L. Esterowitz, and G. H. Rosenblatt, "Tm3+:YLF laser continuously tunable be-

tween 2.20 and 2.46 μm," Opt. Lett. **19**(12), 883-885 (1994).
(3) K. van Dalfsen, S. Aravazhi, C. Grivas, S. M. García-Blanco, and M. Pollnau, "Thulium channel waveguide laser with 1.6 W of output power and$\sim$ 80% slope efficiency". *Optics letters*, **39**(15), 4380-4383.

(4) M. F. Joubert, S. Guy, and B. Jacquier, "Model of the photon-avalanche effect," Phys. Rev. B **48**(14), 10031-10037 (1993).
(5) A. Tyazhev, F. Starecki, S. Cozic, P. Loiko, L. Guillemot, A. Braud, F. Joulain, M. Tang, T. Godin, A. Hideur, and P. Camy, "Watt-level efficient 2.3 μm thulium fluoride fiber laser". *Optics Letters*, **45**(20), 5788-5791 (2020).
(6) A. Tyazhev, J.E. Bae, M. Gaulke, P. Loiko, J. Heidrich, M. Golling, S. Idlahcen, L. Guillemot, T. Godin, P. Camy, U. Keller, and A. Hideur "Upconversion-pumped femtosecond thulium laser at 2309 nm mode-locked by a GaSb-based SESAM". *Optics Express*, **32**(9), 15093-15105 (2024).
(7) H. Dupont, T. Lenfant, L. Guillemot, P. Loiko, X. Delen, P. Loiseau, B. Viana, T. Georges, P. Georges, P. Camy, and F. Druon "High-power 2.3 μm Tm: YLF laser with intracavity upconversion pumping by a Nd: ASL laser at 1051 nm". *Optics Letters*, **49**(8), 2093-2096 (2024).
(8) P. Loiko, E. Kifle, L. Guillemot, J.L. Doualan, S. Starecki, A. Braud, M. Aguiló, F. Díaz, V. Petrov, X. Mateos, and P. Camy, "Highly efficient 2.3 μm thulium lasers based on a high-phonon-energy crystal: evidence of vibronic-assisted emissions". *Journal of the Optical Society of America B*, **38**(2), 482-495 (2021).
(9) P. Loiko, R. Soulard, L. Guillemot, A. Tyazhev, G. Brasse, J.-L. Doualan, A. Braud, A. Hideur, F. Druon, and P. "Efficient Tm:LiYF4 Lasers at 2.3μm: Effect of Energy-Transfer Upconversion". *IEEE Journal of Quantum Electronics*, **55**(6), 1-12 (2019).
(10) C. Bader, and I. Krejci, "Indications and limitations of Er: YAG laser applications in dentistry". *American journal of dentistry*, **19**(3),178 (2006).
(11) V. Jambunathan, S. Normani, P. Loiko, K. Veselský, L. Basyrova, A. Benayad, P. Camy, A. Hideur, and A. Braud "Effect of doping concentration on the performance of 2.8 μm Er: CaF2 lasers". *Optics Letters*, **50**(6), 2081-2084 (2025).
(12) S. Normani, P. Loiko, Z. Pan, E. Dunina, L. Fomicheva, A. Kornienko, A. Braud, W. Chen, U. Griebner, V. Petrov, and P. Camy, "Spectroscopy and 2.8 μm laser operation of disordered Er: CLNGG crystals". *Optics Letters*, **48**(10), 2567-2570 (2023).
(13) S. Normani, S. Idlahcen, P. Loiko, S. Hatim, P.-H. Hanzard, A. Rodrigues De Paula, L. Guillemot, T. Godin, T. Berthelot, S. Cozic, S. Poulain, E. Koivusalo, M. Guina, P. Camy, and A. Hideur "2.8-μm polarization-maintaining Er fiber laser mode-locked by a GaSb-based SESAM". *Optics Express*, **32**(9), 15106-15114 (2024).

Associative ionisation of H(1s)+H(ns): a semi-classical description

Pierre Guichard *† 1, Paul-Antoine Hervieux‡ 1, Xavier Urbain§ 2

1 Institut de Physique et Chimie des Matériaux de Strasbourg – université de Strasbourg, Centre National de la Recherche Scientifique, Matériaux et Nanosciences Grand-Est, Réseau nanophotonique et optique, Réseau nanophotonique et optique – France

2 Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain – Belgium

Associative ionisation (AI), a fundamental atomic collision process, plays a crucial role in atomic physics, plasma physics and astrophysics, contributing to the ionisation of atoms and the formation of molecules. In this work we study AI in low-energy hydrogen atom collisions, in particular the reaction H(1s) + H(ns) $\rightarrow$ H_2^+ + e- with $2 \leq n \leq 10$, using a semi-classical approach. We extend the Duman-Shmatov-Mihajlov-Janev (DSMJ) model (1) to include short-range interactions and multistate transitions, thereby improving the predictive capabilities for low-energy AI processes. While the approach in (2) provided valuable insights, it relied on highly sophisticated quantum mechanical calculations and is therefore limited to collisions with $n \leq 4$. In contrast, our semi-classical model reproduces the results of (2) very well at significantly lower computational cost and gives a better intuition of the underlying physical processes, making it a more efficient alternative while remaining in good agreement with the experimental data (3). This work not only aims at reproducing these results, but has also been used to explore the regime with $n \gg 1$.

References:

(1) R. K. Janev and A. A. Mihajlov, *Excitation and de-excitation processes in slow collisions of Rydberg atoms with ground-state parent atoms*, Physical Review A **20**, 1890–1904 (1979).
(2) J. Hörnquist et al., *Associative ionization in collisions of H+ + H- and H(1s) + H(ns)*, Physical Review A **108**, 052811 (2023).
(3) F. Brouillard and X. Urbain, *Associative Ionisation in Low Energy Collisions*, Phys. Scr. T **96**, 86 (2002).

---

[*] Speaker

[†] Corresponding author: pierre.guichard@ipcms.unistra.fr

[‡] Corresponding author: paul-antoine.hervieux@ipcms.unistra.fr

[§] Corresponding author: xavier.urbain@uclouvain.be

Exploring proton microsolvation in noble gas complexes through data-driven modeling

María Judit Montes De Oca-Estévez * [1], Rita Prosmiti [1]

[1] Institute of Fundamental Physics, IFF-CSIC – Spain

For a long time, space was considered a hostile environment characterized by its extreme conditions, where the formation of any molecular system was rather unlikely or even impossible. However, advances in molecular astrophysics field have made it possible to discard this false belief with the detection of more than 300 molecules in the interstellar medium (ISM) (1). With each new discovery, answering the question "What comes next?" becomes increasingly complex, as the number of potential species continues to grow. One of the most revolutionary discoveries within this field is the detection of the noble gas hydride cations complexes, HeH^+ and ArH^+ (2), indicating the need of a much better understanding of noble gas chemistry. In this context, the main objective of our research is tis to identify trends and develop models by performing computational quantum chemistry calculations. These calculations aim to provide astrochemically relevant data for the identification of new small finite-size Ng_nH^+ clusters (3,4,5,6), which could potentially be detected in the ISM. To achieve this, we explore simplified sum-of-potentials approaches by employing kernel-based machine-learning potential models trained on CCSD(T)-F12 data. These models included expansions of up to two-body, three-body, and four-body terms to represent the underlying interactions as the number of Ng atoms increases. The most accurate model is then used for EP optimization calculations. When compared to *ab initio* data, this approach has provided valuable insights into the nature and balance of the underlying interactions that influence the growth process of these clusters. The results obtained here provide a deeper insight into the energy and structural properties of Ng_nH^+ clusters, while also clarifying the interactions that occur during the microsolvation of protons by argon atoms. These findings contribute to a comprehensive understanding of the energetic stability and structural characteristics, as wellas to the assignment of growth patterns observed experimentally.

---

[*] Speaker

18 Jun 2025

Ultrafast dynamics of ionized molecules and molecular clusters in the gas phase

Sergio Díaz-Tendero *† 1,2,3

[1] Universidad Autonoma de Madrid – Spain
[2] Institute of Advanced Research in Chemical Sciences (IAdChem) – Spain
[3] Condensed Matter Physics Center (IFIMAC) – Spain

When ionizing radiation interacts with molecules or clusters in the gas phase, it induces their ionization and excitation. This phenomenon is observable regardless the type of ionizing radiation used, including collisions with multiply charged ions, energetic synchrotron radiation, or intense laser fields. The direct consequence of this interaction is the formation of molecular species with high degrees of excitation and ionization, leading to fragmentation into two or more positively charged moieties which repeal each other, the so-called Coulomb explosion. However, alongside this process, a variety of other phenomena occur in competition; these include intramolecular charge transfer (1,2), hydrogen migration (3-7), roaming of a neutral fragment (8) or even intermolecular reactivity in a cluster forming larger species (9-12). These reactions are triggered by ionization and excitation and can only be observed if they occur within the femtosecond timescale characteristic of the Coulomb explosion. In this communication I will review the main characteristics of these unexpected processes presenting some recent examples.

References

(1) P. Rousseau et al. *Sci. Adv.* **7**, eabg9080 (2021).
(2) F. Aguilar-Galindo et al. *Phys. Chem. Chem. Phys.* **26**, 7638 (2024).
(3) S. Maclot et al. *J. Phys. Chem. Lett.* **5**, 3903 (2013).
(4) N.G. Kling et al. *Nat. Commun.* **10**, 2813 (2019).
(5) M. McDonnell et al. *J. Phys. Chem. Lett.* **11**, 6724 (2020).
(6) F. Ota et al. *Phys. Chem. Chem. Phys.* **23**, 20174 (2021).
(7) T. Kuraoka et al. *J. Phys. Chem. A* **128**, 1241 (2024).
(8) D. Mishra et al. *Phys. Chem. Chem. Phys.* **24**, 433 (2022).
(9) B. Oostenrijk et al. *Phys. Chem. Chem. Phys.* **21**, 25749 (2019).
(10) P. Rousseau et al. *Nat. Commun.* **11**, 3818 (2020).
(11) S. Ganguly et al. *Commun. Chem.* **5**, 16 (2022).
(12) O. Licht et al. *Angew. Chem. Int. Edit.* **62**, e202218770 (2023).

---

[*] Speaker

[†] Corresponding author: sergio.diaztendero@uam.es

VUV Photoionization of cyano substituted PAHs

Madhusree Roy Chowdhury *† [1,2], Gustavo Garcia-Macias [3], Christine Joblin [4], Helgi Hrodmarsson [5], Dusan Bozanic [6], Jean-Christophe Loison [7], Laurent Nahon [2]

[1] University of Kassel – Germany
[2] Synchrotron SOLEIL – Synchrotron SOLEIL – France
[3] Synchrotron SOLEIL – Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UR1 – France
[4] Institut de recherche en astrophysique et planétologie (IRAP) – CNRS, Université de Toulouse Paul Sabatier, CNES – France
[5] Laboratoire Interuniversitaire des Systèmes Atmosphériques – Université Paris-Est Créteil Val-de-Marne - Paris 12 – France
[6] Department of Physical Chemistry [Vinča Institute] – Serbia
[7] ISM – Institut des Sciences Moléculaires, The French National Centre for Scientific Research, Bordeaux, France – France

Polycyclic Aromatic Hydrocarbons (PAHs) are ubiquitous in the interstellar medium (ISM), accounting for a major source of carbon and playing an important role in the physics and chemistry of the ISM. The signature of their existence in the interstellar and circumstellar environments had been confirmed for a long time by the observance of the aromatic infrared emission bands (AIBs). Although their presence is well acknowledged, direct detection of the PAHs is notoriously difficult due to their highly symmetric structures. In such cases, searches focused on substituted PAHs have led to the identification of cyanonaphthalene (CNN) isomers in the cold TMC-1 (1). In the interstellar and circumstellar medium, the PAHs are exposed to VUV radiation. Upon absorbing the VUV radiation, the PAHs relax via ionization and photodissociation in competition to radiative cooling (including IR emission). Ionization leads to gas heating by thermalization of emitted electrons (2). Free PAHs are produced by evaporation of carbonaceous very small grains (C-VSGs) under VUV irradiation.

The experiments were carried out at the VUV undulator based DESIRS beamline of the SOLEIL Synchrotron radiation facility. The molecular beam chamber is coupled to a double imaging photoelectron photoion coincidence spectrometer DELICIOUS 3 (3). The state-selected fragmentation pattern obtained for the CNN cation and further comparison with the unsubstituted PAH sheds light on the photostability of cyano-substituted PAHs. The present measurements can also be used to estimate the contribution of PAHs to the gas heating of the ISM since the experimentally obtained kinetic energy distributions of the photoelectrons as a function of photon energy can be employed to model the photoelectric heating for any incoming photon flux spectral distribution (4). In addition to studying the contribution of free PAHs to gas heating, the project has been extended further to study the photoelectron spectroscopy of nanoparticles of PAHs.

---

[*] Speaker

[†] Corresponding author: madhusree@physik.uni-kassel.de

References
(1) B. A. McGuire *et. al.* *Science* **371,** 1265 (2021)
(2) O. Berné *et. al.* *A&A* **667,** A159 (2022)
(3) G. A. Garcia *et. al.* *Rev. Sci. Inst.* **84,** 053112 (2013)
(4) M. Roy Chowdhury *et. al.* *ApJ* **963**, 29 (2024)

Interparticle Coulombic electron capture beyond the virtual photon approximation

Jan Šenk *† [1,2], Vincent Graves [3], Jimena D. Gorfinkiel [3], Přemysl Kolorenč [2], Nicolas Sisourat [1]

[1] Sorbonne Université, CNRS, Laboratoire de Chimie Physique – Matière et Rayonnement, UMR 7614, F-75005 Paris – LCPMR – France
[2] Institute of Theoretical Physics, Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, 180 00 Prague – Czech Republic
[3] School of Physical Sciences, The Open University – Walton Hall, Milton Keynes, MK7 6AA, United Kingdom

Interparticle Coulombic Electron Capture (ICEC) is an environment-enabled electron capture process where the excess energy is released by ionization or excitation of a neighboring particle. Both the capturing particle and the neighbor can be atoms, molecules, or ions. ICEC was theoretically predicted in 2009 (1, 2) and is expected to be significantly more efficient than competing photorecombination. It has since been studied using analytical approximations (3), theoretical models (4), and *ab initio* calculations (5). It has yet to be experimentally observed.

Our work has focused on improving the previously used asymptotic approximation, which has been shown to severely underestimate the ICEC cross section when the distance between the two particles is comparable to their size. The asymptotic approximation treats the whole process as two independent events: virtual photorecombination at the capturing particle and virtual photoionization of the neighbor. These are linked by the transfer of the excess energy. It therefore neglects the correlation between the electrons of the two particles and especially the possibility of an electron transfer from the neighbor to the capturing particle. We have proposed an analytical model of the electron transfer mechanism of ICEC, and benchmarked it with *ab initio* R-matrix scattering calculations for several systems (6).

In comparison to the original asymptotic approximation, our model improved the agreement with the *ab initio* results at relevant inter-particle distances while keeping its simplicity. The model ICEC cross section can be evaluated simply using tabulated properties of the participating particles.

References

(1) K. Gokhberg, L. S. Cederbaum, J. Phys. B: At. Mol. Opt. Phys. 2009, 42, 231001.
(2) K. Gokhberg, L. S. Cederbaum, Phys. Rev. A 2010, 82, 052707.
(3) A. Molle, O. Zatsarinny, T. Jagau, A. Dubois, N. Sisourat, J. Chem. Phys. 2023, 158, 134306.
(4) F. M. Pont, A. Bande, L. S. Cederbaum, J. Phys.: Condens. Matter 2016, 28, 075301.
(5) N. Sisourat, T. Miteva, J. D. Gorfinkiel, K. Gokhberg, L. S. Cederbaum, Phys. Rev. A 2018, 98, 020701.
(6) J. Šenk, V. Graves, J. D. Gorfinkiel, P. Kolorenč, N. Sisourat, J. Chem. Phys. 2024, 161, 174113.

---

*Speaker
†Corresponding author: jan.senk@sorbonne-universite.fr

High-harmonic generation in solids from a high-energy fiber laser system

Anastasiia Mikhneva *† [1,2], Djamila Boukhaoui [3], Saïd Idlahcen [2], Jonathan Houard [3], Ivan Blum [3], Thomas Godin [2], Leo Guiramand [2], Foued Amrani [4], Frédéric Gerome [4,5], Fetah Benabid [4,5], David Gauthier [6], Hamed Merdji [7], Willem Boutu [6], Angela Vella [3], Ammar Hideur [2]

[1] Groupe de physique des matériaux – Université de Rouen Normandie, Institut national des sciences appliquées Rouen Normandie, Centre National de la Recherche Scientifique, Institut de Recherche sur les Matériaux Avancés – France
[2] Complexe de recherche interprofessionnel en aérothermochimie – Université de Rouen Normandie, Institut national des sciences appliquées Rouen Normandie, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR6614 – France
[3] Groupe de physique des matériaux – Université de Rouen Normandie, Institut national des sciences appliquées Rouen Normandie, Centre National de la Recherche Scientifique, Institut de Recherche sur les Matériaux Avancés – France
[4] GLOphotonics S.A.S. – GLOphotonics S.A.S. – France
[5] XLIM – Université de Limoges, Centre National de la Recherche Scientifique – France
[6] Laboratoire Interactions, Dynamiques et Lasers (ex SPAM) – Université Paris-Saclay, CY Cergy Paris Université – France
[7] Laboratoire d'optique appliquée – École Nationale Supérieure de Techniques Avancées, Ecole Polytechnique, Centre National de la Recherche Scientifique – France

High harmonic generation (HHG) is a well-established process used to produce light in the extreme ultraviolet (EUV) range. High harmonics of the driving laser frequency can be generated by tightly focusing a high-energy laser into a nonlinear medium, such as a gas, solid, or plasma. Historically, HHG has been primarily driven by lasers with wavelengths around 800 nm. However, mid-infrared (mid-IR) lasers have gained increasing interest due to their ability to extend the harmonic cutoff, enabled by the quadratic wavelength scaling of the ponderomotive energy (1). Additionally, mid-IR drivers offer improved damage thresholds, making them attractive for high-intensity applications.
Optical Parametric Chirped-Pulse Amplification (OPCPA) and Optical Parametric Amplifier (OPA) systems have proven effective in achieving these results, but their inherent complexity highlights the need for more compact, efficient, and scalable EUV generation techniques (1, 2, 3). In this context, ultrafast mid-IR fiber lasers have emerged as a promising alternative for HHG. However, their pulse energies remain limited to the nanojoule range, posing a challenge for generating high-flux EUV radiation (4).

In this work, we demonstrate high-order harmonic generation in bulk crystals using a high-energy fiber laser system operating near 1550 nm. The system delivers few-cycle pulses with durations below 50 fs, microjoule-level pulse energies, and a repetition rate of 660 kHz. This is achieved by

---

*Speaker

†Corresponding author: anastasiia.mikhneva@univ-rouen.fr

combining a high-energy chirped-pulse amplifier featuring erbium-doped fibers, initially producing 600 fs pulses, with a post-compression stage based on an Argon-filled hollow-core photonic crystal fiber (HC-PCF) (5, 6). The compressed pulses are then focused into an MgO crystal to generate EUV high-order harmonics. The EUV spectra were measured using a home-built spectrometer and analyzed as a function of the crystal orientation relative to the laser polarization, and the driving laser intensity. As a result, harmonic orders up to the 31st were detected, with a total photon flux reaching 5 × 10 photons per second.

References:
(1) S. Ghimire, et al. "Observation of high-order harmonic generation in a bulk crystal, " Nat. Phys.7, 138-141 (2011).
(2) V. E. Nefedova, et al. "Enhanced extreme ultraviolet high-harmonic generation from chromium-doped magnesium oxide," Appl. Phys. Lett., 118, 20 (2021).
(3) S. Gholam-Mirzaei, et al. "High harmonic generation in ZnO with a high-power mid-IR OPA," Appl. Phys. Lett., 110, 6 (2017).
(4) D. Franz, et al. "All semiconductor enhanced high-harmonic generation from a single nanostructured cone," Sci. Rep., 9, 5663 (2019).
(5) F. Amrani, et al. "Low-loss single-mode hybrid-lattice hollow-core photonic-crystal fibre," LSA, 10, 7, (2021).
(6) D. Boukhaoui, et al. "High-harmonic generation in solids from a high-energy fiber laser system." APL Photonics 10.2 (2025).

Single-particle mass analysis : nanospray ionization coupled to a linear charge detection array ion trap spectrometer

Tessa Reinert *† [1], Lilou Duplantier [1], Sylvain Maclot [1], Guillaume Montagne [1], Christian Clavier [1], Xavier Dagany [1], Clothilde Comby-Zerbino [1], Michel Kerleroux [1], Rodolphe Antoine [1]

[1] ILM - Institut Lumière Matière – Université Claude Bernard Lyon 1, CNRS, Institut Lumière Matière (iLM), UMR 5306, 10 rue Ada Byron, 69622 Villeurbanne Cedex, France – France

Mass spectrometry (MS) is a worldwide established analyitical strategy for the rapide and reliable identification and characterization of biomolecules. For instance, MS can be used to understand the structure, biology and interactions of protein samples, which is essential for the advancement of life sciences and can significantly contribute to the development of new therapies and vaccines (1). However, conventional MS, which measures the mass-to-charge ratio (m/z) of an ensemble of ions, faces upper limits around the MDa masses. Recently, charge-detection mass spectrometry (CDMS) has emerged as a key MS-based technique that allows single-particle analysis in the megadalton range (2,3). By measuring the mass of individual particles, CDMS can reveal subtle differences in protein stoichiometry within macromolecular complexes, differences that are typically lost in conventional ensemble measurements.
We have developed an in-house CDMS that integrates an eight-tube detector array capable of measuring the induced current from ions passing through it. From this charge image, it is possible to determine both the m/z and the charge of each particle that has been previously ionized by a nano-electrospray source. This instrument can therefore generate and characterize multiply charged macromolecular complexes from a liquid solution. The high mass range, from MDa to GDa, of the CDMS allows the analysis of large biomolecules in their native structures. In addition, we have installed conical electrodes at both ends of the array to trap the ions. Trapping induces the multiplication of measurements of each particle, reducing charge and mass uncertainties.

This state-of-the-art design was applied to viruses, DNA and RNA structures to determine their molecular weight distribution. The instrument was able to record ions in transmission mode (linear array) and ion trapping mode, allowing precise measurements of time-of-flight (related to m/z) and charge at the single particle level. Measurement of the molecular weight distribution of these biomolecules provided important information about their composition and heterogeneity and can be relevant for their assembly and disassembly processes, for exemple (4).

The instrument can also be easily switch to a trapping mode, were trapped single ions oscillate back and forth through the detector array, allowing multiple charge measurements. We have successfully trapped noroviruses and adenoviruses for tens of ms, reducing charge uncertainties from 10 charges

---

[*] Speaker

[†] Corresponding author: tessa.reinert@univ-lyon1.fr

for linear array transmission to ± 1.5 charges for ions trapped for 20 ms. In addition, the ability to switch between trapping and transmission modes facilitates calibration and improves mass accuracy.

Single-particle mass analysis uses a linear array for fast data acquisition and ion trapping for improved mass and charge resolution. The instrument has enabled the characterization of a wide range of high molecular weight bioparticles.

(1) S. Zoratto et al, 2023, Viruses, doi: 10.3390/v15061361
(2) D.Z. Keifer et al, 2017, Analyst, doi: 10.1039/C7AN00277G.
(3) R. Antoine et al, 2020, Rapid Comm Mass Spectrometr, doi: 10.1002/rcm.8539.
(4) L.F. Barnes et al, 2022, Anal. Chem. doi: 10.1021/acs.analchem.1c02439.

A new electrochemical property of hydrogen-bonded solids at 10 K: negative charge transport by proton-hole transfer

Kensei Kitajima *† [1,2], Yoichi Nakai [3], Masashi Tsuge [1], Hiroshi Hidaka [1], Wmc Sameera [4], Naoki Watanabe [1]

[1] Institute of Low Temperature Science, Hokkaido University – Japan
[2] National Institute of Science and Technology Policy, MEXT – Japan
[3] Radioactive Isotope Physics Laboratory, RIKEN Nishina Center – Japan
[4] Department of Chemistry and Molecular Biology, University of Gothenburg – Sweden

The electrochemical behavior of water ice is of particular interest in astrophysical chemistry and atmospheric chemistry. Much research has shown that ice can be a p-type semiconductor due to the conduction of excess protons along the hydrogen bonds (1). Although the proton transfer mechanism is well understood, knowledge on proton–hole transfer (PHT) involving proton abstraction by anions such as OH^- remains limited. To gain the knowledge on PHT, experimental and computational studies of H_2O, H_2S, and NH_3 solids have been performed (2-4). In recent years, negative charge transport in H_2O ice at temperatures below 50 K, which is governed by PHT, has been demonstrated (2,3). This phenomenon is observed when ice is simultaneously exposed to UV light and electrons. The negative charge transport is confirmed by measuring the negative current at the metal substrate beneath the ice. Using a combination of photostimulated desorption and resonance-enhanced multi-photon ionization (PSD-REMPI) methods, we verified the role of surface OH radicals in PHT (3). Quantum chemical calculations also indicate that potential energies of the ice–metal system, including the OH^- in ice, decrease gradually along with the location of OH^- from the vacuum–ice to ice–metal boundary. We propose that once OH adsorbate captures an electron on ice surface, the surface OH^- trigger the flow of negative current by the sequential PHT in ice.

In addition to ice, we have recently examined other typical hydrogen-bonded molecules, H_2S and NH_3 (4). Similarly to the case of ice, negative currents were observed in H2S and NH3 solids simultaneously exposed to electrons and 193 nm UV at 10 K. Using the PSD-REMPI methods, the role of HS radicals in PHT in H_2S solids was also confirmed. In bilayer H_2S/H_2O and NH_3/H_2O solids, where H_2O is the lower layer, a significant negative current was observed only in the NH_3/H_2O solid. The behavior is attributed to the exothermic proton abstraction reaction of NH_2^- from H_2O at the bilayer interface. In contrast, no negative current was observed in the H_2S/H_2O solid since the proton abstraction reaction of HS^- from H_2O is endothermic. These result strongly support the PHT mechanisms in these solids at 10 K. Through these experiments, we, for the first time, demonstrated PHT-induced electrochemical behavior in hydrogen-bonded solids other than ice.

In this talk, we discuss our recent findings on PHT-induced electrochemical properties of hydrogen-bonded solids, including H_2O, H_2S, and NH_3 at 10 K.

---

*Speaker

†Corresponding author: kitajima@nistep.go.jp

References

(1) D. Marx, 2006, ChemPhysChem, 7, 1848.
(2) N. Watanabe, W.M.C. Sameera, H. Hidaka, A. Miyazaki, A. Kouchi, 2019, Chem. Phys. Lett., 737, 136820.
(3) K. Kitajima, Y. Nakai, W.M.C. Sameera, M. Tsuge, A. Miyazaki, H. Hidaka, A. Kouchi, N. Watanabe, 2021, J. Phys. Chem. Lett., 12, 704.
(4) K. Kitajima, Y. Nakai, M. Tsuge, N. Watanabe, 2024, J. Phys. Chem. Lett., 12, 704.

Chirality Effects and Electronic Properties of LuI3-Based Nanotubes

Costanza Borghesi * [1,2], Giacomo Tanzi Marlotti [3,4], Enric Canadell† [4],
Giacomo Giorgi‡ [2,5,6], Riccardo Rurali§ [4]

[1] CNR-NANO, Via Campi 213/A, 41125 Modena – Italy
[2] Department of Civil Environmental Engineering (DICA), Università degli Studi di Perugia, Via G. Duranti 93, 06125 Perugia – Italy
[3] Department of Physics "Aldo Pontremoli", Università degli Studi di Milano, Via Celoria 16, I-20133 Milano – Italy
[4] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, 08193 Bellaterra – Spain
[5] CNR-SCITEC, 06123 Perugia – Italy
[6] CIRIAF - Interuniversity Research Centre, University of Perugia, Via G. Duranti 93, 06125 Perugia – Italy

This study employs density functional theory to investigate the electronic structure of nanostructures based on the hexagonal layers of LuI_3. Both bulk and slabs with one to three layers exhibit large, indirect bandgaps. These layered structures can be used to generate various families of nanotubes. Two distinct chiralities of semiconducting nanotubes were examined, with the direct or indirect nature of their optical gaps dependent on the chirality and a simple explanation for this dependence can be provided based on band folding. Notably, a metastable form of armchair LuI_3 nanotubes can be achieved by rearranging the structure, causing some iodine atoms to segregate toward the center and form chains of dimerized iodines. These nanotubes, with an Lu_2NI_5N backbone, are predicted to be metallic and resistant to Peierls distortion. The iodine chains in the interior are weakly bound to the backbone, allowing for their potential removal to produce a new series of neutral Lu_2NI_5N nanotubes, which may exhibit unique magnetic properties. Given that the LuI3 structure is found in many lanthanide and actinide trihalides, tuning the optical, transport, and possibly magnetic properties of these nanotubes opens up an exciting opportunity for future experimental research.

---

*Speaker

†Corresponding author: canadell@icmab.es

‡Corresponding author: giacomo.giorgi@unipg.it

§Corresponding author: rrurali@icmab.es

Photoelectron quantum state tomography

Hugo Laurell [1,2], Sizuo Luo [1], Robin Weissenbilder [1], Mattias Ammitzböll [1], Edoardo Boati [1], Gustav Arvidsson [1], Hugo Söderberg [1], Shahnawaz Ahmed [3], Leon Petersson [4], Christoph Dittel [1,5], Daniel Finkelstein-Shapiro [6], Mathieu Gisselbrecht [1], Cord Arnold [1], Anton Frisk-Kockum [3], Andreas Buchleitner [5], Eva Lindroth [4], Anne L'huillier [1], David Busto *† [1]

[1] Lund University – Sweden
[2] University of California [Berkeley] – United States
[3] Chalmers University of Technology [Göteborg] – Sweden
[4] Stockholm University – Sweden
[5] Freiburg University – Germany
[6] Universidad Nacional Autónoma de México = National Autonomous University of Mexico – Mexico

The photoelectric effect is a fundamental quantum phenomenon that is used in various spectroscopy and microscopy techniques. The advent of attosecond science has opened the possibility to study the dynamics of photoemission on its natural time scale by measuring the amplitude and phase of the emitted photoelectron wave packets. This description of the photoelectron is appropriate when it can be described by a wave function, i.e. the photoelectron quantum state is pure. In contrast, if the photoelectron is described a statistical mixture, the density matrix formalism must be used to accurately describe the photoelectron quantum state. In many cases, photoionisation leads to the formation of an entangled ion-photoelectron bipartite system. In this case, if only the photoelectron is measured, it's reduced quantum state is described by a statistical mixture. As a result, standard attosecond interferometric methods cannot correctly describe the photoelectron. In this talk, I will discuss how to experimentally measure the photoelectron density matrix using a combination of ultrashort extreme ultraviolet pulses and spectrally tailored infrared laser fields. Using our quantum state tomography protocol, KRAKEN, we measure the density matrix describing photoelectrons originating from helium and argon atoms. Our measurements show that, in helium, photoelectrons are in a pure state that can be described by a wave function. In contrast, in argon, the purity of the photoelectron is strongly reduced due to ion-photoelectron entanglement induced by spin-orbit interaction. Potential extensions of the KRAKEN protocol to speed up the measurement process will also be discussed.

---

[*] Speaker

[†] Corresponding author: david.busto@fysik.lth.se

Measurement of Charge Exchange Cross Sections in Collisions of Ne^{8+} Ions with H_2 and He

Pufang Ma * [1,2], Tianming Meng [1], Mingxuan Ma [1], Hao Yin [1], Yijiao Wu [1], Xu Tan [1], Bingsheng Tu [1], Yaming Zou [1], Amine Cassimi† [2], Baoren Wei‡ [1]

[1] Institute of Modern Physics, Key Laboratory of Nuclear Physics and Ion-Beam Application (MOE), Fudan University – China
[2] Centre de recherche sur les Ions, les MAtériaux et la Photonique – Université de Caen Normandie, Institut Rayonnement Matière de Saclay (DRF), Ecole Nationale Supérieure d'Ingénieurs de Caen, Centre National de la Recherche Scientifique, Institut de Recherche sur les Matériaux Avancés – France

Charge exchange (CX) or electron capture (EC), which predominates all other types of inelastic collisions at impact velocities less than one atomic unit ($<$ 25keV/u), affects the ionization balance and results in spectral line emissions in astrophysical regions or fusion devices. It is one of the most significant processes that occur during collisions between highly charged ions (HCIs) and atomic or molecular species. Neon ions are considered an important component of the solar wind and are one of the primary impurities appearing at various relative energies and ionization stages in plasmas. For these applications, there is a strong demand for accurate data on the cross sections of EC.
The experiment was performed on the 150 kV highly charged ion collision platform at Fudan University to measure the total and state-selective EC cross sections (1,2). The HCIs beam, generated by an ECR ion source, was directed to collide with neutral gases in a gas cell to measure the total EC cross sections. Through a thorough analysis of the systematic uncertainties associated with the experimental setup and measurement procedures, the experimental error for the absolute cross sections of single electron capture (SEC) was found to be less than 9%. For the relative state-selective EC cross sections, measurements were performed using a cold target recoil ion momentum spectroscopy (COLTRIMS) apparatus (3).

The total and *n*-resolved state-selective cross sections of SEC between Ne^{8+} ions and H_2 and He were measured in the impact energy of 2.8 and 40 keV/u, covering velocities corresponding to fast solar wind and coronal mass ejections. The total EC cross section is crucial for assessing the probability of capturing electrons, however, it does not elucidate electron transition mechanisms in detail. By normalizing the relative state-selective SEC cross sections to the absolute total SEC cross sections, the absolute state-selective SEC cross sections of Ne^{8+} colliding with He and H_2 gases were determined over a wide energy range(4).

The present CX cross section data fill the gaps in the relevant collision energy range, which can

---

[*] Speaker
[†] Corresponding author: amine.cassimi@ganil.fr
[‡] Corresponding author: brwei@fudan.edu.cn

be valuable for establishing accurate plasma models to analyze the interstellar gas distribution and to interpret the observation of the diffuse soft X-ray emission.

References
(1) J. Han et al., *APJS.* **(2021)** 253, 6.
(2) T. Meng et al., *New J. Phys.* **(2023)** 25, 093026.
(3) Z.H. Xia et al., *APJ.* **(2022)** 933, 207.
(4) P. Ma et al., *APJ*. **(2025)** 978, 6.

Moving with the Times: Electronic-Decay-Process Spectra Including Nuclear Degrees of Freedom

Alexander V. Riegel * 1,2, Elke Fasshauer† 1,2,3

1 Institute of Physical and Theoretical Chemistry [Tübingen] – Germany
2 Center for Light-Matter Interaction, Sensors Analytics (LISA+) [Tübingen] – Germany
3 Physical and Theoretical Chemistry Laboratory [Oxford] – United Kingdom

Breakthroughs in femto- to attosecond experiments (1) have made possible the time-resolved measurement of nuclear and electronic motion, the very heart of chemistry. We can now directly observe how photoinduced rearrangements of electrons can significantly change nuclear degrees of freedom in atoms and molecules, up to dissociation events, as for example in Auger–Meitner decay or Interparticle Coulombic Decay (ICD) (2). Interpreting such observations, though, requires reliable theoretical models for these ultrafast processes.
Having already established an analytical framework for the calculation and analysis of spectra for electrons which are emitted during electronic decay processes (3) focussing solely on the electronic states, we now significantly advance our approach by the inclusion of nuclear dynamics (4). The combination of Fano's theory of resonances (5) with the Born–Oppenheimer approximation and time-dependent perturbation theory yields improved analytical expressions. These permit a deeper understanding of the interaction between electronic and nuclear motion in these processes and enable us to extract characteristic energy spacings and lifetimes from interference patterns.

To illustrate the merits of our improved description, we examine several systems with known eigenstates by calculating time-resolved kinetic-energy spectra and analyzing signal distributions, peak shapes and oscillation patterns. The selected cases encompass different bound states and also final states with a repulsive potential (6), which are important for ICD processes that result in a Coulomb explosion.

References:
(1) I. Orfanos, I. Makos, I. Liontos, E. Skantzakis, B. Förg, D. Charalambidis, P. Tzallas, APL Photonics 2019, 4, 080901.
(2) L. S. Cederbaum, J. Zobeley, F. Tarantelli, Phys. Rev. Lett. 1997, 79, 4778.
(3) E. Fasshauer, L. B. Madsen, Phys. Rev. A 2020, 101, 043414.
(4) A. V. Riegel, E. Fasshauer, Phys. Rev. A 2025, 111, 013112.
(5) U. Fano, Phys. Rev. 1961, 124, 1866.
(6) A. V. Riegel, E. Fasshauer, 2025, in preparation.

---

[*] Speaker
[†] Corresponding author: elke.fasshauer@gmail.com

Posters

1	A Monte Carlo approach for electron impact on molecules under local plasma approximation: For application to electron beam induced deposition process	Jureddy Chinmai Sai
2	Collision and coagulation of rare-gas atoms in helium nanodroplets by zero-point averaged dynamics	Bonhommeau David
3	Dissociative electron Attachment to Iodomethane	Saha Samrat
4	Dynamics of alkali atoms and clusters in helium nanodroplets by zero-point averaged dynamics	Bonhommeau David
5	Electronic structure calculations for electron driven reactivity of PH+	Jonas Tibor
6	ESPECDAS – A Database of Ab Initio Calculated Transitions in Small Molecules for Identification of Potential DIB Carriers	Gatt Michael
7	First principles construction of Newns-Anderson Hamiltonians for hydrogen chemistry at surfaces	Hertl Nils
8	Fragmentation of naphthalene and quinoline dications produced under oxygen ion impact	Srivastav Sumit
9	From perturbation theory to model potential for alkali rare gas molecules	Gervais Benoit
10	Hydrogen atom diffraction through free-standing single-layer graphene	Guichard Pierre
11	Isotope effects for Hydrogen scattering on W(110) surface	Bombín Escudero Raúl
12	Laboratory experiments for chemical kinetics at very low temperature: a new viewpoint	Durif Olivier
13	Low temperature collisional cross-sections of molecules of astrophysical interest	Jureddy Chinmai Sai
14	Measuring ion-induced biomolecular fragmentation using a Velocity Map Imaging spectrometer	Bourgeteau Antonin
15	Multi-Channel Quantum Scattering Calculation of fine structure quenching and electronic excitation exchange between ultracold meta-stable Sr+ and ground state Rb atoms	Jonas Tibor
16	Payloads for plasma characterization and mass spectroscopy in planetary ionosphere	Raghunandanan Sreeja
17	Reaction Mechanisms Between Atomic Carbon C(3Pj) and Cyclopentadiene Using Synchrotron-Based Photoionization Mass Spectrometry and Theoretical Quantum Calculation	Bourgalais Jeremy
18	State-selected dissociation of formic acid upon carbon core-shell excitation studied by Auger/photoelectron photoion coincident spectroscopy at PLEIADES/SOLEIL	Milosavljevic Aleksandar
19	Tailoring perovskites through chemical substitution for "à la carte" optoelectronic properties: a Quantum Chemistry approach	Aguilar-Galindo Fernando
20	The influence of water on the modified amino acid phosphotyrosine: A multiscale study using soft X-ray radiation	Leroux Juliette
21	The vibrational structure of excited RbHe molecule	Gervais Benoit
22	Theoretical investigation of excited electronic states of the KAr molecule	Gervais Benoit
23	Theoretical study of electron-molecule collisions for plasma simulations	García-Muñoz Alejandro L.
24	Vibrational properties and photodegradation of 4-Nitroguaiacol isolated in cryogenic matrices: An experimental and theoretical approach	Camacho Granados Daniel
25	Watching a disulide bond break in real time	Robertson Patrick
26	Towards the identification of structure and function of biological ions: a native MS based approach	Meloottayil Vinitha

A Monte Carlo approach for electron impact on molecules under local plasma approximation: For application to electron beam induced deposition process

Chinmai Sai Jureddy *† [1,2], Juraj Fedor [3], Ivo Utke [1]

[1] Swiss Federal Laboratories for Materials Science and Technology [Thun] – Switzerland
[2] Institut de Physique de Rennes – Université de Rennes, Centre National de la Recherche Scientifique – France
[3] J. Heyrovský Institute of Physical Chemistry – Czech Republic

Focused Electron Beam Induced Deposition (FEBID) is an advanced 3D nanofabrication technique in which an electron beam locally decomposes adsorbed precursor molecules, resulting in a material deposition at the irradiated site. The process is controlled by a complex interplay of surface phenomena, including adsorption, desorption, dissociation, and diffusion. The deposition rate and composition are influenced by the electron-induced dissociation cross-sections, molecular fragmentation pathways, and other contributing mechanisms. To support the continuum-scale modeling of FEBID, which requires dissociation cross-sections, we have developed a theoretical model that yields ionization cross-sections and fragmentation yields. The model employs a Monte Carlo approach to compute the mean energy loss distribution of electrons interacting with molecules under the local plasma approximation. This distribution is then used to derive ionization cross-sections. Additionally, by convolving the mean energy loss distribution with a parabola-shaped internal energy distribution in molecules upon electron impact, we obtain the total internal energy deposition profile. Based on a thermochemical fragmentation model, we estimate the resulting fragmentation yields. We will present the model results in comparison with experimental data and discuss its application to FEBID.

---

*Speaker

†Corresponding author: chinmai-sai.jureddy@univ-rennes.fr

Collision and coagulation of rare-gas atoms in helium nanodroplets by zero-point averaged dynamics

Brendan Fixot [1], Elsa Louaas [1], David Bonhommeau * [2]

[1] Laboratoire Analyse, Modélisation et Matériaux pour la Biologie et l'Environnement – Université d'Évry-Val-d'Essonne, Institut de Chimie - CNRS Chimie, Université Paris-Saclay, Centre National de la Recherche Scientifique, CY Cergy Paris Université – France
[2] Laboratoire Analyse, Modélisation et Matériaux pour la Biologie et l'Environnement – CNRS – France

The experimental capture of rare-gas atoms (RG) by helium nanodroplets in pickup chambers is well known to yield the formation of rare-gas clusters within the droplet. In the present study, the coagulation process of these rare-gas atoms is investigated by zero-point averaged dynamics (ZPAD) where He-He and He-RG interactions are described by pseudopotentials to take into account the quantum nature of helium atoms without entering the complexity of time-consuming quantum calculations. Simulations were performed for RG + $RG_n He1000$ ($n = 1$ to 4) collisions for all rare-gas atoms, including radon (1). Comparisons with TDDFT, RPMD, and former ZPAD-like simulations carried out on argon atoms emphasize the enhanced suitability of the current method. Despite the lack of superfluidity in the model, coagulation was found to be very efficient for heavy rare-gas atoms (Xe and Rn). Moreover, when coagulation does not occur, the projectile is not immobile but roams in a limited region of the droplet. The low computational cost of ZPAD approaches is expected to make them appropriate to tackle the dynamics of larger droplets and embedded heliophilic species.

Reference:

(1) B. Fixot, E. Louaas, and D. A. Bonhommeau, J. Chem. Phys. **161**, 044307 (2024).

---

*Speaker

Dissociative electron Attachment to Iodomethane

Samrat Saha * [1,2], Juraj Fedor [1], Pamir Nag [1]

[1] J. Heyrovský Institute of Physical Chemistry of the CAS – Czech Republic
[2] Dept. of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University – Czech Republic

Low-energy electron molecule scattering often leads to the formation of anionic states via resonant electron capture, which may result in dissociative electron attachment (DEA). In Prague, we have a unique DEA-VMI (velocity map imaging) spectrometer combined with a trochoidal electron monochromator (1) which is capable of recording the VMI images at electron energies as low as 0.01 eV. Here we present our results on DEA to iodomethane (CH_3I) using this spectrometer. We observed three DEA fragments: I^-, CH_2^- and CH^-. The strongest fragments I- shows a peak at zero eV as well as a weaker peak at around 8.5 eV incident electron energies. The second strongest fragment, CH_2^-, produces a peak around 8.5 eV and another weaker peak around 4 eV.

To get the angular and kinetic energy distributions we measured the velocity map images of I^- fragments around the zero eV resonance and also around the second resonance at 8.5 eV. For ions exhibiting resonance near zero eV, a strong angular distribution is observed, with ions predominantly formed in the forward and backward directions. However, for 8.5 eV resonance we saw isotopic angular distribution. We also measured the kinetic energy distribution of the I- fragments for all the four different incident electron energies and it showed a peak around 0.07 eV.

This is the first time that the dynamics of any DEA process close to 0 eV has been probed by VMI, we are not aware of any other electron collision VMI setup which could reach such low energies in a controlled way.

References
P. Nag, M Polášek, J. Fedor (2019) *Phys. Rev. A,* **99**, 052705.

---

*Speaker

Dynamics of alkali atoms and clusters in helium nanodroplets by zero-point averaged dynamics

David Bonhommeau * [1], Yannick Jeanvoine [2]

[1] Laboratoire Analyse, Modélisation et Matériaux pour la Biologie et l'Environnement – CNRS – France
[2] Laboratoire Analyse, Modélisation et Matériaux pour la Biologie et l'Environnement – Université d'Évry-Val-d'Essonne, Institut de Chimie - CNRS Chimie, Université Paris-Saclay, Centre National de la Recherche Scientifique, CY Cergy Paris Université – France

Unlike rare-gas atoms, alkali atoms colliding with helium nanodroplets remain at the surface of the droplet due to their heliophobic nature. Although TDDFT simulations can model the creation of vortices and capillary waves upon collision of alkali atoms (eg, Cs) with the droplet, these methods do not predict any capture of these atoms at experimental velocities (400 m/s) but the piercing of the droplet. On the contrary, recent zero-point averaged dynamics (ZPAD) simulations have demonstrated that collisions of Cs atoms on He1000 could yield the impurity capture at velocities up to 500 m/s even if this capture may be preceded by a transient submersion of the alkali atom (1). This heliophobic behavior of alkali atoms is however expected to vanish for sufficiently large clusters. As an example, sodium clusters were experimentally found to sink into the droplet for sizes exceeding 21 atoms (2). A parallelized version of our program has been developed in order to tackle alkali submersion in helium nanodroplets close to experimental sizes ($N <$ 100 000 He atoms) by ZPAD simulations. First results on these calculations will be discussed and compared with experimental expectations.

References:

(1) D. A. Bonhommeau, J. Chem. Phys. **161**, 184302 (2024).
(2) L. An der Lan, P. Bartl, C. Leidlmair, H. Schöbel, R. Jochum, S. Denifl, T. D. Märk, A. M. Ellis and P. Scheier, J. Chem. Phys. 135, 044309 (2011).

---

*Speaker

Electronic structure calculations for electron driven reactivity of PH^+

Tibor Jonas * [1,2,3], Nadia Bouloufa-Maafa [4], Olivier Dulieu [4], Jonathan Tennyson [5,6], Ioan Schneider [6,4], Andrea Orban [7], Janos Zsolt Mezei [1]

[1] HUN-REN Institute for Nuclear Research – Hungary
[2] University of Debrecen – Hungary
[3] Université Paris-Saclay – Université Paris-Saclay, CNRS, Laboratoire Aimé Cotton, 91405 Orsay, France – France
[4] Université Paris-Saclay, CNRS, Laboratoire Aimé Cotton – Université Paris-Saclay, CNRS, Laboratoire Aimé Cotton, 91405 Orsay, France – France
[5] University College London, Dept. of Physics and Astronomy – United Kingdom
[6] Université le Havre Normandie, CNRS, Laboratoire Ondes et Milieux Complexes – Université le Havre Normandie, CNRS, Laboratoire Ondes et Milieux Complexes – France
[7] HUN-REN Institute for Nuclear Research – Hungary

Measurements of trace gases in the atmosphere of Venus indicate the presence of phosphine (PH_3) and other phosphorus hydrides (1). Thus the chemistry of PH_3 is assummed to play an important role in the atmosphere of Venus. The simplest among phosphorus-hydrides is the PH and its cation, PH^+. The electron impact recombination of molecular cations is in the heart of the molecular reactivity in cold ionised media (2). To study the dissociative recombination (DR) of PH^+ we need to calculate the potential energy curves (PEC) followed by nuclear dynamical calculations. For a consistent dynamical model all PECs and couplings have to be calculated at the same level of theory. We have performed the calculation of the PECs of PH^+ with the multireference configuration interaction (MRCI) method including the 2,4 $\Sigma-$, 2,4 $\Sigma+$, 2,4 Π, 2,4 - states followed by the determination of the PECs of PH with the same approach for 1,3 $\Sigma-$, 1,3 $\Sigma+$, 1,3 Π, 1,3 states with MOLPRO (3) and R-matrix method (4). These PECs provide the possible reaction paths for DR, either through autioionizing doubly excited valence states or mono-excited Rydberg states. The calculated cross sections and rate coefficients will be useful in the interpretation of the observations of ESA EnVision mission (2031). The work is supported by the EKÖP-24-3-II-DE-347 University Research Scholarship Program of the Ministry for Culture and Innovation from the source of the National Research, Development and Innovation Fund.

References:

(1) J. S. Greaves et al., Nature Astronomy 5 (2021)
(2) I. F. Schneider, O. Dulieu, J. Robert, eds., EPJ WoC 84 (2015)
(3) H.-J. Werner et al. WIREs Compute. Mol. Sci. 2, 242 (2012)
(4) J. Tennyson, Phys. Rep. 491, 29 (2010)

---

*Speaker

ESPECDAS – A Database of Ab Initio Calculated Transitions in Small Molecules for Identification of Potential DIB Carriers

Michael Gatt *† [1], Gabriel Schöpfer [1], MilanOnčák [1]

[1] Department of Ion Physics and Applied Physics, University of Innsbruck – Austria

Diffuse Interstellar Bands (DIBs) are a long-standing mystery in astrophysics, with over 500 absorption features detected in the interstellar medium, yet only one carrier, C60+, has been ultimately identified (1). The nature of most DIB carriers remains unknown, but small molecules, particularly transition metal compounds, are considered promising candidates (2). Identifying these carriers requires accurate spectroscopic data, which is often lacking for many potential species, requiring ad hoc exploratory calculations (3).

Our new Electronic Spectroscopy Database for Astrochemical Studies (ESPECDAS) aims to be a comprehensive resource, collecting *ab initio* calculated transitions using Multireference Configuration Interaction (MRCI, (4)) for small molecules relevant to the astrochemical space. The database focuses on diatomic molecules, particularly transition metal oxides, carbides, nitrides, and hydrides, as well as selected triatomic species such as SiO2 and TiO2. The database will include both neutral and charged species, with energy ranges up to 7 eV. The underlying calculations will be mostly automated, employing methods for automated selection of the active space within the multireference calculations.

Users will be able to explore all calculated transitions for a given molecule, including electronic excitations, ionization, and electron attachment processes. A key feature allows users to search for transitions corresponding to a specific DIB by filtering based on electronic or vibrational transitions. By providing systematic spectroscopic data, ESPECDAS aims to serve as a tool for helping to identify potential DIB carriers.

References

(1) E. K. Campbell, M. Holz, D. Gerlich, J. P. Maier, *Nature*. **523** (2015).
(2) M. Juanes, S. Jin, R. T. Saragi, C. van der Linde, A. Ebenbichler, N. Przybilla, M. Ončák, M. K. Beyer, *J. Phys. Chem. A*. **128**, 1306–1312 (2024).
(3) A. Ebenbichler, M. Ončák, N. Przybilla, H. R. Hrodmarsson, J. V. Smoker, R. Lallement, A. Farhang, C. Bhatt, J. Cami, M. Cordiner, P. Ehrenfreund, N. L. J. Cox, J. Th. van Loon, B. Foing, *Astronomy and Astrophysics*. **695**, A212 (2025).
(4) H. Werner, P. J. Knowles, *J. Chem. Phys.* **89** (1988).

---

[*] Speaker

[†] Corresponding author: Michael.Gatt@uibk.ac.at

First principles construction of Newns-Anderson Hamiltonians for hydrogen chemistry at surfaces

Nils Hertl *† 1,2, Zsuzsanna Koczor-Benda 1, Reinhard J. Maurer 1,2

1 Department of Chemistry, University of Warwick, CV4 7AL, Coventry, UK – United Kingdom
2 Department of Physics, University of Warwick, CV4 7AL, Coventry, UK – United Kingdom

Adsorption of atomic and molecular hydrogen on surfaces is the gateway to many important chemical processes in nature. For realistic simulations of adsorption of hydrogen atoms or molecules at metal surfaces, or light-driven desorption, accurate couplings between the gaseous particles and the substrate's electronic states are essential. However, their acquisition and utilisation for molecular dynamics is not straightforward if one wishes to account for the spectral properties of the substrate.

Here, we present a pragmatic protocol based on the projection-operator diabatisation (POD) approach (1, 2) that allows the acquisition of electronic couplings between adsorbate and metallic substrates. Since the POD approach relies on partitioning the states of the total system into an adsorbate subset and a substrate subset, it has primarily been applied to weakly interacting systems, whilst its applicability to strongly interacting systems has been questioned (1, 2). Here, we will present a strategy to overcome this issue and apply our workflow to strongly interacting systems, i.e., atomic hydrogen adsorbed on metal surfaces. We show that we can verify the validity of this projection by reconstructing the projected density of states of the adsorbate and extracting electron-tunnelling rates. We further connect these electronic couplings to vibrational relaxation rates due to electron-hole pair (ehp) excitation. This allows us to compare our acquired results to reflective IR measurements and pump-probe experiments (3, 4) and computational reference data acquired from density functional theory based time-dependent perturbation theory (5).

Finally, we outline how this approach allows for the construction of Newns-Anderson Hamiltonians, the standard model in gas-surface dynamics, to describe the interaction of a single adsorbate state with a continuum of metal states.

(1) S. Ghan, C. Kunkel, K. Reuter and H. Oberhofer, J. Chem. Theory Comput., 2020, 16, 7431–7443.
(2) S. Ghan, E. Diesen, C. Kunkel, K. Reuter and H. Oberhofer, J. Chem. Phys., 2023, 158.
(3) C. Lamont, B. Persson and G. Williams, Chemical Physics Letters, 1995, 243, 429–434.
(4) D. Palecek, G. Tek, J. Lan, M. Iannuzzi and P. Hamm, J. Phys. Chem. Lett., 2018, 9, 1254–1259.
(5) R. J. Maurer, M. Askerka, V. S. Batista and J. C. Tully, Phys. Rev. B, 2016, 94, 115432.

---

[*] Speaker

[†] Corresponding author: Nils.Hertl@warwick.ac.uk

Fragmentation of naphthalene and quinoline dications produced under oxygen ion impact

Sumit Srivastav *† [1], Sylvain Maclot [1], Alicja Domaracka [1], Patrick Rousseau‡ [1]

[1] Université de Caen Normandie – Normandie Université, Normandie Univ., ENSICAEN, UNICAEN, CEA, CNRS, CIMAP, 14000 Caen, France – France

For more than a decade, the ionization and subsequent fragmentation of polycyclic aromatic hydrocarbons (PAHs) and their nitrogen analogues (PANHs) upon interaction with various source of perturbation has been a topic of study due to its presence in a large variety of environments, such as planetary atmospheres and the interstellar medium. In situ measurements by the Cassini Huygens mission has demonstrated the importance of the 10 to 100 keV energy range of charged ion collisions in the dynamics of Titan's ionosphere.

Here, we attempt to understand the dissociation of naphthalene dications (Nap^{2+}) and quinoline dications (Q^{2+}) created under the impact of O^{6+} ion at 48 keV energy. The experiment is performed using COLIMACON setup (a time-of-flight mass spectrometer) at the ARIBE platform of GANIL, Caen, France. In total mass spectra, we observe that the m/z 51 amu ($C_8H_2^{2+}$) is one of the dominant fragments corresponding to the C_2H_2 /HCN-loss fromparent dications, which is contrary to the earlier observation of photodissociation study. We find that the intensity ratio of $C_8H_6^{2+}$ to the respective parent dication is 2.7 times higher in case of quinoline than that of naphthalene, indicating the first instance of prompt HCN-loss from Q^{2+} in our study.

Using the coincidence map of time-of-flight (TOF) of first fragment versus the TOF of second fragment, the branching ratio (BR) of the two-body breakup, H-loss and C_2H_2-loss from both molecules dications and with an additional HCN-loss from Q^{2+} are determined. For Q^{2+} , BR of two-body breakup, H-loss and C2H2 -loss are comparatively suppressed, however, the HCN-loss is higher than the corresponding C2H2 -loss from Nap^{2+} . The combined contribution of C2H2 and HCN-loss from Q^{2+} is even more significant than the C2H2 -loss from Nap^{2+}. It suggests that in present collision system, Q^{2+} is comparatively more likely to fragment through C2H2 /HCN-loss, and when it comes to H-loss, Nap^{2+} is relatively more prone than Q^{2+}. Interestingly, in H-loss, we have also identified the complete H-stripping process through the dissociation channels C_3^+ /C_7^+ and C_2N^+/C_7^+ from Nap and Q, respectively. In addition to dicationic metastable decay into fragment ion pairs, we have also observed a monocation $C_8H_5^+$ showing a delayed fragmentation into $C_6H_3^{2+}$ ion through C_2H_2 neutral loss.

---

*Speaker

†Corresponding author: sumitsrivastav2708@gmail.com

‡Corresponding author: patrick.rousseau@ganil.fr

From perturbation theory to model potential for alkali rare gas molecules

Benoit Gervais * [1], Julie Douady [2], Erwan Hochard [2]

[1] Centre de recherche sur les Ions, les MAtériaux et la Photonique – Institut Rayonnement Matière de Saclay (DRF) – France
[2] Centre de recherche sur les Ions, les MAtériaux et la Photonique – Université de Caen Normandie – France

We present a derivation of an ab intio model potential (AIMP) based on the Van Vleck Perturbation theory. Our approach provides a formal background for the empirical potential often used to study molecular systems made of one alkali atom interacting with rare gas atoms. In contrast with standard core polarization potential used so far, the use of AIMP, which keeps the nodal structure of the orbitals, allows us to take into account accurately the spin-orbit relativistic correction. Its application to alkali-rare gas diatomic molecules allows us to reproduce rather well the known experimental and the best ab initio calculations at a lower computational cost. In particular, the heavy-element effect, which consists in a magnification of the spin-orbit splitting of the alkali bound to Ar or heavier rare gas, is very well predicted by the model.

---

*Speaker

Hydrogen atom diffraction through free-standing single-layer graphene

Pierre Guichard *† [1], Arnaud Dochain [2], Raphaël Marion [3], Pauline De Crombrugghe De Picquendaele [2], Nicolas Lejeune [2,4], Benoit Hackens [2], Paul-Antoine Hervieux * [1], Xavier Urbain [2]

[1] Institut de Physique et Chimie des Matériaux de Strasbourg – université de Strasbourg, Centre National de la Recherche Scientifique, Matériaux et Nanosciences Grand-Est, Réseau nanophotonique et optique – France
[2] Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain – Belgium
[3] Royal Observatory of Belgium (ROB-ORB) – Belgium
[4] Ephec – Belgium

We report the observation of fast atom diffraction through single-layer graphene. High resolution images have been recorded with hydrogen atoms at kinetic energies ranging from 150 eV to 1200 eV, following the experimental protocol suggested by Brand et al. (1). The commercial suspended graphene samples were characterized using micro-Raman spectroscopy, prior to and after beam exposure for the quantification of defects. When placed on the beam path in ultra-high vacuum, the samples were subjected to high temperature to induce thermal desorption of contaminants. Monocrystalline domains within the illuminated area produced characteristic hexagonal diffraction patterns. A negligible energy loss was recorded by time-of-flight tagging of individual atom detection events, making such an experimental approach suitable for matter-wave interferometry.

Density functional theory calculations with pseudopotentials (2) have been performed to determine the H-graphene interaction potential over the whole unit cell. The total energy of the system was calculated as a function of the position of the hydrogen atom relative to the graphene surface. The energies of the isolated graphene sheet and the hydrogen atom were then subtracted from the total energy of the system. Nice agreement with the calculations of Ehemann et al (3) is found, who used the Self-Consistent Charge-Density Functional Tight Binding method. In particular, our calculations confirm the presence of a long-range potential well reminiscent of the C-H bond. In order to simulate diffraction images, we generate a phase mask by integrating the three-dimensional potential along the coordinate normal to the graphene plane and performing an eikonal treatment of the scattering events.

References:

(1) C. Brand, M. Debiossac, T. Susi, F. Aguillon, J. Kotakoski, P. Roncin, and M. Arndt, New Journal of Physics 21, 033004 (2019)

(2) P. Giannozzi, S. Baroni, N. Bonini, et al., Journal of Physics: Condensed Matter 21, 395502 (2009)

---

[*] Speaker

[†] Corresponding author: pierre.guichard@ipcms.unistra.fr

(3) R. C. Ehemann, P. S. Krstić, J. Dadras, P. R. C. Kent, and J. Jakowski, Nanoscale Research Letters 7:198 (2012)

Isotope effects for Hydrogen scattering on W(110) surface

Raúl Bombín Escudero *† [1]

[1] Institut des Sciences Molecularies - Université de Bordeaux – Université de Bordeaux (Bordeaux, France), Institut des Sciences Moléculaires, The French National Centre for Scientific Research, Bordeaux, France – France

An understanding of the dynamics of hydrogen atom scattering on metal surfaces is of great importance for a number of applications, including catalysis and material science. Of particular interest is the case of tungsten surfaces, as it will be the material of plasma facing components in future fusion reactors. In this study, we investigate the scattering of hydrogen atoms on the W(110) surface, employing both classical and quantum dynamics approaches to elucidate the importance of quantum effects in this system.

The focus of this study is on several key observables, including the sticking probability and diffraction channels, which are used to characterize the scattering process. Furthermore, the vibrational excitation spectra of H atom adsorbed on the tungsten surface is studied at both the semiclassical and quantum levels. This enables the quantification of quantum effects by direct comparison with classical molecular dynamics results(1,2)

References

(1) R. Martin-Barrios *et al.* Phys. Chem. Chem. Phys. **24**, 20813-20819 (2022)
(2) C. Ibarguen Becerra *et al.* Surf. Science. **701** 121678 (2020)

---

*Speaker

†Corresponding author: raul.bombin@u-bordeaux.fr

Laboratory experiments for chemical kinetics at very low temperature: a new viewpoint

Olivier Durif * [1]

[1] Department of Chemistry, KTH, Royal Institute of Technology, Stockholm, Sweden – Sweden

The kinetic increase of gas-phase reactions with decreasing temperature is counter-intuitive, but well established in the scientific literature for almost all chemical systems at very low temperatures (< 100K). This is what has been reported from experimental studies conducted in uniform supersonic flow over the past few decades. (1)
These experimental results are used to feed databases for the modeling of astrochemistry, and recently, a study based on astronomical observations has re-examined the disagreement between some experimental laboratory measurements and theoretical results. (2)

In this presentation, I will review experimental measurements and defend a new reading of the vast majority of laboratory results relevant to the chemistry of the cold interstellar medium. I will show that in these experiments, the reaction signal, monitored following the reactant, is actually driven by the density fall of the adiabatic expansion under the effect of gaseous mixing (3). I will explain why this interpretation has been missed until now and how this controversy can be resolved simply by examining existing data with this new point of view. Finally, I will also discuss new experimental approaches to mitigate this dramatic effect.

In conclusion, with these highlights, I will argue that the question recently asked to scientists: "Can astronomical observations be used to constrain crucial chemical reactions? The case of methoxy" has a positive answer.

Références

(1) 1. A. Potapov, A. Canosa, E. Jiménez, B. Rowe, Uniform Supersonic Chemical Reactors: 30 Years of Astrochemical History and Future Challenges. *Angewandte Chemie International Edition* **56**, 8618–8640 (2017).
(2) N. Balucani, C. Ceccarelli, F. Vazart, F. Dulieu, D. Skouteris, M. Rosi, F. Pirani, E. Bianchi, P. Caselli, C. Codella, Can astronomical observations be used to constrain crucial chemical reactions? The methoxy case. SOLIS XVIII. *Monthly Notices of the Royal Astronomical Society* **528**, 6706–6719 (2024).
(3) O. Durif, Commentary Regarding the CRESU-SIS Experiment: Concerns About the Uniform Supersonic Flow Reactor. ArXiv (2023).

---

*Speaker

Low temperature collisional cross-sections of molecules of astrophysical interest

Chinmai Sai Jureddy * [1], Alberto Macario Farto [1], Myriam Drissi [1], Omar Abedelkader Khedaoui [1], Ian Sims† [1,2]

[1] Institut de Physique de Rennes – Université de Rennes, Centre National de la Recherche Scientifique – France

[2] Institut Universitaire de France – Ministère de l'Education nationale, de l'Enseignement supérieur et de la Recherche – France

Low temperature collisional cross-sections of molecules are important for modelling spectral lines to retrieve the physical conditions of astrophysical environments. The collisional rate coefficients become necessary in non-local thermal equilibrium environments.
Theoretical methods are being developed for calculating the collisional rate coefficients in extra-terrestrial environments (1). The computational demand and complexity increase with increase in the size of the molecule and in addition, the long range interactions between collisional partners are enhanced in low temperature conditions which requires accurate modelling of interaction potentials. This calls for the experimental investigation of these collisional rate coefficients to benchmark the theoretical calculations.

Several experimental methods exist to determine the collisional rates (1). The CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme or reaction kinetics in uniform supersonic flow) technique generates a wall-less collisional environment by gas expansion through convergent-divergent (Laval) nozzles. It can be combined with laser and millimeter-wave techniques to determine absolute collisional cross-sections (2,3). The uniform supersonic flows comprise a cold isentropic core surrounded by boundary layers, which are at different temperatures and complicate the measurements when the rotational transitions are probed directly. To avoid this, a method of producing the molecules of interest through photodissociation of a precursor exclusively in the cold isentropic core was implemented (2). This technique also enables the measurement of collisional cross-sections of exotic or unstable species.

We are interested in measuring low temperature (< 150 K) H_2CO, HCN and HNC collisional cross-section with colliding partners He, N_2 and CO for astrophysical applications. For H2CO, tetrahydrofuran, 2,3-dihydrofuran, and oxetane are tested as photodissociation sources for H_2CO at 193.3 nm in a supersonic jet expansion. A chirped pulse millimeter wave spectrometer is used to detect the H2CO and to retrieve collisional cross-section in uniform flows. For HCN and HNC production in cold core, vinyl cyanide used in previous experiments of Hays et al., 2022 (2) will be used. The collisions of interest are with heavy colliders N_2 and CO. To improve the S/N, Laval nozzles working for N_2 at low pressures are designed and tested and will be used for studying collisional cross-sections.

---

*Speaker

†Corresponding author: ian.sims@univ-rennes.fr

References

(1) Roueff E et al 2013 *Chem. Rev.* **13.12** 8906 8938.
(2) Hays, B.M et al 2022 *Nat. Chem.* **14** 811–815
(3) Labiad, H et al 2022 *Phys. Rev A* **105.2** L020802
(4) Hays, B. M et al 2020 J. Quant. Spectrosc. Radiat. Transf.) **250** 107001.

Measuring ion-induced biomolecular fragmentation using a Velocity Map Imaging spectrometer

Antonin Bourgeteau * [1], Alain Méry [2], Jimmy Rangama [3], Jean-Yves Chesnel [4], Violaine Vizcaino [3]

[1] Université de Caen Normandie – Normandie Université – France
[2] Centre de recherche sur les Ions, les MAtériaux et la Photonique – Université de Caen Normandie – France
[3] Centre de recherche sur les Ions, les MAtériaux et la Photonique – Centre National de la Recherche Scientifique – France

With the development of hadrontherapy, a method for treating cancers with ion beams, it is relevant to study the interactions between ion beams and biomolecules such as nucleobases, nucleosides, amino acids or peptides. The interactions between the energetic ions and the biomolecular target leads mostly to ionisation and excitation of the biomolecules. The ionized or excited states can then relax by molecular fragmentation. To better quantify the fragmentation channels and the collision processes, it is interesting to measure the differential cross-sections of the created fragments in both kinetic energy (KE) and emission angle. To do so, a Velocity Map Imaging (VMI) spectrometer initially designed to measure ion-induced electron emission from biologically relevant molecules (1) has been adapted to study fragmentation dynamics.
In the experimental set-up, the pulsed projectile ion beam and the biomolecular target beam produced from an effusive cell cross perpendicularly. The fragments formed in the interaction volume are velocity focused by a multi-electrode VMI spectrometer onto the 2D position sensitive detector (PSD) mounted after a flight tube. The time-of-flight (ToF) arrival signals are used to distinguish the fragments according to their m/q ratio with m and q, the mass and the charge state of fragment respectively. The detector is pulsed in order to image only a specific m/q specie determined by its ToF. To reconstruct the initial velocity vector and deduce both kinetic energy spectra and emission angle we then perform an inverse Abel transform to the image. To improve the mass resolution we have designed a longer flight tube, which allows us to study fragments of complex molecules such as biomolecules that we could not separate before.

In this contribution, we will present the experimental set-up and its characterisation as well as our methodology to retrieve the fragments velocity. In particular, we will discuss the influence of the target beam initial velocity on the images of fragments that leave with a low kinetic energy. Indeed, due to Maxwell-Boltzmann velocity distribution of the target beam, the images are shifted and distorted, presenting a more elliptical shape. A deconvolution method using a Wiener filter has been implemented on the experimental images to remove the influence of the target initial speed with rather satisfactory results. And finally recent results on the different fragmentation pathways of Uracil and Adenine upon 120keV-$Ar^{8}+$collision will be discussed based on the KE spectra measured.

---

*Speaker

Reference:

(1) Nicolas Sens, Michal Ryszka, Jean-Christophe Poully, Alain Méry, Jean-Yves Chesnel, and Violaine Vizcaino. A velocity map imaging spectrometer for measuring absolute differential cross sections for ion-induced electron emission from molecules. *Rev. Sci. Instrum.* 93, 085103 (2022)

Multi-Channel Quantum Scattering Calculation of fine structure quenching and electronic excitation exchange between ultracold meta-stable Sr+ and ground state Rb atoms

Tibor Jonas * [1,2,3], Romain Vexiau [3], Nadia Bouloufa-Maafa [3], Eliane Luc [3], Andrea Orban [4], Olivier Dulieu [3]

[1] HUN-REN Institute for Nuclear Research – Hungary
[2] University of Debrecen – Hungary
[3] Université Paris-Saclay – Université Paris-Saclay, CNRS, Laboratoire Aimé Cotton, 91405 Orsay, France – France
[4] HUN-REN Institute for Nuclear Research – Hungary

Our work is related to ongoing hybrid trap experiments, where usually a single ion is injected in the middle of an atomic gas cloud. We focus on the theoretical modelling of the dynamics of ion-neutral system at ultra low temperature (â‰ª 1K) in order to design ways for their full quantum control. In the experiments alkaline earth ion and alkali atom are used. Due to the laser cooling scheme a metastable d-level of the ion is considerably populated in the experiments, e.g. in the case of 88 Sr+ ion embedded in the ultracold 87 Rb atomic cloud (1) or 138 Ba+ in 6 Li cloud (2, 3). Due to the large internal energy of the ion several inelastic processes can take place, like charge-exchange (CE), fine structure quenching (FSQ) or electronic excitation exchange (EEE).

We perform detailed atomic and molecular structure calculations and we perform dynamical calculations based on the multi-channel quatum scattering (MCQS) description of the collision between an ion and atom. Hund's case (a) potential energy curves, rotational and spin-orbit couplings are involved in our theoretical description.

We determine state-to-state cross sections and rate coefficients, which can be compared to experimental ones.

References

(1) R. Ben-Shlomi, R. Vexiau, Z. Meir, T. Sikorsky, N. Akerman, M. Pinkas, O. Dulieu, R. Ozeri, Phys. Rev. A 102 ,031301(R)

(2) P. Weckesser, F. Thielemann, D. Wiater, A. Wojciechowska, L. Karpa, K.Jachymski, M.

---

*Speaker

Tomza, T.
Walker, T. Schaetz, Nature 600, 429 (2021)
(3) X. Xing, P. Weckesser, F. Thielemann, T. Jónás, R. Vexiau, N. Bouloufa-Maafa, E. Luc-Koenig, K. W.
Madison, A. Orbán, T. Xie, T. Schaetz, O. Dulieu, J. Phys. B:At. Mol. Opt. Phys. 57, 245201 (2024)
(4) T. Jónás, R. Vexiau, N. Bouloufa-Maafa, E. Luc-Koenig, A. Orbán, O. Dulieu, in preparation

Payloads for plasma characterization and mass spectroscopy in planetary ionosphere

Sreeja Raghunandanan *† [1], Anoop C S [1], Muthuamirthambal S [1], Sudharshan Kaarthik [1], Sreehari B N [1], Sreelakshmi Palakkal [1], Sooraj V S [1], Veena C P [1], Vishnumaya A [1], Umesh Ramakant Kadhane‡ [1]

[1] Indian Institute of Space and Science Technology – India

Planetary ionosphere is an excellent environment to study a diverse phenomenon at a large scale. These include, space weather dynamics and associated effects on earth, accelerated atmospheric losses in Mars, extremely dynamic Bow-shock region of Venus or seeding of large organic molecules in the Titan, etc. These and many more multidisciplinary and interdisciplinary problems demand purpose built, space born, in-situ measurement instrumentation. The applications of such research include solar physics, atmospheric sciences, space weather and space asset protection, planetary evolution and even genesis and evolution of molecular seeds of life.

At SPDL, IIST efforts are being made to establish instrumentation capabilities for such research. The work started with investigating the plasma parameters in Low Earth Orbit (LEO) using Advanced Retarding Potential Analyzer for Ionospheric Studies (ARIS) payload. This payload was developed at SPDL and deployed as part of missions launched by the Indian Space Research Organisation (ISRO). The first version, ARIS101F was launched on board the Polar Satellite Launch Vehicle (PSLV) during the PSLV-C45 mission, while the second, upgraded version, ARIS201F was deployed in the PSLV-C55 mission. The Polar Orbiting Experiment Platform (POEM) on PSLV enables cost-effective experimentation by facilitating efficient data transfer and system interfacing. The ARIS payload comprises both electron and ion retarding potential analyzers, designed to measure ionospheric plasma properties. ARIS has successfully collected data over 3000 orbits. Analysis of the Electron Retarding Potential Analyzer (ERPA) and Ion Retarding Potential Analyzer (IRPA) datasets has revealed variations in ion and electron densities, as well as temperature fluctuations across different orbits. Deploying multiple sensors like ARIS across different altitudes and orbits will enhance global space weather monitoring, contributing to improved space asset management and operational readiness.

Building upon the experience of the two ARIS missions, SPDL, IIST was given the responsibility to develop a compact plasma diagnostics package for the upcoming TDS01 geostationary communication satellite mission by the Indian space agency which will use plasma thrusters for the orbit raising and orbit maintenance. The package will be monitoring the health of the plasma engines over the entire life of the satellite. In addition a new project is initiated to develop an orbitrap mass spectrometer future interplanetary missions in order to search for molecules of life outside the boundaries of earth.

---

[*] Speaker

[†] Corresponding author: sreeja.raghunandanan@ganil.fr

[‡] Corresponding author: umeshk@iist.ac.in

Reaction Mechanisms Between Atomic Carbon C(3Pj) and Cyclopentadiene Using Synchrotron-Based Photoionization Mass Spectrometry and Theoretical Quantum Calculation

Mohammed Mounsif Abbes [1], Fabien Goulay [2], Sébastien Le Picard [3], Jeremy Bourgalais *† [4]

[1] Université Gustave Eiffel – Université Gustave Eiffel, Université Gustave Eiffel – France
[2] University of West Virginia – United States
[3] Institut de Physique de Rennes – Université de Rennes, Centre National de la Recherche Scientifique – France
[4] Institut de Physique de Rennes – Centre National de la Recherche Scientifique - CNRS, Université de Rennes I – France

Polycyclic aromatic hydrocarbons (PAHs) are critical intermediates in the combustion of fuels such as gasoline, diesel, and kerosene. However, their incomplete combustion generates carcinogenic compounds harmful to both human health and the environment. Understanding their formation and conversion mechanisms is essential, particularly in the context of plasma-assisted combustion (PAC), a promising technology that uses plasma to enhance combustion efficiency and reduce emissions. PAC leverages the generation of highly reactive species, such as ground-state carbon atoms ($C(^3P_j)$), ions, and radicals, to initiate and sustain combustion under conditions where traditional methods fail, such as in lean or low-temperature environments. These carbon atoms are generated through processes such as the dissociation of hydrocarbons, fragmentation of excited carbon-containing species, and interactions with plasma-generated ions and radicals. Their high reactivity enables unique reaction pathways that influence PAH and soot formation, making them crucial for optimizing combustion efficiency and reducing pollutant emissions. This study focuses on the interaction between atomic carbon and 1,3-cyclopentadiene (CP), a key precursor in PAH growth, to refine chemical kinetic models used in combustion simulations and pollutant formation predictions. The reaction of C + CP was investigated using a synchrotron-based experimental setup at the Advanced Light Source (CA/USA). Pulsed laser photolysis in a gas flow tube initiated the reactions, and the products were ionized using tunable vacuum ultraviolet light, followed by detection via time-of-flight mass spectrometry. This approach allows for the precise differentiation of isobaric and isomeric species, which are compared with theoretical quantum chemical calculations to provide consistent insights into the fundamental reaction mechanisms at play. These findings contribute to a better understanding of PAH formation pathways and support the development of accurate combustion models.

---

*Speaker

†Corresponding author: jeremy.bourgalais@cnrs.fr

State-selected dissociation of formic acid upon carbon core-shell excitation studied by Auger/photoelectron photoion coincident spectroscopy at PLEIADES/SOLEIL

Aleksandar Milosavljevic *† [1], Antoine Gloriod [2], Ayad Bellili [3], Christophe Nicolas [4], Jérôme Palaudoux [5], Majdi Hochlaf‡ [6]

[1] Synchrotron SOLEIL – Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UR1 – France
[2] Université Gustave Eiffel, COSYS/IMSE, 5 Bd Descartes, 77454, Champs Sur Marne, France – Université Gustave Eiffel – France
[3] U. Houari Boumediene des Sciences et Technologies, LTMM – Algeria
[4] Synchrotron SOLEIL – Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UR1 – France
[5] Laboratoire de Chimie Physique - Matière et Rayonnement (LCPMR) – Sorbonne Universite, Centre National de la Recherche Scientifique : UMR7614 – 11 Rue Pierre et Marie Curie 75231 Paris Cedex 05, France
[6] Université Gustave Eiffel, COSYS/IMSE, 5 Bd Descartes 77454 Champs sur Marne, France – Université Gustave Eiffel, COSYS – France

We will present the capabilities of the experimental setup EPICEA available at the PLEIADES beamline at the SOLEIL synchrotron to probe the state-to-state dynamics upon inner-shell single photon ionization. For illustration, we will focus on the processes occurring after removal of an electron from the C 1s of formic acid.
The experimental setup has been developed to perform Auger/photoelectron photoion photoion coincident (PEPIPICO/AEPIPICO) measurements (1-3). It is based on a double toroidal electron analyser (DTA) and a time of flight (TOF) ion detector with 3D focusing capabilities. The detected electron makes a start trigger for the ion TOF.

We will discuss the most recent results dedicated to the investigation of state-selected dissociation of isolated formic acid molecule upon C 1s excitation/ionisation. We have obtained a high resolution C1s NEXFAS of formic acid by measuring total ion yield (TIY) and then acquired several coincident spectra at either resonant photon energies related to C1s excitation or at the energy above the C1s ionisation potential, where the Auger electron kinetic energy distribution was recorded in coincidence with the ion TOF and momenta distribution. Therefore, we could produce good quality AEPICO maps showing strong m/z – electronic state correlation, as well as PIPICO and KERBECO (Kinetic Energy Release Binding Energy COincident) maps resolving dissociation processes and released kinetic energy.

---

[*] Speaker
[†] Corresponding author: aleksandar.milosavljevic@synchrotron-soleil.fr
[‡] Corresponding author: Majdi.hochlaf@u-pem.fr

The experimental results obtained are analysed with the help of advanced *ab initio* electronic structure calculations. These computations consist on the determination of the energetics and the structures of the ionic final species (singly and doubly charged) and intermediates and on the mapping of their multi-dimensional potential energy surfaces. We found that these reactions take place, as expected, in the ground ionic potentials and more intriguing on the electronic excited states potentials after intercrossing, spin-orbit conversions and roaming leading to unexpected obvious products. Therefore, the present work contributes to the profound understanding of the photoinduced dissociation and complex processes associated with the soft x-ray interaction with the important class of chemical compounds possessing -COOH group. Furthermore, the present results could help improve our understanding of the abiotic molecular oxygen production through the ionic pathways upon molecular photodissociation/photoionisation as observed recently after double ionizing SO_2 molecule (4).

References:
(1) Bozek, Miron, Journal of Electron Spectroscopy and Related Phenomena., 204(Part.B): 269-276. (2015).
(2) Liu et al, Scientific Reports., 7: art. n○ 2898. (2017).
(3) Ganguly et al, PCCP - Physical Chemistry Chemical Physics., 24(47): 28994-29003. (2022).
(4) Wallner et al., Sci. Adv. 8, eabq5411 (2022).

Tailoring perovskites through chemical substitution for ”à la carte” optoelectronic properties: a Quantum Chemistry approach.

Fernando Aguilar-Galindo *† 1,2, Cristina Reviejo *

3, Alberto Muzas 3

1 Departamento de Química, Universidad Autónoma de Madrid – Spain
2 Institute for Advanced Research in Chemical Sciences, Universidad Autónoma de Madrid – Spain
3 Departamento de Química-Física Aplicada, Universidad Autónoma de Madrid – Spain

Perovskites are a diverse class of materials with exceptional optical and electronic properties, making them ideal for applications in light-emitting diodes, photodetectors, and solar cells. Their properties can be finely tuned through chemical composition modifications, enabling the rational design of materials for specific technological applications (1).

In this communication, we employ Density Functional Theory (DFT) to investigate the electronic structure and tunability of perovskite materials. We analyze the impact of exact exchange in hybrid functionals (2) and explore how chemical substitutions influence the balance between ionic and covalent bonding, directly affecting the optical band gap. Additionally, we examine the substitution of lead with alternative, less toxic metals, providing insights into the design of environmentally friendly and sustainable perovskites (3). Our findings enhance the understanding of structure-property relationships in perovskites, guiding their optimization for improved optoelectronic performance.

(1) H. Gouadria et al. Submitted
(3) P. Umari et al. Scientific Reports, 4, 4467 (2014)
(2) C. Reviejo et al. In preparation

---

*Speaker
†Corresponding author: fernando.aguilar-galindo@uam.es

The influence of water on the modified amino acid phosphotyrosine: A multiscale study using soft X-ray radiation

Juliette Leroux * [1,2], Jean-Yves Chesnel [3], Carlos Mahecha [4], Aarathi Nair [1], Bart Oostenrijk [5], Laura Pille [5], Florian Trinter [6], Ilchen Markus [2,5], Nicolas Velasquez [6], Lucas Schwob [7], Sadia Bari [5]

[1] The Hamburg Centre for Ultrafast Imaging – Germany
[2] Department of Physics, University of Hamburg – Germany
[3] Centre de recherche sur les Ions, les MAtériaux et la Photonique – Université de Caen Normandie, Institut Rayonnement Matière de Saclay (DRF), Ecole Nationale Supérieure d'Ingénieurs de Caen, Centre National de la Recherche Scientifique, Institut de Recherche sur les Matériaux Avancés – France
[4] Hamburg University of Technology – Germany
[5] Deutsches Elektronen-Synchrotron [Hamburg] – Germany
[6] Fritz-Haber-Institut der Max-Planck-Gesellschaft – Germany
[7] Deutsches Elektronen-Synchrotron [Hamburg] (DESY) – Notkestraße 85 D-22607 Hamburg, Germany

The isolation of biomolecules in the gas phase eliminates all interactions with the solvent, allowing for stepwise control of these interactions by progressively increasing the number of bound water molecules, thereby bridging the gap between isolated molecules and aqueous conditions. A single water molecule can already induce significant structural changes in the molecule, such as the location of the protonation site. Over the past thirty years, efforts have been made to develop experimental techniques for studying hydrated species in the gas phase. Comparing the gas-phase structure with the singly hydrated gas-phase structure provides insight into the influence of molecular water on its properties. In contrast, performing a liquid-phase study allows us to gain insights into the influence of water as a solvent and approach the conditions relevant to biology.

Soft X-ray radiation provides a local probe into the atomic environment based on the electronic excitations of core electrons to unoccupied molecular orbitals, thus capturing both the electronic and geometric structures of the system under investigation. In this multiscale study, we first combined X-ray absorption spectroscopy with tandem mass spectrometry to obtain information about the electronic structure of singly hydrated, protonated phosphotyrosine. We further explore the influence of the solvent on phosphotyrosine by performing liquid-jet photoelectron spectroscopy in the soft X-ray range and extending it to the tender X-ray domain.

In this presentation, I will discuss our results on the electronic and geometrical structures of singly hydrated phosphotyrosine and how they can be compared with the liquid phase structure. Furthermore, I will discuss the influence of the water solvation shell on electron dynamics at the phosphorus K-edge, which highlights the importance of solvent interactions in biomolecular studies.

---

*Speaker

The vibrational structure of excited RbHe molecule

Benoit Gervais * [1], Erwan Hochard [2], Julie Douady [2], Augustin Lecoeur [2]

[1] Centre de recherche sur les Ions, les MAtériaux et la Photonique – Institut Rayonnement Matière de Saclay (DRF) – France

[2] Centre de recherche sur les Ions, les MAtériaux et la Photonique – Université de Caen Normandie – France

Recent experiment of phase-modulated electronic wave packet interferometry revealed high-resolution spectra of excited RbHe molecules (1). We analyse these results with the help of *ab initio* model core polarization potential (AIM-CPP) recently developed to investigate alkali-rare gas molecules (2). We focus here on the 2P1/2, 2P3/2, 2D3/2 and 2D5/2 states correlating asymptotically with the excited 5d Rb configurations, populated by excitation from the 5p 2P1/2 state of the RbHe diatomic molecule. The computed spectrum reproduces quite faithfully the experimental observation. Our analysis shows that the rotational couplings among the 2D states are significant, as shown by the doubling of the 5p 2P1/2 - 5d 2D transitions. This theoretical study on RbHe suggests that the experiment was performed on rotationally cold molecules.

(1) L. Bruder, M. Mudrich and F. Stienkemeier, Phys.Chem.Chem.Phys., **17**, 23877 (2015)
(2) E. Hochard, submitted to International Journal of Quantum Chemistry

---

*Speaker

Theoretical investigation of excited electronic states of the KAr molecule

Benoit Gervais * [1], Erwan Hochard [2], Julie Douady [2], Augustin Lecoeur [2]

[1] Centre de recherche sur les Ions, les MAtériaux et la Photonique – Institut Rayonnement Matière de Saclay (DRF) – France

[2] Centre de recherche sur les Ions, les MAtériaux et la Photonique – Université de Caen Normandie – France

Using *ab initio* model core polarization potential (AIM-CPP) recently developed for alkali-rare gas molecules (1), we investigate the electronic excited states of the KAr molecule. We focus here on the 2Sstates correlating asymptotically with the excited 5d and 7s K atomic configurations. These two states exhibit an avoided crossing and the dynamical couplings play a significant role in the vibrational structure. Our model allows us to compute the potential energy and the dynamical couplings between these two electronic states in the same footing. Our calculations explain rather well the experimental observation reported by Michalak and Zimmermann (2), which reveals a rather irregular structure of the vibrational states. Our calculation shows the potentiality and the accuracy of the AIM-CPP approach for such kind of excited molecules.

(1) E. Hochard, submitted to International Journal of Quantum Chemistry

(2) R. Michalak and D. Zimmermann, Journal of Molecular Spectroscopy **193,** 260–272 (1999)

---

*Speaker

Theoretical study of electron-molecule collisions for plasma simulations

Alejandro L. García-Muñoz * [1,2], Zdeněk Mašín [3], Nicolas Sisourat [4]

[1] Laboratoire de Chimie Physique - Matière et Rayonnement – LCPMR – France
[2] Institute of Theoretical Physics, Charles University – Czech Republic
[3] Institute of Theoretical Physics, Charles University – Czech Republic
[4] Sorbonne Université, CNRS, Laboratoire de Chimie Physique – Matière et Rayonnement, UMR 7614, F-75005 Paris – LCPMR – France

Electron-molecule collisions are crucial to many scientific and technological applications, from atmospheric chemistry to astrophysics and satellite propulsion. A novel example of the latter involves electron collisions with iodine molecule (I2) which can be used as a propellant in satellite propulsion. Indeed, a French start-up successfully launched the first satellite propelled by iodine in 2020 (1), making a significant milestone in electric propulsion technology. Nevertheless, the processes during electron-I_2 collisions are not well understood. This is due to the fact that simulating heavy atoms, such as iodine, in addition to needing to describe a large number of electrons correctly (which is computationally expensive) it is also relevant to include relativistic effects.
The R-matrix approach (2) is the method of choice to study electron-molecule collisions. This approach is efficiently implemented in the UKRmol+ program (3). However, relativistic effects are currently not considered within the R-matrix approach (except for atomic targets). In order to tackle this important issue, Effective Core Potentials (ECPs) (4) have been implemented into the UKRmol+ code. Under this approach, for every atom, core electrons are substituted by a potential which acts over the valence electrons. The latter potentials are built in order to include relativistic effects between the inner electrons. In this project the implementation of ECPs in UKRmol+ was optimized and used in the study of the iodine molecule.

References
(1) D. Rafalskyi, J. M. Martínez, L. Habl, E. Zorzoli Rossi, P. Proynov, A. Boré, T. Baret, A. Poyet, T. Lafleur, S. Dudin, et al., Nature, 2021, 599(7885), 411–415.
(2) P. G. Burke, R-matrix theory of atomic collisions: Application to atomic, molecular and optical processes, Vol. 61, Springer Science & Business Media, 2011.
(3) Z. Mašín, J. Benda, J. D. Gorfinkiel, A. G. Harvey, and J. Tennyson, Computer Physics Communications, 2020, 249, 107092.
(4) M. Reiher and A. Wolf, Relativistic quantum chemistry: the fundamental theory of molecular science, John Wiley & Sons, 2014.

---

*Speaker

Vibrational properties and photodegradation of 4-Nitroguaiacol isolated in cryogenic matrices: An experimental and theoretical approach

Daniel Camacho Granados *† [1], Alejandro Gutiérrez-Quintanilla [2], Karinne Miqueu [2]

[1] Université de Pau et des Pays de l'Adour – IPREM, CNRS-UPPA, Pau, France – Avenue de l'Université - BP 576 - 64012 Pau Cedex, France
[2] Université de Pau et des Pays de l'Adour – IPREM, CNRS-UPPA, Pau, France – France

4-Nitroguaiacol is an aromatic compound detected in the atmosphere as a result of both primary emissions, mainly from the combustion of lignin, and secondary formation through the reaction of BTEX compounds (benzene, toluene, ethylbenzene, and xylenes) with major atmospheric oxidants. Due to its environmental relevance and potential role in atmospheric chemistry, understanding its molecular properties under isolated conditions is of significant interest. Matrix isolation FT-IR spectroscopy was employed to investigate the vibrational properties of 4-nitroguaiacol isolated in argon and nitrogen matrices at cryogenic temperatures. The experimental spectra were analyzed and compared with theoretical vibrational frequencies and intensities obtained through DFT (Density Functional Theory) calculations at the B3LYP-D3/aug-cc-vpdz level. Special attention was given to the influence of the matrix environment on spectral features, including shifts in characteristic bands and changes in relative intensities. In addition, the photodegradation of 4-nitroguaiacol was studied under broadband UV irradiation (Hg lamp) in both argon and nitrogen matrices in order to try to understand the early steps of its photochemical transformation in the atmosphere.

---

*Speaker

†Corresponding author: decgranados@univ-pau.fr

Watching a disulide bond break in real time

Patrick Robertson *† [1], Felix Allum [2], David Heathcote [3], Till Jahnke [4], Hannes Lindenblatt [2], James Merrick [3,5], Benoit Richard [6], Sergey Usenko [7], Tiffany Walmsley [3,8], Rebecca Boll [9], Rebecca Ingle [10], Fabiano Lever [2], Tommaso Mazza [11], Dennis Mayer [2], Pedro Nunes [12], Dirk Raiser [13], Conor Rankine [14], Jennifer Rigden [8], Philipp Schmidt [13], Björn Senfftleben [13], James Thompson [8], Markus Guehr [2], Adam Kirrander [5], Claire Vallance [3], Michael Meyer [13], Matthew Robinson‡ [13]

[1] School of Chemistry, University of Nottingham – United Kingdom
[2] Deutsches Elektronen-Synchrotron [Hamburg] – Germany
[3] Chemistry Research Laboratory, Department of Chemistry, University of Oxford – United Kingdom
[4] University of Frankfurt – Germany
[5] Physical and Theoretical Chemistry Laboratory [Oxford] – United Kingdom
[6] Center for Free-Electron Laser Science – Germany
[7] European XFEL – Germany
[8] Central Laser Facility, STFC Rutherford Appleton Laboratory – United Kingdom
[9] European XFEL – Germany
[10] Department of Chemistry [University College of London] – United Kingdom
[11] European XFEL – Albert-Einstein-Ring 19 22761 Hamburg, Germany
[12] DIAMOND Light source – United Kingdom
[13] European XFEL – Germany
[14] University of Newcastle – United Kingdom

Disulfide bonds play an important role in biology, acting to stabilise the tertiary structures of proteins. Disulfide bonds are vulnerable to photochemical and oxidative damage, and when excited by ultraviolet (UV) light, undergo an ultrafast homolytic bond fission. Knowledge of how this bond-breaking event occurs gives us a deeper understanding of the early-stages biological processes such a protein unfolding, or radiative damage to biomolecules. 1,2-dithiane, a heterocyclic molecule containing a two adjacent sulfur atoms, is one of the simplest model systems for studying disulfide photochemistry. Past experimental and theoretical work has suggested that the system undergoes a coherent cyclic ring-opening and closing process with a period of 350 fs following the fission of the disulfide bond. Until recently, these dynamics have not been explicitly captured with structural methods on an ultrafast time frame. We present experimental results from a recent beamtime at the SQS endstation of the European XFEL. Using the REMI apparatus, we have captured the evolving nuclear structure of 1,2-dithiane following photoexcitation at 265 nm via x-ray Coulomb explosion imaging (CEI) induced by ionisation at the sulfur K-edge. Our results show the initial ring-opening process, subsequent evolution of the nuclear wavepacket, and ring-closing attempt are directly observable in the relative emission angle of coincidently detected sulfur ions. The timescale of this process is measured to be 400 fs, showing outstanding quantiative agreement with theory.

---

[*] Speaker

[†] Corresponding author: patrick.robertson@nottingham.ac.uk

[‡] Corresponding author: matthew.robinson@xfel.eu

We believe that this represents one best-resolved CEI experiments to date and expect that it will provide new insight to the early-stage dynamics of everyday biologically-relevant processes.

Towards the identification of structure and function of biological ions: a native MS based approach

Meloottayil V. Vinitha *† [1], R. Mattossovich [2], R. Merlo [2], J. Leon Moro [3], E. Roubieu, [3], J. Chiarinelli [1], L. Avaldi [1], A. Parracino [3], A. López Cortajarena [3], A. Valenti [2], P. Bolognesi [1]

[1] CNR-ISM, Area della Ricerca di Roma 1, via Salaria km. 29.300, Monterotondo Scalo (Rome) – Italy
[2] CNR-IBBR, Area della Ricerca di Napoli, Via Pietro Castellino 111, Naples – Italy
[3] Uppsala University, Uppsala Biomedicinska Centrum (BMC), Husarg Uppsala – Sweden

Establishing a link between function and structure of biological ions remains one of the main challenges in biology since it involves real-time analysis of macromolecular ions during a given biological process. To the best of our knowledge none of the established experimental methods can probe the biochemical modifications that a complex biological ion might undergo during its function. The goal of the "iSenseDNA" project is to exploit supercoiled plasmid DNA as a nano-transducer that modifies its conformation in a well-defined manner depending on the function of the interacting biomolecule, similarly as to in-vivo processes.

In this activity of the project, we are trying to set up an experimental methodology based on native mass spectrometry (MS) to assess the structural changes of a MDa sized supercoiled DNA plasmid in presence of a target protein, for example, α-synuclein. It is known that charge state distribution of electrosprayed-macromoleuclar ions reflect their topology [1]. Several authors have already applied this method to understand biochemical reactions of biomolecules of different sizes (from few tens to few hundreds of kDa) [2,3]. In this poster we will present the conditions for micro-electrospray ionization mass spectrometry to characterize structural modifications of MDa-sized plasmid DNAs upon interaction with model proteins, along with preliminary results.

Acknowledgement:
This work is funded by the European Union under grant agreement No 101046920, project "iSenseDNA-Computational-driven development of in vivo-like-DNA-nanostructures to study the dynamics of interaction DNA-protein in real-time".

References :
Lohra M. Miller et al.J. Am. Soc. Mass Spectrom. 2024, 35, 19691975.
Deterding, Leesa J., et al. Bioconjugate Chemistry 2000, 11.3, 335-344.
Basri Gulbakan et al. J. Am. Chem. Soc. 2018, 140, 74867497.

---

*Speaker
†Corresponding author: vinitha.meloottayil@mlib.ism.cnr.it

19 Jun 2025

LIBS imaging: Recent advances and perspectives

Vincent Motto-Ros * [1]

[1] Institut Lumière Matière (ILM) – CNRS : UMR5306, Université Claude Bernard - Lyon I (UCBL) – UMR5306 CNRS Université Claude Bernard Lyon 1 Domaine Scientifique de La Doua Bâtiment Kastler, 10 rue Ada Byron 69622 Villeurbanne CEDEX, Franc, France

The imaging capability of laser-induced breakdown spectroscopy (LIBS) has a high potential in various domains including biology, industry, geology and medicine (1,2). This approach can be distinguished by its ease in use, multi-elemental capability, detection of light elements, as well as operation at ambient conditions. This is furthermore the only all-optical technique providing space-resolved elemental information with ppm-scale sensitivity and μm-range resolution. These advantages, make LIBS imaging very attractive to be used in research laboratories for routine investigations.

However, advanced technological solutions must be found for this application since elemental imaging requires high sensitivity, sharp spatial resolution, high speed of acquisition as well as the ability to process a huge quantity of data. In this presentation, we will summarize the recent progresses made in the Light and Matter Institute concerning the implementation of the LIBS imaging. In particular, different examples of breakthrough applications, such as biomedical or industrial will be shown with the aim of illustrating the specificities and the great potential of LIBS imaging. Different perspectives will be finally discussed.

References:
(1) B. Busser, S. Moncayo, J.-L. Coll, L. Sancey, V. Motto-Ros, Coordination Chemistry Reviews 358, 70-79 (2018).
(2) V. Gardette, V. Motto-Ros, C. Alvarez-Llamas, et al., Analytical Chemistry 95, 49-69 (2023).

---

*Speaker

Exploring charge transfer mediated by rotational dynamics in dissociating molecules

Björn Senfftleben * [1]

[1] European X-Ray Free-Electron Laser – Germany

Charge transfer is a fundamental process relevant to many complex chemical processes. Forming a detailed understanding of such processes on a molecular level requires an understanding of the involved elementary dynamics. Here, in particular, the interplay of structural dynamics and the likelihood of transferring charges is of interest. For small molecules, a combined measurement of the structure and the ability to transfer charges can be achieved by combining site-selective ionization by intense X-ray pulses and the Coulomb explosion imaging technique. Combined with an ultra-short pump-pulse to trigger a two-body photo-dissociation of the molecule, the probability of charge transfer at different distances of the two forming fragments and in different charge state configurations can be studied. The first experiments studying the charge transfer probability dependence on fragment distance found the inhibition of charge transfer beyond a critical distance that a classical over-the-barrier model describes well (1-6).

In the experiment presented here, we increase the complexity of the studied photo-dissociation process to include effects due to fragment orientation. We employed a velocity map imaging spectrometer with an MCP-phosphor stack detector and a Timepix3-based optical ns-timestamping camera to isolate the kinetic energy, delay, mass, and charge-dependent signals of the studied samples - bromoiodomethane and chloroiodomethane. As for other dihalomethanes, upon cleavage of the carbon iodine bond, the remaining halomethyl group starts to rotate because its center of mass is off-axis from the cleaved bond (6-8). By site-selectively ionizing the iodine atom, we can map the charge transfer probability by distance and orientation for a wide range of charge states. We especially investigate those charge states for which, due to the halomethyl group's rotation, the critical distance is expected to be crossed multiple times based on the classical over-the-barrier model.

(1) Erk et al., Science 345, 288-291 (2014). (2) Schnorr et al., PRL 113, 073001 (2014). (3) Amini et al., Structural Dynamics 5, 014301 (2018). (4) Boll et al., Structural Dynamics 3, 043207 (2016). (5) Allum et al., Faraday Discuss., 2021, 228, 571-596. (6) Köckert et al., J. Phys. B: At. Mol. Opt. Phys. 55 (2022) 014001. (7) Burt et al., Phys. Rev. A 96, 043415 (2017). (8) Murillo-Sánchez et al., Phys. Chem. Chem. Phys., 2018, 20, 20766

---

[*] Speaker

Comparative Study of Elastic Electron Scattering Cross Sections for Halothane, Isoflurane, and Sevoflurane at 200 eV in the Gaseous Phase

Jelena Vukalović * [1,2], Bratislav Marinković [1], Francisco Blanco [3], Gustavo García [4], Jelena Maljkovic [5]

[1] Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, – Serbia
[2] Faculty of Science, University of Banja Luka, Mladena Stojanović a 2, 78000 Banja Luka, Republic of Srpska – Bosnia and Herzegovina
[3] Departamento de Fısica Atomica, Molecular y Nuclear, Universidad Complutense de Madrid, – 28040 Madrid, Spain, Spain
[4] Instituto de F ísica Fundamental, Consejo Superior de Investigaciones Cientificas, Serrano 121, 28006 Madrid – Spain
[5] Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, – Serbia

Motivated by the significant contribution of anesthetic molecules to global warming and ozone depletion, we performed both theoretical and experimental investigations of elastic electron scattering from halothane, sevoflurane, and isoflurane at 200 eV. Research indicates that the majority of anesthetics administered to patients are exhaled unchanged into the atmosphere, and this release has been increasing over time. As halogenated compounds, these anesthetics have high Global Warming Potentials (GWP) and, in some cases, significant Ozone Depletion Potentials (ODP) (1).

The experimental setup used a crossed-beam apparatus that included an electron gun, a capillary gas needle, and a channeltron detection system. To normalize the measured relative cross sections, we employed the relative-flow method with argon as the reference gas. Theoretical calculations of the differential cross sections were carried out using the Independent Atom Model combined with the Screening Corrected Additivity Rule and interference effects (IAM-SCAR+I). The experimental and theoretical data were compared, offering valuable insights into the behavior of these anesthetic molecules at 200 eV (2,3,4).

Understanding the electron scattering cross sections of volatile anesthetics is important for assessing their potential impact on climate change. These cross sections are key parameters in atmospheric modeling, helping to improve predictions of their long-term behavior in the environment.

This research was supported by the Science Fund of the Republic of Serbia, Grant No.6821, Project title – ATMOLCOL

References

---

[*] Speaker

(1) Langbein, T., Sonntag, H., Trapp, D., Hoffmann, A., Malms, W., Röth, E.P., Mörs, V., Zellner, R.: 1999, Br. J. Anaesth., 82, 66–73.
(2) Maljković, J.B., Vukalović, J., Pešić, Z.D., Blanco, F., García, G., Marinković, B.P.: 2023, Eur. Phys. J. Plus, 138, 349.
(3) Vukalović, J., Maljković, J.B., Blanco, F., García, G., Predojević, B., Marinković, B.P.:2022, Int. J. Mol. Sci., 23, 21.
(4) Vukalović, J., Marinković, B. P., Rosado, J., Blanco, F., García, G., Maljković, J. B.: 2024, Phys. Chem. Chem. Phys., 26, 985-991.

Modeling a Low-Temperature Plasma to Study Analogous Conditions of Titan's Atmosphere

David Dubois *† [1], Ella Sciamma-O'brien [1], Farid Salama [1]

[1] NASA Ames Research Center – United States

Titan, Saturn's largest moon, is the only moon in our solar system to have its own dense atmosphere. The atmosphere is subject to strong dynamical, season, and photochemical effects that lead to an abundant distribution of organic molecules extending up to 1500 km in altitude. In the study presented here, we model the gas phase chemistry induced by plasma discharge at low temperature (150 K) in the NASA Ames COSmIC Simulation Chamber (COSmIC) using a 1D multi-fluid plasma model named CO-PRISM (COSmIC Plasma Reactivity and Ionization Simulation Model) to characterize ionized conditions analogous to Titan's upper atmosphere. Our model incorporates an extensive chemical reaction network to simulate the neutral-neutral and ion-neutral reactions occurring in the COSmIC experiments when using N2-CH4-based gas mixtures relevant to Titan's atmosphere. Our reaction network now includes crucial reactions involving the first electronically-excited state of atomic nitrogen, recent electron collision cross-sections, and radical chemistry. In particular, we have investigated the influence of C_2H_2 on the gas phase polymeric growth and the elemental composition of the chemical products, and we have compared our findings to recently published solid phase (tholin) analyses. The modeling results are consistent with experimental measurements of N_2-CH_4-C_2H_2 plasmas on COSmIC, showing the production of C_6H_x intermediates and precursors of larger organics, as well as methanimine in small concentration. Our numerical results point to cationic pathways enabling efficient intermediate-sized and nitrogen-rich C_2H_2-driven chemistry driving *tholin* production. Comparison of the modeled gas phase elemental composition with elemental composition of the solid phase samples produced in COSmIC reveal similar trends, with C/N increasing when C_2H_2 is present in the gas mixture. Finally, our results demonstrate the importance of such synergistic studies using low-temperature plasma chemistry experiments combined with modeling efforts to improve our understanding of cold planetary and astrophysical environments.

---

*Speaker

†Corresponding author: david.f.dubois@nasa.gov

Few-fs charge dynamics in molecular systems

Federico Vismarra * [1,2]

[1] Laboratory for Physical Chemistry, ETH Zürich, Vladimir-Prelog-Weg 1-5/10 8093 Zürich Switzerland – Switzerland
[2] Dipartimento di Fisica [Politecnico Milano] – Italy

The interaction of molecules with attosecond pulses provides a powerful means to investigate the earliest stages of coupled electron–nuclear dynamics.
Among the key processes accessible in this ultrafast regime are charge migration (CM)-the purely electronic rearrangement of charge density occurring immediately after ionization-and charge transfer (CT), in which nuclear motion drives the charge displacement across molecular subunits. While CM and CT are often considered separately, their interplay is fundamental to understanding how coherent electronic motion impacts long-range charge redistribution in photoexcited molecular systems.

In a recent study conducted at Politecnico di Milano (Nat. Chem. 16, 2017–2024 (2024)), we investigated this interplay in nitroaniline donor–π–acceptor molecules. Using attosecond XUV-pump/few-femtosecond IR-probe spectroscopy in combination with advanced many-body quantum chemistry simulations, we resolved the ultrafast evolution of electronic and nuclear degrees of freedom following XUV ionization. We observed that the initial CT-like step-driven by the rapid planarization of the amino donor group-occurs within 10 fs, as the nitrogen lone pair reorganizes into the adjacent C–N π-system. This structural change corresponds to an orbital hybridization switch (from sp^3 to sp^2) and marks the beginning of any subsequent longer-range CT in the studied donor–π–acceptor compounds.
Looking ahead, a central goal is to deepen our fundamental understanding of the intricate connection between CM and CT by enabling site-selective tracking of charge dynamics with high-temporal resolution. To this end, we are developing a novel experimental approach at ETH Zürich based on soft X-ray attosecond spectroscopy, capable of probing element-specific core-level transitions with attosecond temporal resolution. This technique will provide direct access to the spatiotemporal evolution of electronic charge at individual atomic sites, opening new frontiers in our ability to observe and disentangle ultrafast photoinduced processes in complex molecular systems.

---

*Speaker

Investigation of dehydrogenation process in PAHs using kinetic energy correlated ToF measurements

Vinitha M V *† [1,2], Arya M Nair [3], Umesh Kadhane [1]

[1] Indian Institute of Space and Science Technology – India
[2] Istituto di Struttura della Materia – Italy
[3] Government College, Karyavattom, University of Kerala, Thiruvananthapuram, 695581, Kerala – India

Several mechanisms related to Hydrogen (H) migration, H loss or H2 loss mechanisms in PAHs (polycyclic aromatic hydrocarbons) are reported in the past by several authors using various theoretical and experimental methodologies or combination of both (1-4). But direct evidence for the loss of hydrogen molecule in any PAHs is not experimentally demonstrated to the best of our knowledge. But such events are very important in the astronomical context for explaining large abundance of molecular hydrogen observed in the vicinity of PAH systems present in various star's environment (5). In this context we were able to directly demonstrate in the laboratory that loss of molecular hydrogen can be a dissociation pathway in smaller PAHs using a kinetic energy correlated-ToF experimental methodology developed as part of my PhD thesis in Atomic and molecular Research laboratory in Indian Institute of Space Science and Technology (IIST) in India (6). This experimental method, with the help of a dedicated Monte-Carlo modelling allowed us to quantify gas phase kinetics of molecular dissociation occurring in microseconds to millisecond time scales, which is normally difficult to achieve with a standard ToF mass analyzer (7). Further very recently, with the help of this technique we were able to uncover some important intermolecular dissociation channels in nitrogenated PAH clusters produced at room temperature. The kinetic energy correlated ToF mass spectrometric experimental method, its implications on investigating statistical dissociation channels in large carbonaceous molecules such as PAHs will be discussed in detail in the talk.

References:
(1) F. Jolibois et al. A & A 444 (2) (2005)
(2) T. Kumakura et al. Chem. Phys. Lett. 714 (2019)
(3) Chen, Tao, et al. JCP.142.14 (2015).
(4) Désesquelles, Pierre, et al. Chem. Phys. Chem. 25.1 (2024).
(5) Combes et al. Molecular hydrogen in space. Cambridge University Press, 2000.
(6) Vinitha, M. V., et al. Int. J. Mass Spectrom. 471,116704 (2022)
(7) M.V. Vinitha et al. Rev. Sci. Instrum. 90, 103304, (2019).

---

[*] Speaker
[†] Corresponding author: vinithamvv@gmail.com

Electron induced processes in liquid microjets : a step towards quantifying solvated electrons

Pamir Nag * [1], Samrat Saha [1], Cécile Sicard-Roselli [2], Miloš Ranković [1],
Volodymyr Malynovskyy [1], Juraj Fedor [1]

[1] J. Heyrovský Institute of Physical Chemistry of the CAS – Czech Republic
[2] Université Paris-Saclay, CNRS, Institut de Chimie Physique – Université Paris-Saclay, CNRS – France

We recently developed a new experimental setup to study electron beam-induced processes in liquid- and solvated-phase molecules. One of the motivations for this work is to understand the radiation-induced damage to living cells and biologically important molecules in their natural environment – i.e. in aqueous solvated form. The experimental results will also enable us to understand the effect of the liquid environment in electron-induced reactions. The experimental setup is equipped with a high-vacuum compatible recirculating liquid micro-jet source and an electron gun producing an electron beam with tunable energy ranging from 60 to 800 eV. The irradiated sample can be collected for ex-situ analysis or recirculated for further irradiation experiments.

To test the setup, we recently studied electron-beam induced reactivity in water-solvated TRIS (2-Amino-2-(hydroxymethyl) propane-1,3-diol) molecule. Around 19.3 mM aqueous solution of TRIS was irradiated with a 300 eV electron beam, and the irradiated solution was collected and analysed using UV-VIS spectroscopy. We were able to clearly observe reaction of TRIS with the OH radicals created by electron-induced dissociation of H_2O molecules.

To understand the electron-induced damage to biologically important molecules, including DNA strand breaks, it is necessary to quantify the electron dose in the liquid. Until now, accurate estimation of the electron dose for solvated molecules has been challenging. To quantify the solvated electron dose, we irradiated water solvated $NaNO_3$ with an electron beam at incident energies ranging from 60 to 600 eV and collected the irradiated sample to study the two-electron reduction of nitrate ions (NO_3^-) to nitrite (NO_2^-). The irradiated samples are collected and mixed with 2,3-diaminonaphthalene, which only reacts with NO_2^- and produces fluorescent 2,3-naphtotriazole (2,3-NAT). By measuring the florescent yield, it is possible to quantify the electron dose inside the liquid micro-jet. We irradiated the sample at four different incident electron energies, and for each energy, we irradiated the sample for eight cycles. We measured the fluorescence spectra for each cycle at all fixed incident electron energies to quantify the concentration of solvated electrons.

---

*Speaker

Covariance Analysis of Phenyl Cation Fragmentation Dynamics

Tiffany Walmsley * [1,2], Felix Allum [3,4], James R Harries [5], Yoshiaki Kumagai [6], Suzanne Lim [1], Joseph W Mcmanus [1], Kiyonobu Nagaya [7], Mathew Britton [3,4], Mark Brouard [1], Philip H Bucksbaum [4], Mizuho Fushitani [8], Ian Gabalski [9,10], Tatsuo Gejo [11], Paul Hockett [12], Andrew J Howard [4,10], Hiroshi Iwayama [13], Edwin Kukk [14], Chow-Shing Lam [1], Russell S Minns [15], Akinobu Niozu [16], Sekito Nishimuro [17], Johannes Niskanen [14], Shigeki Owada [18,19], Weronika O Razmus [15], Daniel Rolles [20], James Somper [1], Kiyoshi Ueda [21], James Unwin [1], Shin-Ichi Wada [22], Joanne L Woodhouse [15], Ruaridh Forbes [3], Michael Burt† [1], Emily M Warne‡ [1]

[1] Chemistry Research Laboratory, Department of Chemistry, University of Oxford – United Kingdom
[2] Central Laser Facility, STFC Rutherford Appleton Laboratory – United Kingdom
[3] Linac Coherent Light Source, SLAC National Accelerator Laboratory – United States
[4] PULSE Institute, SLAC National Accelerator Laboratory – United States
[5] National Institutes for Quantum Science and Technology (QST), SPring-8 – Japan
[6] Department of Applied Physics, Tokyo University of Agriculture and Technology – Japan
[7] Department of Physics, Kyoto university – Japan
[8] Department of Chemistry, Graduate School of Science, Nagoya University – Japan
[9] PULSE Institute, SLAC National Accelerator Laboratory – United States
[10] Department of Applied Physics, Stanford University – United States
[11] Graduate School of Material Science, University of Hyogo – Japan
[12] National Research Council of Canada – Canada
[13] Institute for Molecular Science – Japan
[14] Department of Physics and Astronomy, University of Turku – Finland
[15] School of Chemistry, University of Southampton – United Kingdom
[16] Graduate School of Humanities and Social Sciences, Hiroshima University – Japan
[17] Department of Chemistry, School of Science, Tokyo Institute of Technology – Japan
[18] Japan Synchroton Radiation Research Institute – Japan
[19] RIKEN SPring-8 Center – Japan
[20] J. R. Macdonald Laboratory, Department of Physics, Kansas State University – United States
[21] Department of Chemistry, Tohoku University – Japan
[22] Graduate School of Advanced Science and Engineering, Hiroshima University – Japan

Extreme ultra-violet (XUV) laser pulses are frequently used to probe time-resolved excited state structural dynamics. XUV photons can highly ionise molecules by removing inner-shell electrons and ensuing Auger-Meitner decay processes. This typically induces highly energetic Coulomb explosions, which produce ionic fragments whose momenta are related to the instantaneous geometry

---

*Speaker

†Corresponding author: michaelburt@trentu.ca

‡Corresponding author: chemistry@emilywarne.co.uk

of the exploding structure. However, the number and complexity of competing Coulomb explosion and fragmentation pathways accessible to the XUV probe alone increase with the size of the molecule, which complicates time-resolved spectra. Therefore, sophisticated analysis procedures are required to disentangle the nuclear dynamics of concurrent and multi-step XUV fragmentation channels. We employed advanced covariance analysis techniques(1,2) to separate and examine a range of phenyl (mono/poly)cation fragmentation channels accessed by site-selective XUV ionisation of the iodine 4d electrons of iodobenzene.(3) Ionic products were recorded by velocity map imaging and three-dimensional momentum information was recovered for each ion detected. Comprehensive correlations between fragment momenta were used to characterise the (in)stability of various phenyl cations and the nuclear dynamics of the most probabilistic fragmentation pathways. The results demonstrate the potential to extend these analytical methods to in-depth studies of the competitive photochemistry of larger, more chemically complex systems that react to form unstable or long-lived intermediates.

References:

(1) McManus, J.W., et al. "Disentangling sequential and concerted fragmentations of molecular polycations with covariant native frame analysis." PCCP 24.37 (2022): 22699-22709.
(2) Walmsley, T., et al. "The role of momentum partitioning in covariance ion imaging analysis." The Journal of Physical Chemistry A 128.22 (2024): 4548-4560.
(3) Walmsley, T., et al. "Distinguishing the XUV-induced Coulomb explosion dynamics of iodobenzene using covariance analysis." Journal of Physics B: Atomic, Molecular and Optical Physics 57.23 (2024): 235101.

Studying radical species of astrochemical interest through VUV photoionisation

Myriam Drissi * [1], Bérenger Gans [2], Séverine Boyé-Péronne [2], Hai-Linh Le [2], Mengxu Jiang [2], Laurent Nahon [1], Gustavo Garcia [1], Jean-Christophe Loison [3]

[1] Synchrotron SOLEIL – Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UR1 – France
[2] Institut des Sciences Moléculaires d'Orsay – Université Paris-Saclay, Centre National de la Recherche Scientifique, Centre National de la Recherche Scientifique : UMR8214 – France
[3] ISM – Institut des Sciences Moléculaires, The French National Centre for Scientific Research, Bordeaux, France – France

Radicals and ions are known to be important drivers of the rich chemistry in astronomical media. The identification and characterisation of such reactive species are therefore necessary to gain knowledge on the gas-phase processes occurring in such environments. Vacuum-ultraviolet (VUV) photoionisation can be used, not only to characterize the electronic structure of molecules through photoelectron spectroscopy, but also to study their photochemistry under VUV irradiation. Additionally, in the past decade, synchrotron-based photoelectron spectroscopy has been coupled to mass spectrometry in search of a universal detection method able to probe the presence of products and intermediates in complex chemical reactions. Here, I will present the current experimental setup installed at the DESIRS VUV beamline (Synchrotron SOLEIL) allowing the production of radicals inside a flow tube reactor with a microwave discharge and coupled to a i^{2}PEPICO (double imaging photoelectron photoion coincidence) spectrometer to measure their mass-selected photoelectron spectra with vibrational resolution. I will present the different applications of this experiment including the spectroscopy of radical species, such as HCCS, and the study of radical-atom reactions which are both essential to improve astrochemical models. In addition, I will also discuss short-term critical developments to the existing set-up to improve our detection limit for trace species, needed to broaden our scientific scope from astrophysical to atmospheric/combustion media.

---

*Speaker

Elucidating Dissociation Kinetics in Hydrated Ions through Multiple Isomer Master Equation Modelling

Gabriel Schöpfer *† [1], Magdalena Salzburger [1], Michael Gatt [1], Olivia O'neill [2], Christian Van Der Linde [1], Martin K. Beyer [1], Milan Ončák [1]

[1] Leopold Franzens Universität Innsbruck - University of Innsbruck – Austria
[2] The University of Edinburgh – United Kingdom

Anthropogenic climate change has become a scientific fact. However, many processes in the atmosphere are still only poorly understood. In particular, aerosol-related processes like their formation and dissociation are still not fully understood on a molecular level.
In this contribution, I show how to properly describe hydrated superoxide radical anions O_2•–$(H_2O)_{1-7}$, which play an important role in the atmosphere and might serve as aerosol precursor molecules. Strikingly, already for this relatively small number of water molecules, many isomers exist and might be reached during the dissociation process. And – as the water molecules are relatively loosely bound – isomerization happens with a very high rate.

We developed a new approach to consider these circumstances and describe the dissociation kinetics of such multiple isomer systems, the so-called AWATAR RRKM MEM (**A**ll **W**ells **A**nd **T**ransition States **A**re **R**elevant **R**ice-**R**amsperger-**K**assel **M**arcus **M**aster **E**quation **M**odelling),(1) serving as an extension to the standard RRKM MEM. The idea is to use RRKM MEM to model the dissociation kinetics, but instead of describing only the pathway from one global minimum isomer to one dissociated isomer, this new approach treats all desired isomers on the same footing, allowing for several reactant isomers and several isomers for the dissociated form. We have already shown that high-lying isomers play a significant role in dissociation kinetics because of entropic effects.(2)
With this new approach, we now employ thousands of isomers to reliably model the dissociation kinetics of O_2•–$(H_2O)_{1-7}$ under the influence of black body radiation and compare the predictions with our experimental results obtained using mass spectrometry.

Potential energy surface exploration was performed using our in-house genetic algorithm (3) using the semi-empirical xTB approach, followed by a graph-based structure clustering (4) and reoptimization with DFT methods.

(1) J. C. Hartmann, S. J. Madlener, C. van der Linde, M. Ončák, and M. K. Beyer. *Phys. Chem. Chem. Phys.*, 2024, **26**, 10904-10918. https://doi.org/10.1039/D4CP00357H
(2) M. Salzburger, M. Ončák, C. van der Linde, and M. K. Beyer. *J. Am. Chem. Soc.* 2022, 144, 47, 21485–21493. https://doi.org/10.1021/jacs.2c07060

---

*Speaker
†Corresponding author: Gabriel.Schoepfer@uibk.ac.at

(3) G. Schöpfer, M. Gatt, M. Ončák: https://git.uibk.ac.at/c7441332/genetic-algorithms
(4) M. Gatt, G. Schöpfer, M. Ončák: https://git.uibk.ac.at/csaz7810/structure-clustering

Molecular collisional cross-sections in low temperature cold uniform supersonic flows

Chinmai Sai Jureddy * [1], Alberto Macario Farto [1], Myriam Drissi [1], Omar Abdelkader Khedaoui [1], Ian Sims† [1,2]

[1] Univ Rennes, CNRS, IPR (Institut de Physique de Rennes) - UMR 6251, F-35000 Rennes, France. – Université Rennes – France

[2] Institut Universitaire de France – Ministère de l'Education nationale, de l'Enseignement supérieur et de la Recherche – France

Molecular collisions at low temperatures ($<$ 150 K) are important for modelling spectral lines to retrieve the physical conditions of low temperature astrophysical environments. Collisional rate coefficients for rotational energy transfer are required for radiative transfer calculations when non-LTE (local thermodynamic equilibrium) conditions prevail. Theoretical methods are being developed for determining these collisional rate coefficients at low temperatures (1). The computational demand and complexity increase with increase in the size of the molecule and in addition, the long-range interactions between collisional partners are enhanced in low temperature conditions which requires accurate modelling of interaction potentials. This calls for the experimental investigation of these collisional rate coefficients to benchmark the theoretical calculations.
Several experimental methods exist to determine the collisional rates (1). The CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme or reaction kinetics in uniform supersonic flow) technique generates a wall-less collisional environment by gas expansion through convergent-divergent (Laval) nozzles. It can be combined with laser and millimeter-wave techniques to determine absolute collisional cross-sections (2,3). The uniform supersonic flows comprise a cold isentropic core surrounded by boundary layers, which are at different temperatures and complicate the measurements when the rotational transitions are probed directly. To avoid this, a method of producing the molecules of interest through photodissociation of a precursor exclusively in the cold isentropic core was implemented (2). This technique also enables the measurement of collisional cross-sections of exotic or unstable species.

We are interested in measuring low temperature H_2CO collisional cross-section with colliding partners He, N_2 and CO for astrophysical applications. Tetrahydrofuran, 2,3-dihydrofuran, and oxetane are tested as photodissociation sources for H_2CO at 193.3 nm in a supersonic jet expansion. A chirped pulse millimeter wave spectrometer is used to detect the H_2CO. We will present the retrieved collisional cross-sections.

(1) Roueff E et al 2013 *Chem. Rev.* **13.12** 8906 8938.
(2) Hays, B.M et al 2022 *Nat. Chem.* **14** 811–815
(3) Labiad, H et al 2022 *Phys. Rev A* **105.2** L020802

---

*Speaker

†Corresponding author: ian.sims@univ-rennes.fr

Influence of Hydrogen Coverage on Energy Dissipation in Hydrogen-Tungsten Collisions: A Theoretical Study

Raidel Martin Barrios *† [1], Oihana Galparsoro [2], Cédric Crespos [1], Pascal Larregaray [3]

[1] Institut des Sciences Moléculaires, U. Bordeaux/ CNRS – Univ. Bordeaux, CNRS, Bordeaux INP, ISM, UMR-5255, F-33400 Talence – France
[2] Kimika Fakultatea, Euskal Herriko Unibertsitatea UPV/EHU, Donostia-San Sebastián 20018 – Spain
[3] Institut des Sciences Moléculaires, U. Bordeaux/ CNRS – Univ. Bordeaux, CNRS, Bordeaux INP, ISM, UMR-5255, F-33400 Talence – France

Recent studies have shown that when hydrogen atoms collide with metal surfaces at energies of a few electron volts, the loss of translational energy is mainly due to electron-hole pair excitations. Here, quasi-classical trajectory simulations have been carried out to investigate the energy transfer during the scattering of hydrogen atoms from hydrogen-covered tungsten surfaces, W(110) and W(100). The theoretical approach investigates the effect of hydrogen coverage, collision energy and direction of incidence on the energy loss. The scattering can be explained by three different dynamical mechanisms, the contribution of which varies depending on the scattering conditions. These results help to explain why the energy loss spectra are significantly different when analysed in the whole space or only at the scattering plane. Furthermore, a previously unknown reflection channel at low energy and grazing incidence at high coverage is suggested, resulting from changes in the potential energy surface.

---

*Speaker

†Corresponding author: raidel.martin-barrios@u-bordeaux.fr

List of posters

1	A Monte Carlo approach for electron impact on molecules under local plasma approximation: For application to electron beam induced deposition process	Jureddy Chinmai Sai
2	Collision and coagulation of rare-gas atoms in helium nanodroplets by zero-point averaged dynamics	Bonhommeau David
3	Dissociative electron Attachment to Iodomethane	Saha Samrat
4	Dynamics of alkali atoms and clusters in helium nanodroplets by zero-point averaged dynamics	Bonhommeau David
5	Electronic structure calculations for electron driven reactivity of PH+	Jonas Tibor
6	ESPECDAS – A Database of Ab Initio Calculated Transitions in Small Molecules for Identification of Potential DIB Carriers	Gatt Michael
7	First principles construction of Newns-Anderson Hamiltonians for hydrogen chemistry at surfaces	Hertl Nils
8	Fragmentation of naphthalene and quinoline dications produced under oxygen ion impact	Srivastav Sumit
9	From perturbation theory to model potential for alkali rare gas molecules	Gervais Benoit
10	Hydrogen atom diffraction through free-standing single-layer graphene	Guichard Pierre
11	Isotope effects for Hydrogen scattering on W(110) surface	Bombín Escudero Raúl
12	Laboratory experiments for chemical kinetics at very low temperature: a new viewpoint	Durif Olivier
13	Low temperature collisional cross-sections of molecules of astrophysical interest	Jureddy Chinmai Sai
14	Measuring ion-induced biomolecular fragmentation using a Velocity Map Imaging spectrometer	Bourgeteau Antonin
15	Multi-Channel Quantum Scattering Calculation of fine structure quenching and electronic excitation exchange between ultracold meta-stable Sr+ and ground state Rb atoms	Jonas Tibor
16	Payloads for plasma characterization and mass spectroscopy in planetary ionosphere	Raghunandanan Sreeja
17	Reaction Mechanisms Between Atomic Carbon C(3Pj) and Cyclopentadiene Using Synchrotron-Based Photoionization Mass Spectrometry and Theoretical Quantum Calculation	Bourgalais Jeremy
18	State-selected dissociation of formic acid upon carbon core-shell excitation studied by Auger/photoelectron photoion coincident spectroscopy at PLEIADES/SOLEIL	Milosavljevic Aleksandar
19	Tailoring perovskites through chemical substitution for "à la carte" optoelectronic properties: a Quantum Chemistry approach	Aguilar-Galindo Fernando
20	The influence of water on the modified amino acid phosphotyrosine: A multiscale study using soft X-ray radiation	Leroux Juliette
21	The vibrational structure of excited RbHe molecule	Gervais Benoit
22	Theoretical investigation of excited electronic states of the KAr molecule	Gervais Benoit
23	Theoretical study of electron-molecule collisions for plasma simulations	García-Muñoz Alejandro L.
24	Vibrational properties and photodegradation of 4-Nitroguaiacol isolated in cryogenic matrices: An experimental and theoretical approach	Camacho Granados Daniel
25	Watching a disulide bond break in real time	Robertson Patrick
26	Towards the identification of structure and function of biological ions: a native MS based approach	Meloottayil Vinitha

List of participants

- Abbes Mohammed Mounsif
- Aguilar-Galindo Fernando
- Anastasiia Mikhneva
- Bombín Escudero Raúl
- Bonhommeau David
- Borghesi Costanza
- Bou Debes Daniel
- Bouchard De La Poterie Ignace
- Bourgeteau Antonin
- Busto David
- Camacho Granados Daniel
- Campbell Eleanor
- Chesnel Jean-Yves
- Demes Sándor
- Diaz-Tendero Sergio
- Domaracka Alicja
- Douady Julie
- Drissi Myriam
- Du Chalard Michel
- Dubois David
- Durif Olivier
- García Alejandro
- Gatt Michael
- Gervais Benoit
- Godin Thomas

- Guichard Pierre
- Guillemot Lauren
- Hertl Nils
- Infuso Maxime
- Irusta Yako
- Jacquet Emmanuelle
- Jonas Tibor
- Jureddy Chinmai Sai
- Kadhane Umesh
- Kensei Kitajima
- Lecoeur Augustin
- Leroux Juliette
- M V Vinitha
- Ma Pufang
- Maclot Sylvain
- Maljkovic Jelena
- Martin Barrios Raidel
- Mery Alain
- Milosavljevic Aleksandar
- Montes De Oca Judit
- Motto-Ros Vincent
- Nag Pamir
- Nair Aarathi
- Ngono Yvette
- Pacary Vincent
- Paliwal Prerna
- Paul Anirban
- Piekarski Dariusz G.
- Porcelli Francesco
- Radloff Robert
- Raghunandanan Sreeja
- Rangama Jimmy

- Reinert Tessa
- Riegel Alexander
- Robertson Patrick
- Rodrigues De Paula Alisson
- Rothard Hermann
- Rousseau Patrick
- Roy Chowdhury Madhusree
- Saha Samrat
- Schöpfer Gabriel
- Senfftleben Bjoern
- Srivastav Sumit
- Tímár-Grósz Tímea
- Vismarra Federico
- Vizcaino Violaine
- Vukalović Jelena
- Walmsley Tiffany
- Šenk Jan

Author Index