July 25 - August 1, 2023

icpeac2023.ca

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icpeac

2023

Conference Program

Welcome!

It is our great pleasure to welcome you to the XXXIII International Conference on Photonic, Electronic and Atomic Collisions, held in Ottawa, Ontario, Canada's capital.

ICPEAC 2023 has been long in the making. We made our first pitch to host ICPEAC in Canada in spring 2015 and were confirmed as the local organizers of the 2021 conference a few months later at the XXIX ICPEAC in Toledo, Spain. We started to lay the groundwork soon thereafter, got serious and enlisted professional help in 2019, only to see our plans thwarted by the coronavirus pandemic in the following year; the 2021 meeting was turned into a virtual one (ViCPEAC) while we were put on hold.

Luckily, we were able to postpone our plans and existing contracts by two years. Everything else, of course, kept moving and, unsurprisingly, the world of 2023 is somewhat different from the vision of 2021 we had back in 2015. But be that as it may, we are delighted to finally meet at the Shaw Centre in Ottawa for the first in-person ICPEAC since 2019! With the help of the ICPEAC Executive and General Committees we have put together an excellent invited program which, with your help, is complemented by an equally outstanding contributed program of more than 550 poster presentations from the whole community. Let's make the most of it and spend this week discussing collisions involving photons, electrons, atoms, ions, molecules, clusters, surfaces, and exotic particles, and with sharing the latest developments in ultracold, attosecond, and strong-field atomic and molecular physics and related areas.

Besides enjoying physics, catching up with old friends and making new ones, we hope that you will have a chance to also enjoy some of the abundant beauty in and around Ottawa. Canada's capital is a city with a rich cultural life and many attractions, known for its welcoming spirit and charm. It is surrounded by beautiful nature, and there are plenty of options to experience the great outdoors without going too far. However you spend your time while you are here, have a blast and get back home safely with fond memories and fresh ideas!

On the next pages, you will find some general information about ICPEAC 2023, a program overview, a more detailed day-by-day program with the abstracts of all invited talks, a listing of the poster presentations, and an index of the presenting authors. The Program Book is accompanied by a Book of Abstracts of all poster contributions, which is available online. We hope that you will find both volumes useful – at the conference and beyond.

Once again, welcome to Ottawa and to ICPEAC 2023!

Tom Kirchner
Chair of the Local Organizing Committee

André Staudte
Co-Chair

François Légaré
Co-Chair

IUPAP Policies

ICPEAC 2023 abides by IUPAP Policy on Conferences, in particular the two following statements:

1. Free Circulation of Scientists: The principle of the Universality of Science is fundamental to scientific progress. This principle embodies freedom of movement, association, expression and communication for scientists, as well as equitable access to data, information and research materials. In pursuing its objectives with respect to the rights and responsibilities of scientists, the International Union of Pure and Applied Physics (IUPAP) actively upholds this principle, and, in so doing, opposes any discrimination on the basis of such factors as ethnic origin, religion, citizenship, language, political stance, gender, or age. IUPAP should only sponsor conferences and events at institutions and in countries that uphold this principle. If scientists are excluded from attending IUPAP-sponsored international conferences by a host institution or country on the basis of any of these factors, IUPAP should register its concern at the highest level of that institution or country, and should not sponsor any future events in that country until such exclusions have been eliminated.

2. Harassment at Conferences: It is the policy of the International Union of Pure and Applied Physics (IUPAP) that all participants at an IUPAP-supported Conference will enjoy a comfortable experience, and that they will treat each other with respect at all times. The conference organisers will name an advisor who will consult with those who have suffered from harassment and who will suggest ways of redressing their problems, and an advisor who will counsel those accused of harassment.

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General Information

Food & Beverages

AM and PM coffee breaks will be held in the exhibition area. Lunch is not included, however there are plenty of options nearby for delegates to go and purchase their lunch (please refer to the map on p.6).

Internet Access

Network Name: ICPEAC23
Password: canadaicpeacrocks

Mobile Phones

As a courtesy to other delegates, please ensure all mobile telephones are turned off or are in silent mode during all sessions and social functions.

Name Badge

Your name badge is your entry into the conference sessions, exhibition, morning/afternoon coffee breaks and social functions (along with a ticket). Please ensure you wear your name badge at all times. If a badge is lost or forgotten onsite, an administrative fee of 10 CAD will be charged for the reprint of the badge after identity verification (passport, driver's license or other recognised identification documents).

Face Masks

Please note that face masks are not mandatory. A limited quantity will be available at the registration desk.

Registration Hours

July 25th: 14:00 – 18:00

July 26th: 8:00 – 16:00

July 27th: 8:00 – 16:00

July 28th: 8:00 – 16:00

July 29th: CLOSED

July 30th: CLOSED

July 31st: 11:00 – 18:00

August 1st: 8:30 – 13:00

Exhibition Hours

July 26th: 10:00 – 18:30

July 27th: 10:00 – 18:30

July 28th: 10:00 – 18:30

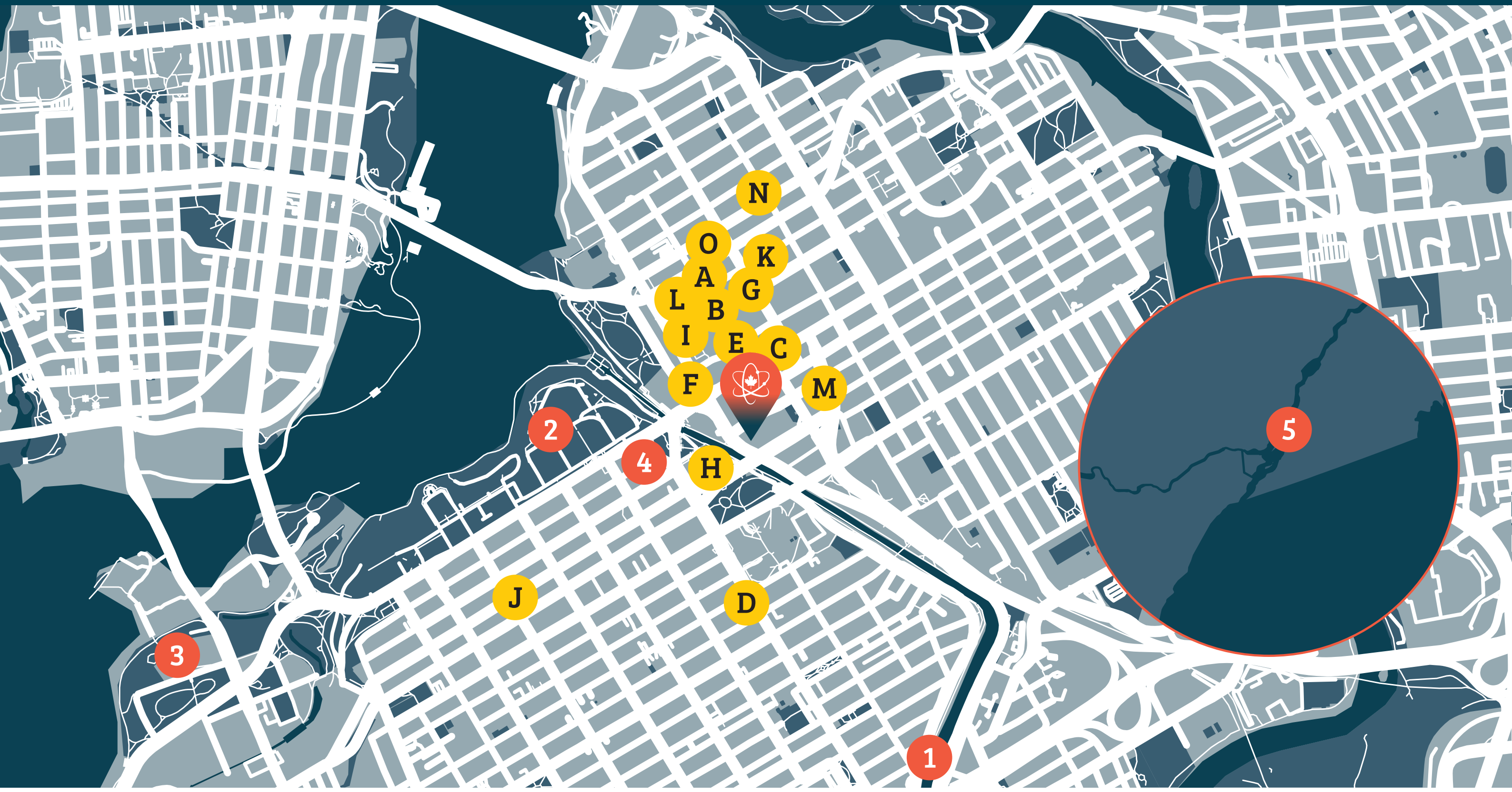
July 29th: CLOSED

July 30th: CLOSED

July 31st: 9:00 – 11:30

Social Media

Follow us on Twitter
@icpeac2023_ca



Ottawa

Points of Interest

1 **Rideau Canal**

2 **Parliament Hill**

3 **Canadian War Museum**

4 **Lady Dive Tour**
Find out more in Program Overview

5 **Montreal (One-Day Tour)**
Find out more in Program Overview

Dining

A **The King Eddy**
Restaurant • $$
613 680 1700

B **Zak's Diner**
Diner • $$
613 241 2401

C **JOEY Rideau**
Restaurant • $$
613 680 5639

D **Johnny Farina**
Italian restaurant • $$
613 680 5639

E **Luxe Bistro**
Steak house • $$$
613 241 8805

F **Metropolitain Brasserie Restaurant**
French restaurant • $$$
613 562 1160

G **Sens House**
Sports bar • $$
613 241 5434

H **1 Elgin Restaurant**
Canadian restaurant • $$$
613 594 5127

I **Restaurant e18hteen**
Restaurant • $$$
613 680 8088

J **Mad Radish**
Health food restaurant • $$
613 421 1356

K **Ahora Mexican Restaurant**
Mexican restaurant • $
613 562 2081

L **Mezzanotte Bistro Italiano**
Italian restaurant • $$$
613 562 3978

M **Norca Restaurant & Bar**
Restaurant • $$
613 691 3218

N **El Taco De Oro**
Mexican restaurant • $$
613 241 4444

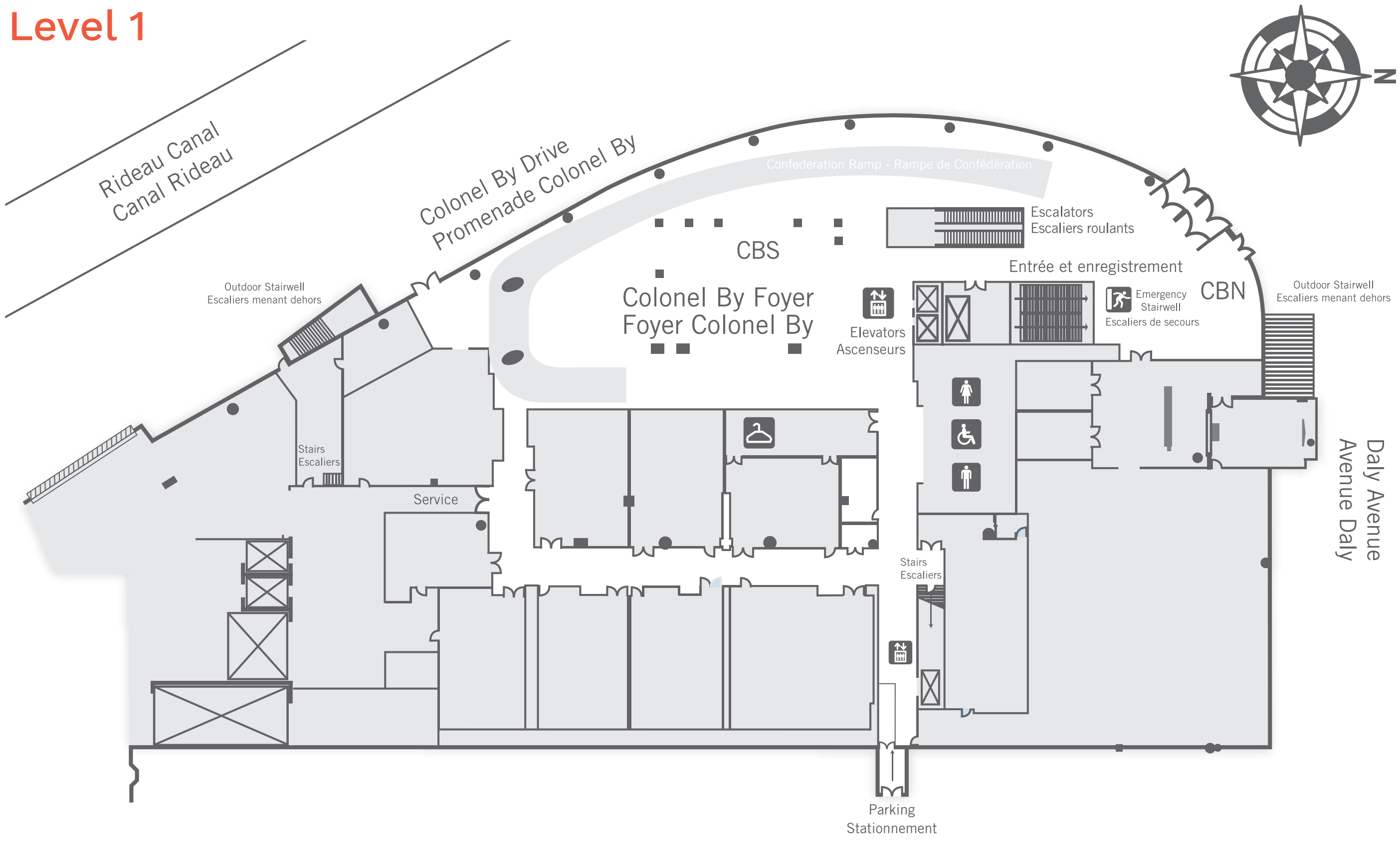
O **Khao Thai Restaurant**
Thai restaurant • $$
613 241 7276

Tutorial Session Location

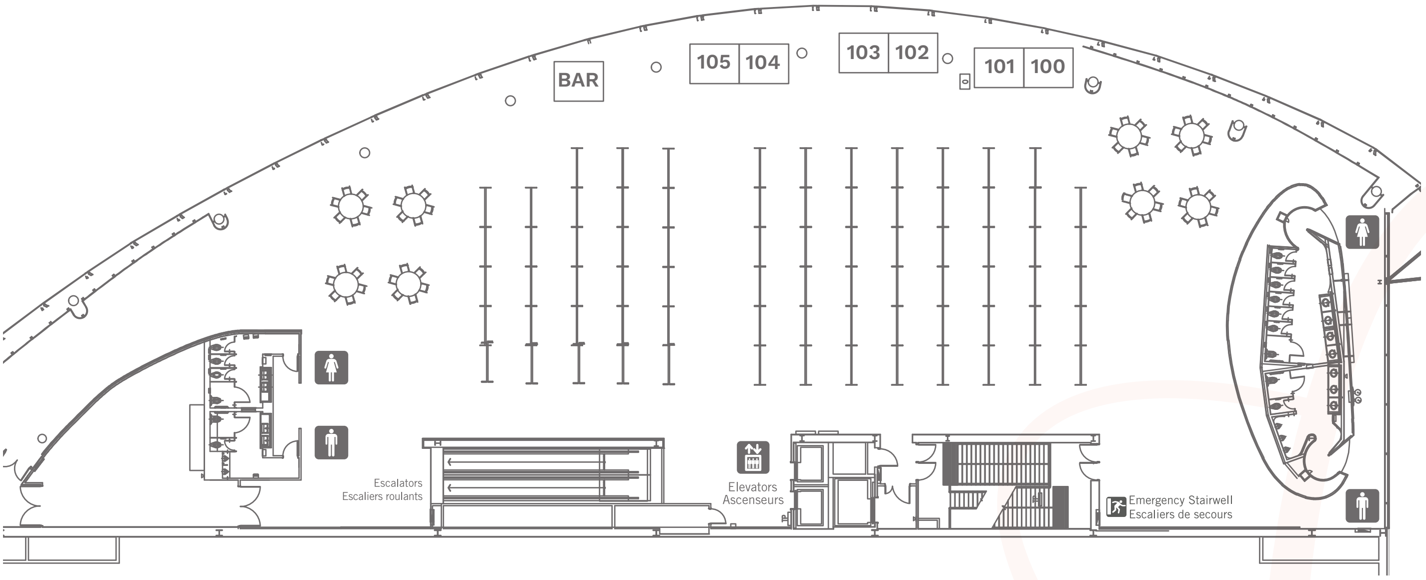
T **Faculty of Social Sciences Building, Room 4007**
120 University Private, Ottawa, ON K1N 6N5

Shaw Centre

Level 1

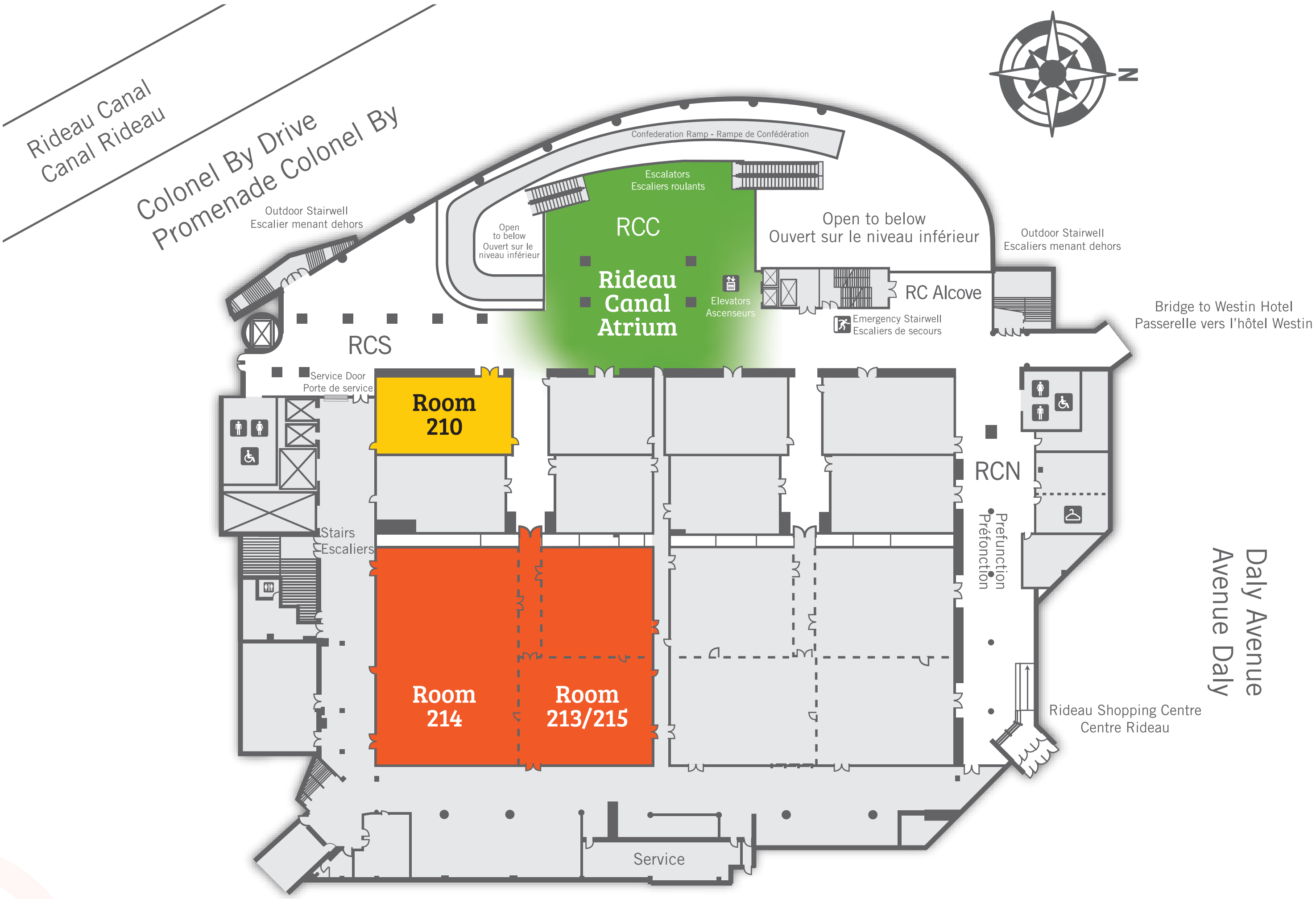


Level 4



Trillium Ballroom • Posters, Exhibition, Gala Dinner

Level 2



🟧 **Room 214** • Plenary, Parallel I, Public Lectures

Room 213/215 • Parallel II

🟨 **Room 210** • Committee Dinner, Committee Lunch

🟩 **Rideau Canal Atrium** • Registration, Welcome Reception

Committees

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Jianmin Yuan China
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Prizes

The IUPAP Early Career Scientist Prize in Atomic, Molecular and Optical Physics 2023

The Early Career Scientist Prize (previously Young Scientist Prize) in Atomic, Molecular and Optical Physics is awarded by the International Union of Pure and Applied Physics (IUPAP) through its Commission C15 (AMO Physics). The 2023 recipient is **Hong-Guang Duan** from Ningbo University, China “for his outstanding contributions to the field of biomolecular lightharvesting and excitation energy transfer, to understand the role of quantum coherence in the exciton transfer dynamics and refine of the tools of nonlinear femtosecond spectroscopy.”

The prize includes a certificate, a medal, a 1,000 € award and an invited presentation at ICPEAC 2023, scheduled for Friday, July 28, 9:30-10:00 am.

The Sheldon Datz Prize for an Outstanding Young Researcher attending ICPEAC

The Sheldon Datz Prize supports an outstanding young researcher (graduate student/post-doc) to attend ICPEAC with a US $1,000 award. The 2023 recipient is **Anna Niggas** from TU Wien, Austria. Anna also happens to be an invited speaker at ICPEAC 2023 (in Parallel Session IX A on Tuesday, August 1, 10:30 – 11:00 am).

Both recipients will be presented with their prize certificates during the Conference Dinner on Monday, July 31.

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Program Overview

XXXIII International Conference on Photonic, Electronic and Atomic Collisions

July 25 - August 1, 2023, Ottawa, Canada

Program Overview

Tuesday, July 25

Tutorial sessions are located at Faculty of Social Sciences Building, Room 4007, 120 University Private, Ottawa, ON K1N 6N5

9:30 - 10:30	**Tutorial I** • Paul B. Corkum • Chair: André Staudte
10:30 - 11:00	**Coffee Break**
11:00 - 12:00	**Tutorial II** • Eva Lindroth • Chair: Tom Kirchner
12:00 - 13:30	**Free Time**
13:30 - 14:30	**Tutorial III** • Emily Lamour • Chair: Marko Horbatsch
14:30 - 15:00	**Coffee Break**
15:00 - 16:00	**Tutorial IV** • Jonathan Tennyson • Chair: Jimena Gorfinkiel
16:00 - 20:00	**Registration and Welcome Reception** • *Rideau Canal Atrium*
18:00	**Executive Committee Meeting and Dinner** • *Room 210*

Wednesday, July 26

8:45 - 9:00	**ICPEAC Opening** • *Room 214*
9:00 - 10:00	**Plenary** • Kenji Ohmori • Chair: Friedrich Aumayr • *Room 214*
10:00 - 10:30	**Coffee Break** • *Trillium Ballroom*
10:30 - 12:30	**Atto I** • Averbukh (PR), Cryan (PR), Douguet (PR), Geyer (SR), Hutcheson (SR) • *Room 214* **Antimatter** • Bray (PR), Nagata (PR), Green (PR), Graves (SR), Nauta (SR) • *Room 213/215*
12:30 - 14:00	**Free Time**
14:00 - 16:00	**Ultrafast** • Centurion (PR), X.Liu (PR), Palacios (PR), Pan (SR), Pajek (SR) • *Room 214* **Astro** • Petrignani (PR), de Barros (PR), Hama (PR), Schneider (PR) • *Room 213/215*
16:00 - 18:30	**Poster Session I** • *Trillium Ballroom*
20:00 - 21:30	**Public Lecture I** • Donna Strickland • Chair: Paul B. Corkum • *Room 214*

Thursday, July 27

9:00 - 10:00	**Plenary** • Ursula Keller • Chair: Dominique Vernhet • *Room 214*
10:00 - 10:30	**Coffee Break** • *Trillium Ballroom*
10:30 - 12:30	**FEL** • Hishikawa (PR), Callegari (PR), Rohringer (PR), Nandi (PR) • *Room 214* **Bio** • Andersen (PR), Rousseau (PR), Kočišek (PR), Lozano (PR) • *Room 213/215*
12:30 - 14:00	**Free Time**
14:00 - 16:00	**Cold I** • Wester (PR), Steinberg (PR), Ishida (PR), Coté (SR), Bouloufa-Maafa (SR) • *Room 214* **Exotic Methods** • Y.Liu (PR), Choubisa (PR), Ngoko Dijokap (PR), Osaku (SR), Giovanetti (SR) • *Room 213/215*
16:00 - 18:30	**Poster Session II** • *Trillium Ballroom*
20:00 - 21:30	**Public Lecture II** • Teresa Scassa • *Room 214*

Friday, July 28

8:30 - 9:30	**Plenary** • Lorenz Cederbaum • Chair: Kiyoshi Ueda • *Room 214*
9:30 - 10:00	**IUPAP Prize Talk** • Hong-Guang Duan • Chair: Rosario González-Férez • *Room 214*
10:00 - 10:30	**Coffee Break** • *Trillium Ballroom*
10:30 - 12:30	**Atto II** • D.Boll (PR), Ruchon (PR), Kheifets (PR), Weber (SR), Magunia (SR) • *Room 214* **El-Molecule** • Houfek (PR), Sinha (SR), Watanabe (SR), Kopyra (PR), Monteiro-Carvalho (SR), Bondy (SR) • *Room 213/215*
12:30 - 14:00	**Free Time**
14:00 - 16:00	**Imaging** • Blume (PR), Wang (PR), R. Boll (PR), Ibrahim (SR), H.V.Sa Lam (SR) • *Room 214* **Spectroscopy** • Okumura (PR), Hori (PR), Loetzsch (PR), Pfäfflein (SR), Zhou (SR) • *Room 213/215*
16:00 - 18:30	**Poster Session III** • *Trillium Ballroom*

Program Overview

Social Tours

Welcome to Ottawa, the perfect place to experience some of the country's best attractions, cultures, and flavors in one welcoming city.

We hand-picked some of the greatest adventures happening this summer across Ontario & Quebec just for the ICPEAC delegates, special offers included!

Make sure to check them out to get the most out of the trip:

Lady Dive Tours

Immerse yourself to the wonderful city of Ottawa with a 6-hour guided tour!

Transportation included (from/to Shaw Centre). Food is excluded. There will be a market stop during the tour where you may purchase meals.

How to Book: Select the "Lady Dive Tour" tickets when you register for the conference

Price: $30 per person (tax included)

Tour sites: Parliament, Canadian Museum of History, Byward Market Square, ...and more!

One-Day Tour to Montréal

During the weekend while you're staying in Ottawa, there is your perfect opportunity to discover Montréal with its bi-cultural heritage and cosmopolitan blend of the old and new on this comprehensive city tour!

Tour Sites: Mont-Royal's Kondiaronk Belvedere, Notre-Dame Basilica, Olympic Tower, Botanic Garden, Old Montreal Walking-Tour, Montréal Downtown, and more.

What's Included: Tours and transportation by coach to and from Ottawa - Montréal, Step-on English speaking guide, Entrance to Notre-Dame Basilica.

Flash Your Badge!

Your badge is your pass! Ottawa Tourism is offering delegate discounts for conference delegates to local participating attractions, tours, and restaurants!

Delegates can use their conference badge to access discounts for them and a guest at participating businesses.

No need to print a passport, simply present your valid event badge to enjoy!

Please contact the attractions in advance to make a reservation or confirm availability.

Whitewater Rafting Day Trip

Join us on the Ottawa River for a day of Whitewater Rafting!

All ICPEAC 2023 delegates enjoy 20% off either trip. Use the discount code **“ICPEAC”** at checkout.

Bus transportation from the Shaw centre is included in the package.

Perfect for ages 13+ and minimum 90lbs.

Book a trip on Sunday, July 30 by visiting:
https://wildernesstours.com/icpeac-2023-group-booking/

VIA Rail Canada

All ICPEAC 2023 delegates are entitled to 10% discount on fares from all stations throughout the VIA system to Ottawa Ontario and return!

Valid through July 22 – August 3, 2023.

Participants must reference the event’s VIA convention discount code: **14389**

Online booking only at VIA Rail Canada Official Website:
https://www.viarail.ca/en/plan/book-travel

Delegates can use this code to travel and tour within/outside Ottawa during the validity period.

Program Overview

Monday, July 31

9:00 - 11:30	**Poster Session IV** • *Trillium Ballroom*
11:30 - 12:30	**Plenary** • Alexander Dorn • Chair: Emma Sokell • *Room 214*
12:30 - 14:00	**Free Time**
14:00 - 16:00	**Synchrotron** • Ganguly (PR), Milosavljevic (PR), Sisourat (SR), Dutta (SR), Trinter (SR) • *Room 214* **Storage Rings** • Hanstorp (PR), Zettergren (PR), Lestinsky (PR), Chacko (SR), Schmidt-May (SR) • *Room 213/215*
16:00 - 16:30	**Coffee Break** • *Rideau Canal Atrium*
16:30 - 18:00	**Complex** • Schöffler (PR), Varella (PR), Ren (SR), Segui (SR) • *Room 214* **Ion Collisions** • Wei (PR), Wolff (PR), Majima (SR), Yang (SR) • *Room 213/215*
19:00 - 22:00	**Conference Dinner** • *Trillium Ballroom*

Tuesday, August 1

9:00 - 10:00	**Plenary** • Amine Cassimi • Chair: Stefan Schippers • *Room 214*
10:00 - 10:30	**Coffee Break** • *Rideau Canal Atrium*
10:30 - 12:30	**Quantum Potpourri** • Niggas (PR), Sato (PR), Niozu (PR), Sheil (PR) • *Room 214* **Cold II** • Hogan (PR), Arora (PR), Gruber (PR), Erdmann (SR), Xie (SR)
12:30 - 13:00	**Business Meeting** • *Room 214*
13:00 - 14:30	**Free Time**
14:30 - 16:00	**Plasmonics** • Pápa (PR), Gholam-Mirzaei (PR), Jalil (SR), Rivera-Dean (SR) • *Room 214* **Recombination** • Ma (PR), Novotny (PR), Zhang (SR), Kalosi (SR) • *Room 213/215*

End of Conference

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Detailed Program & Abstracts of Invited Talks

XXXIII International Conference on Photonic, Electronic and Atomic Collisions

July 25 - August 1, 2023, Ottawa, Canada

Detailed Program

Tuesday, July 25

Tutorial sessions are located at Faculty of Social Sciences Building, Room 4007, 120 University Private, Ottawa, ON K1N 6N5

9:30 – 10:30	**Tutorial I** • *High-harmonic and attosecond-pulse generation, measurement and application* Paul B. Corkum (University of Ottawa and National Research Council, Canada) Chair: André Staudte (National Research Council, Canada)
10:30 – 11:00	**Coffee Break**
11:00 – 12:00	**Tutorial II** • *Amplitude and phase: from cross sections to delays in photoionization* Eva Lindroth (Stockholm University, Sweden) Chair: Tom Kirchner (York University, Canada)
12:00 – 13:30	**Free Time**
13:30 – 14:30	**Tutorial III** • *Ion-matter collisions: new challenges* Emily Lamour (Sorbonne Université, France) Chair: Marko Horbatsch (York University, Canada)
14:30 – 15:00	**Coffee Break**
15:00 – 16:00	**Tutorial IV** • *Electron molecule collision calculations: a primer* Jonathan Tennyson (University College London, UK) Chair: Jimena Gorfinkiel (The Open University, UK)
16:00 – 20:00	**Registration and Welcome Reception** • *Rideau Canal Atrium*
18:00	**Executive Committee Meeting and Dinner** • *Room 210*

High-Harmonic and Attosecond-Pulse Generation, Measurement and Application

P. B. Corkum and D. H. Ko

Joint Attosecond Science Laboratory, University of Ottawa and National Research Council
25 Templeton Street, Ottawa, ON K1N 6N5, Canada

Synopsis Attosecond technology represents three advances in one. Each implies applications: (1) We introduce a new form of nonlinear optics; (2) We synthesize the world's shortest pulses; (3) We control XUV radiation with long wavelength beams, allowing the XUV beam, for example, to focus even without X-ray optics.

In conventional nonlinear optics, bound states describe an electron moving within a quantum system resulting in harmonic generation, but the system always returns to the initial state when it emits coherent photons. If it were not so, phase-matched radiation would not be possible. With attosecond pulses, continuum states play the role of bound states. Thus, in extreme nonlinear optics (1) we free an electron, (2) the electron moves in the continuum under the influence of the strong laser field and (3) it recombines joining the population already present in the original state [1]. Phase matching is still essential. We can never side-step returning to the initial state of the system.

Without perturbation theory as a guiding approximation to high intensity interactions, for extreme nonlinear optics we use classical physics, or the strong field approximation (a semi-classical generalization) for intuitive insight. This is valid because classical physics well describes the motion of electrons in the continuum. Controlling the continuum electron is critical for generating, measuring or applying attosecond pulses.

There are two similar approaches to measuring attosecond pulses – both rely on manipulating the ionized electron.

1. Often called streaking or RABBIT [2], one uses an attosecond pulse (or train of pulses) that has already been produced to irradiate a well understood quantum system, creating photoelectrons that are born into a time-dependent infrared field. The electron's energy (or even phase) serves as an indelible label relating the photoelectron properties with the electron's spectral phase. For a well understood quantum system, we can determine the range of IR-fields in which the electron is generated – the attosecond pulse duration. Delaying the IR pulse relative to the attosecond pulse provides two-dimensional data for a FROG-like algorithm. Alternatively, we can measure the dynamics of a quantum system of interest with a well understood attosecond pulse.
2. Often called perturbative measurement or *in situ* measurement, one uses an intense infrared pulse that will ionize an electron and ultimately creates an attosecond pulse that we will observe. A perturbing pulse can modify the recollision electron's trajectory between birth and recombination. This changes the XUV spectrum encoding the times of birth and recollision including any phase of the transition moments from the initial (bound) state to the final (bound) state [3]. Delaying the perturbing pulse relative to the strong driving pulse provides two-dimensional data for a FROG-like algorithm.

As with all of ultrafast optics, there are many approaches to measurement. One approach is streaking – we time resolve electrons emitted by an attosecond pulse from different levels (or bands) in atoms (or solids) with an infrared field that labels the spectral phase of any electron ionized by the attosecond pulse.

Transient absorption spectroscopy is extensively applied in conventional ultrafast optics. It can be generalized to attosecond phenomena by using an intense beam as a pump to initiate attosecond dynamics. Changes in the absorption spectrum reveal ultrafast dynamics of the system under investigation stimulated by the pump.

References

[1] Corkum, P.B. 1993 *Phys. Rev. Lett.* **71**, 1994
[2] Paul, P.M. et al. 2001 *Science* **292**, 1689
[3] Brown, G.G. et al. 2022 *Phys. Rev. A.* **105**, 023520

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[*] E-mail: pcorkum@uottawa.ca

Amplitude and Phase: From Cross Sections to Delays in Photoionization

E Lindroth[1] *

[1]Department of Physics, Stockholm University, AlbaNova University Center, SE-106 91 Stockholm, Sweden

Synopsis In this tutorial we will discuss the concept of *delay in photoionization*, how it can be understood and calculated, and in particular how this is connected to our ability to handle photoionization cross sections and atomic structure.

Photoionization is a fundamental process where light interacts with matter and electrons are released. A complete description of the ionized electron wave packet requires the knowledge of both its spectral amplitude and phase. Information about the amplitude has since the first half of the previous century been obtained through cross section measurement. The fantastic development of light sources and techniques since the field was born, from lasers and synchrotrons to high-harmonic generation and free-electron lasers, has over the years produced precise cross section data for a wide range of quantum systems as well as photon energies. The phase of the wave packet was, however, always more elusive. There are some traditional routes to phase information: as the angular dependence of the photoelectrons [1] where the relative phase of different angular momentum channels come into play, or the asymmetric line profiles [2] produced by the interference of different ionization paths, but the attosecond (as) techniques that have been exploding since the beginning of this century, have provided many more ways to obtain phase information.

Through the process of high-harmonic generation, pulses, or trains of pulse, with a sub-femtosecond duration, are produced. The temporal resolution they allow for is routinely in the region of a few ten attoseconds [3]. From Bohr's model of the atom we can estimate the "revolution" time for the electron in the hydrogen ground state to be around 150 as, and thus it clear that we are in the position to study electron dynamics.

In this tutorial lecture I will discuss how the electron dynamics, and especially the *delayed* response to photoabsorption, is encoded in the phase of the electron wave packet. We will see how "old" subjects such as angular anisotropy or resonances due to quasi-bound states can be studied from a new angle when also the phase is accounted for. The focus will be on the theoretical understanding and treatment where the quantum many-body problem remains a challenge.

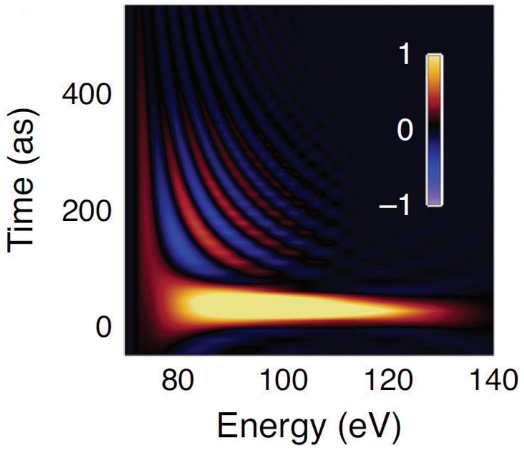

Figure 1. The Wigner representation of photoelectrons emitted after absorption of photon energies in the vicinity of the threshold for $4d$-ionization in xenon showing the different time-scales of the contributing resonances, from Ref. [4]

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Ion-Matter Collisions: new challenges

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Synopsis The objective of this tutorial is to underpin the role of fundamental processes that are involved from the first moments of the interaction between highly charged ions and matter. When they are well known, the knowledge and mastery of these processes allow to probe and/or modify matter in a controlled manner, and even to highlight specific phenomena. We will also discuss what can be learned from ion-ion collisions in a regime where the ion energy loss is maximal.

When multicharged ions interact with matter, the latter is subjected to strong fields (which can reach up to 10^9 V/cm), often for extremely short durations (from femtoseconds to a few attoseconds) inducing electronic dynamics that are more or less understood. In ion-matter collisions, different "velocity" regimes are usually defined but to distinguish them, a collision strength parameter need to be introduced since the ion velocity is not the only relevant parameter.

In the "low velocity regime", typically at center-of-mass energies of a few keV to a few 100 keV, the ion captures target electrons in highly excited states, which is by far the dominant process. On the contrary, in the "high velocity regime", the so-called perturbative regime, the ion mainly loses its electrons (ionization) or they are promoted in excited states (excitation). For those collision regimes, the cross sections of the electronic processes are fairly well reproduced by existing theories. From there, we will wonder if we can use this knowledge to probe, for instance, the magnetic order of a sample surface [1] or to modify/optimize a given ion charge state at the exit of a target [2]. With these two examples we will take the opportunity to give an overview of the experimental techniques implemented at heavy-ion accelerators.

A third collision regime is one in which the ion stopping power is maximum, resulting in the most significant effects on material modifications (including biological material [3]). At the atomic level, there, all the primary electronic processes reach their optimum probability and are of the same order of magnitude. Consequently, the experimental determination of the effective cross section of a single elementary collision process becomes extremely difficult even when dealing with a "simple" ion-atom collision (beyond proton - hydrogen atom collision). In this regime, available theoretical calculations are at their limit of validity and there is a crucial lack of measurements. In other words, this regime corresponds to a real 'terra incognita' for atomic physics of collisions. So how to unravel such complex electronic dynamics? This is only possible if the presence of many electrons can be avoided and/or controlled on each of the collision partners, i.e. the projectile and the target, but the development of an ion-ion collider in this velocity regime remained a real challenge!

In this tutorial, we will see how we can not only investigate the pure 3-body problem (bare heavy ion on hydrogenic target) but also study the role of additional electrons - one by one-bounded to the projectile and/or the target. Beyond the 3-body problem that will serve as a benchmark for theories, we will explore how to quantify a whole series of effects that will be tackled during the presentation. We will also discuss the technical obstacles that need to be overcome, as well as the possibility of using state-of-the-art accelerators available today to perform those hyper-demanding and challenging experiments [4].

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Electron molecule collision calculations: a primer

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Synopsis Electron-molecule collisions are important in a variety of natural processes ranging from lightning to the the chemistry of the interstellar medium, and drive technological plasmas which underpin much of modern industry. This tutorial will discuss the variety of process that occur following an electron collusion appropriate methods for computing cross sections for different electron energy regimes.

There is a great demand for electron molecule collision cross sections driven by the desire to model key process both natural and technological. This demand is largely being met by theory given the difficulty and expense of experiments which also find it difficult to probe key processes ranging from electron impact rotational excitation of molecular ions (important for models of interstellar medium spectra) to electon collisions with open shell molecules (radicals) which form an important driver in cold (molecular) plasmas.

Appropriate methods for treating electron molecule collisions depend on the kinetic energy of the impacting electron. Broadly these can be divided into the low energy regime where the electron has insufficient energy to the ionize the target molecule; the high energy regime (above about 50 eV) where simplified treatments often yield excellent results and the challenging intermediate energy regime which straddles the ionization regime. There is also the case the high energy relativistic regime but this is only important in special circumstances such as cosmic ray ionization.

While some processes such as electron impact ionization can be treated using simplified (semi-empirical) procedures; generally detailed scattering calculations are required to obtain energy-dependent cross sections. In the low energy regime so-called resonances, where the scattering electron is temporarily trapped in a quasi-bound state, provide prominant structures in the cross sections and drive much of the processes. In this regime procedures such as close-coupling bear some similarities with quantum chemistry calculations, albeit with the need to treat processes lying in the continuum. At high energies, electron collisions can often be treated using procedures based on perturbation theory such the Born approximation. At intermediate energy quasi-complete treatments such as the convergent close-coupling or R-matrix with pseudo states have been demonstrated to give excellent results, although so far their application has been restricted to collisions with simple (few electron) molecular targets.

This tutorial lecture will discuss the various processes that can result from electron collisions with molecules and methods available for their study. Attendees will be given a temporary licence to the QEC (Quantemol electron collisions) expert system [1] which drives the UK molecular R-matrix code UKRmol+ [2] to allow them to explore performing electon – molecule collision calculations.

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Detailed Program

Wednesday, July 26

8:45 – 9:00	**ICPEAC Opening** • *Room 214*
9:00 – 10:00	**Plenary Session I** • *Ultrafast quantum simulation and quantum computing with ultracold atom arrays at quantum speed limit* • *Room 214* Kenji Ohmori (Institute for Molecular Science, National Institutes of Natural Sciences, Japan) Chair: Friedrich Aumayr (TU Wien, Austria)
10:00 – 10:30	**Coffee Break** • *Trillium Ballroom*
10:30 – 12:30	**Parallel Session I A: Attosecond Physics I** • *Room 214* Chair: Madhusree Roy Chowdhury (Synchrotron Soleil, France)
10:30	*PR: Quantum coherence and entanglement in attosecond atomic and molecular photoionization* Vitali Averbukh (Imperial College London, UK)
11:00	*PR: Coherent and nonlinear attosecond spectroscopy in molecules* James Cryan (SLAC National Accelerator Laboratory, USA)
11:30	*PR: Theoretical and numerical advances for the study of ultra-fast and strong-field phenomena in atoms and molecules* Nicolas Douguet (Kennesaw State University, USA)
12:00	*SR: Experimental fingerprint of the electron's longitudinal momentum at the tunnel exit in strong field ionization* Angelina Geyer (Goethe-Universität Frankfurt, Germany)
12:15	*SR: Core-resonance line-shape analysis of atoms undergoing strong-field ionization* Lynda Hutcheson (Queen's University Belfast, UK)
10:30 – 12:30	**Parallel Session I B: Antimatter** • *Room 213/215* Chair: Ilya Fabrikant (University of Nebraska-Lincoln, USA)
10:30	*PR: Calculating antihydrogen formation via excited positronium-antiproton scattering* Igor Bray (Curtin University, Australia)
11:00	*PR: Fundamental studies of positronium using a high-quality energy-tunable positronium beam* Yugo Nagata (Tokyo University of Science, Japan)
11:30	*PR: Many-body theory of positron interactions with molecules* Dermot Green (Queen's University Belfast, UK)
12:00	*SR: R-Matrix investigations of low-energy positron scattering from biomolecules* Vincent Graves (The Open University, UK)
12:15	*SR: Ultra-high precision laser spectroscopy of anti-hydrogen* Janko Nauta (Swansea University, UK)

12:30 – 14:00	**Free Time**
14:00 – 16:00	**Parallel Session II A: Ultrafast Dynamics** • *Room 214* Chair: Chitra Rangan (University of Windsor, Canada)
14:00	*PR: Ultrafast imaging of molecular dynamics with electron diffraction* Martin Centurion (University of Nebraska-Lincoln, USA)
14:30	*PR: Ultrafast molecular imaging with intense femtosecond laser fields* Xiaojun Liu (Innovation Academy of Precision Measurement Science and Technology, Chinese Academy of Sciences, China)
15:00	*PR: Attosecond pump-probe spectroscopy: XUV and X-ray induced ultrafast electron* Alicia Palacios (Universidad Autónoma de Madrid, Spain)
15:30	*SR: An ultrafast stopwatch to clock and manipulate molecular dynamics* Shengzhe Pan (East China Normal University, China)
15:45	*SR: Clocking ultrafast relaxation of Rydberg hollow atoms at surfaces by x-rays* Marek Pajek (Jan Kochanowski University, Poland)
14:00 – 16:00	**Parallel Session II B: Astrophysics** • *Room 213/215* Chair: Daniel Savin (Columbia University, USA)
14:00	*PR: Spectroscopy of interstellar complex organic molecules* Annemieke Petrignani (University of Amsterdam, The Netherlands)
14:30	*PR: Ion and photon processing of astrophysical ice analogues* Ana de Barros (Federal Center for Technological Education - CEFET/RJ, Brazil)
15:00	*PR: Experimental approaches towards understanding the surface physics and chemistry of interstellar dust and atmospheric aerosols* Tetsuya Hama (The University of Tokyo, Japan)
15:30	*PR: Electron-induced reactivity of molecular cations relevant for astrochemistry and cold plasmas* Ioan F. Schneider (Université Le Havre Normandie, France)
16:00 – 18:30	**Poster Session I and Exhibition** • *Trillium Ballroom*
20:00 – 21:30	**Public Lecture I** • *Generating high-intensity, ultrashort optical pulses* • *Room 214* Donna Strickland (University of Waterloo, Canada) Chair: Paul B. Corkum (University of Ottawa and National Research Council, Canada)

Ultrafast quantum simulation and quantum computing with ultracold atom arrays at quantum speed limit

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[2] **SOKENDAI (The Graduate University for Advanced Studies), Okazaki**, 444-8585, Japan

Synopsis The ultrafast quantum simulator/computer with ultracold atom arrays that we are developing are based on a new concept where quantum simulators/computers are driven by ultrafast lasers. This new approach allows us to execute a controlled-Z gate, a conditional two-qubit gate essential for quantum computing, in only 6.5 nanoseconds at quantum speed limit. This is faster than any other controlled gates with cold atoms by two orders of magnitude. It is also two orders of magnitude faster than the noise from the external environment and operating lasers, so that the effect of noise can be neglected.

Many-body correlations drive a variety of important quantum phenomena and quantum machines including superconductivity and magnetism in condensed matter as well as quantum computers. Understanding and controlling quantum many-body correlations is thus one of the central goals of modern science and technology. My research group has recently pioneered a novel pathway towards this goal by exciting strongly interacting ultracold Rydberg atoms, far beyond the Rydberg blockade regime, by using an ultrafast laser pulse [1-6]. We first applied our ultrafast coherent control with attosecond precision [2,3] to a random ensemble of those Rydberg atoms in an optical dipole trap, and successfully observed and controlled their strongly correlated electron dynamics on a sub-nanosecond timescale [1]. This new approach is now applied to arbitrary atom arrays assembled with optical lattices or optical tweezers that develop into a pathbreaking platform for quantum simulation and quantum computing on an ultrafast timescale [4-6].

In this ultrafast quantum computing, we have recently succeeded in executing a controlled-Z gate in only 6.5 nanoseconds at quantum speed limit, as schematically shown in Fig. 1, where the gate speed is solely determined by the interaction strength between two atomic qubits [6]. This is faster than any other controlled gates, conditional two-qubit gates essential for quantum computing, with cold-atom hardware by two orders of magnitude. It is also two orders of magnitude faster than the noise from the external environment and operating lasers, whose timescale is in general 1 microsecond or slower, and thus can be safely isolated from the noise. The speed of this controlled gate compares favorably also with the ones demonstrated so far with superconducting qubits [7], paving the way towards high-fidelity quantum computers with neutral atom arrays.

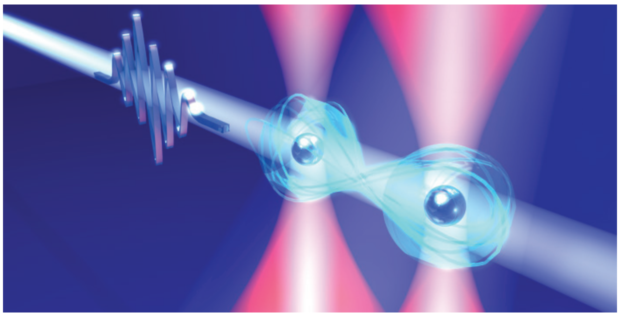

Figure 1. Conceptual diagram of the ultrafast controlled gate for quantum computing. Two single rubidium atoms captured in optical tweezers (red light) with a separation of a few micrometers are entangled by an ultrafast laser pulse (blue light) shone for only ~10 picoseconds [6]. Image source: Dr. Takafumi Tomita (IMS).

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Quantum coherence and entanglement in attosecond atomic and molecular photoionisation

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Synopsis Atomic and molecular photoionisation by attosecond pulses may lead to creation of coherent superpositions of ionic states and as a result to coherent dynamics of the electron hole taking the form of hole migration in molecular ions or electron cloud breathing in atomic ions. The quantum entanglement between the photoelectron and the ion which precludes the ionic state coherence can be probed and verified by the Bell tests.

Molecular photoionisation by attosecond pulses may lead to creation of coherent superpositions of ionic states by coupling of a series of such states to the same continuum wavefunction of the photoelectron. The temporal extent of the resulting coherent hole dynamics that can be seen as a migration of the electron hole across the molecular volume [1] is limited by decoherence stemming from the zero-point energy of the nuclear vibrations, the nuclear motion itself, as well as by the electronic decay of the ionic wavepacket components above the double ionisation threshold. In this presentation, I will discuss the theoretical interpretation of the recent hole migration experiments performed at the LCLS [2] and FLASH [3] X-ray free electron laser facilities and targeting the electronic observables, such as time-dependent Auger electron signal [4]. I will also describe our progress in developing the *ab initio* many-electron theoretical tools, such as B-spline ADC and Fano-ADC [5,6], that allow us to gain insight into the mechanisms of the onset and decay of the coherent hole dynamics. Combining application of such *ab initio* tools with analytical modelling has led us to propose a number of new spectroscopic approaches for direct observation of coherent many-electron dynamics in ionised systems, such as interferometric measurement of Auger decay dynamics and of quantum revivals below the double ionisation threshold [7,8], as well as pump-probe spectroscopy of Auger decay [9]. While these schemes still await their experimental realisation, attosecond measurement of the *resonant* Auger decay of a coherent superposition of core-excited states has been very recently achieved by the angular streaking technique [10].

A central role in the generation of the ionic coherence belongs to the quantum entanglement between the photoelectron and the atomic or molecular ion. We have developed and simulated numerically a Bell test for probing the quantum entanglement in photoionisation [11]. We have designed and simulated the quantum protocol for entanglement quantification for the case of noble gas atoms photoionised by ultrashort, circularly polarised infra-red laser pulses in the strong-field regime, demonstrating robust violation of the Bell inequality. The Bell test developed in our work detects entanglement between the internal states of the Ar^+ and the spin states of the photoelectron by exploiting the spin polarisation of the photoelectron beam.

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Coherent and nonlinear attosecond spectroscopy in molecules

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Synopsis We study the ultrafast motion of electrons using site-specific x-ray spectroscopy.

The ultrafast motion of electrons is a key component of every photochemical process. Given the electron volt-scale energy differences of electronic excited state in small molecular systems, the natural timescale for electronic motion is typically in the few- to sub-femtosecond regime. Consequently, the study of ultrafast electronic phenomena requires light pulses that can access this extreme timescale. At the same time, soft x-ray spectroscopy provides a convenient probe of electronic densities with atomic-site specificity. So, attosecond soft x-ray pulses are a useful tool to elucidate the earliest processes involved in chemical change.

Free Electron Lasers (FELs), such as the Linac Coherent Light Source (LCLS), are a source of high-brightness ultrashort x-ray pulses, with wavelength continuously tunable across the x-ray regime. Schemes to provide isolated, sub-femtosecond pulses from an FEL are being explored at facilities world-wide, and recently we have demonstrated such pulses using the LCLS [1]; opening the door for time-resolved measurements of ultrafast electron dynamics on their natural timescale. In my talk I will highlight our recent developments in probing electonic motion in small molecular systems.

We exploit the interaction between strong-laser fields and x-ray ionized electrons to study the temporal profile of the electron emission pattern using the angular streaking technique [2]. We have observed the creation and subsequent Auger-Meitner decay of a coherent superposition of core-excited states in nitric oxide [3]. We have performed subsequent experiments exploring the time-domain behavior of an entanglement photoelectron/photoion pair.

We have made use of the high peak power pulses from an FEL to develop x-ray nonlinear spectroscopies such as stimulated X-ray Raman scattering (SXRS) [4] and pump/probe spectroscopy. I will also show our first results on attosecond pump/probe experiments of ultrafast charge dynamics following x-ray ionization. These dynamics are probed using x-ray absorption spectroscopy by a time-delayed attosecond x-ray pulse.

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Theoretical and numerical advances for the study of ultra-fast and strong-field phenomena in atoms and molecules

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Synopsis We present our recent theoretical and numerical advances to investigate ultra-fast and strong-field phenomena in atoms and molecules in the gas phase. These developments enable to shade light on the complex electron dynamics in systems subjected to intense optical fields, to explore new effects with twisted light, and to reveal the role of electron correlation in strong fields. These methods are employed to study a variety of processes, such as attosecond streaking, attosecond interferometry, chiral recognition, and high harmonic generation.

The development of intense and ultrashort laser sources has revolutionized our study of light-matter interactions by making it possible to study the electron dynamics in atoms and molecules at its natural time scale. These astonishing advances require the design of always more sophisticated theoretical approaches to describe the interaction of complex targets with intense fields. Here, we present new computational techniques to explore some of the exciting aspects of attosecond science.

The calculation of classical and quantum electron trajectories is first used to provide a different framework to analyze strong-field phenomena in elliptical [1] and linear optical pulses [2]. In particular, quantum trajectories can reveal the transition between photoionization regimes and the effect of the target structure on the electron tunneling dynamics.

Optical vortex beams, i.e., spatially inhomogeneous light carrying orbital angular momentum (OAM), also offer promising applications for dynamical quantum control of matter and high-resolution microscopy. We use time-dependent simulations accounting for the light OAM to explore new streaking and chiral recognition techniques. We also consider high harmonic generation (HHG) with optical vortex beams and analyze the generation of attosecond twisted light with large topological number, including the time evolution of the spatial intensity distribution.

Finally, while processes with intense optical pulses are generally assumed to be dominated by single-electron dynamics, important multi-electron effects, e.g., the removal of an electron from different atomic/molecular orbitals, electron-electron correlation and exchange, as well as the polarization of the photo-ion, can strongly influence the electron dynamics in complex systems. To account for these effects, we have developed a new *ab initio* method, ATTOMESA, that uses a hybrid gaussian and finite-element discretized variable representation (FEDVR) basis set to solve the time-dependent Schrödinger equation (TDSE). ATTOMESA allows us to treat the interaction of multi-electron systems with intense optical pulses, e.g., to study strong-field ionization of poly-atomic systems, or the effect of electron correlation in HHG, as we recently showed it can play an important role [3]. Preliminary results and future applications of ATTOMESA are discussed.

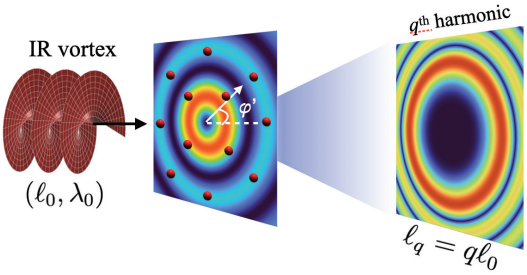

Figure 1. A gas of atoms is illuminated by an optical vortex beam with wavelength λ_0 and topological number ℓ_0, resulting in the generation of high harmonics with large topological number.

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Experimental fingerprint of the electron's longitudinal momentum at the tunnel exit in strong field ionization

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Synopsis We present experimental data on the strong field tunnel ionization of argon in a counter-rotating two-color (CRTC) laser field. We find that the initial momentum component along the tunneling direction changes its sign comparing the rising and the falling edge of the CRTC field. If the initial momentum at the tunnel exit points towards the ion at the instant of tunneling, this manifests as an enhanced Coulomb interaction of the outgoing electron with its parent ion. Our conclusions are in accordance with predictions based on strong field approximation.

The strong field ionization of argon is experimentally investigated using a counter-rotating circularly polarized two-color (CRTC) field. The two-color field (central wavelengths of 390 nm and 780 nm) is generated in an interferometric two-color setup [1]. The intensity of the 780 nm [390 nm] pulse is $8.5 \times 10^{13}\,\mathrm{W/cm^2}$ [$5.6 \times 10^{13}\,\mathrm{W/cm^2}$]. The three-dimensional electron momentum distribution is measured using cold target recoil ion momentum spectroscopy (COLTRIMS) [2].

We experimentally observe a qualitatively new feature in the electron momentum distribution. We find that this feature emerges because the component of the initial momentum at the tunnel exit that points towards or away form the residual ion modifies the Coulomb interaction of the electron with its parent ion after tunneling [4].

Fig. 1(a) shows the measured electron momentum distribution. Electrons that are born on the falling edge of the CRTC field (marked by a black circle) form a wing-like structure. We have performed a simulation using the non-adiabatic classical two-step (NACTS) model to reproduce the measured observables (see Fig. 1(b)) [3]. (c) [(d)] shows the initial momentum perpendicular [parallel] to the time-dependent laser electric field at the instant of tunneling as a function of the instant of tunneling t.

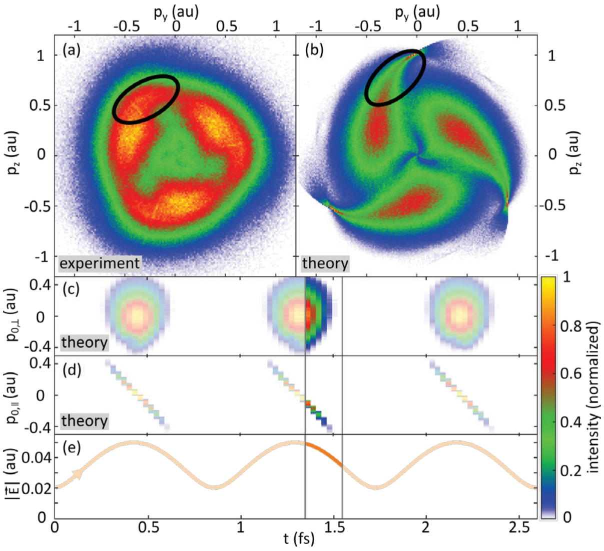

Figure 1. (a) Measured electron momentum distribution for the ionization by a CRTC field. (b) Simulated electron momentum distribution. (c) [(d)] Initial momenta perpendicular [parallel] to the time-dependent laser electric field at the instant of tunneling as a function of the electron's release time t. (e) Absolute laser electric field as a function of t. The events between the two gray lines in (c)-(e) belong to final momenta in the black circle in (a) and (b).

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Core-resonance line-shape analysis of atoms undergoing strong-field ionization

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Synopsis We investigate the build-up of absorption lines in xenon ions as a function of the near-infrared (NIR) pump intensity during strong-field ionization. We observe a half-cycle-periodic change in the line-shape asymmetry of the ionic $4d-5p$ resonances. In particular, we find the phase of the induced dipole emission is modified and the magnitude of this phase modulation decreases with increasing laser intensity. We discuss the influence of ground state depletion on interfering pathways involved in XUV-assisted strong-field ionization.

Attosecond transient absorption spectroscopy (ATAS) is well suited for the time-resolved investigation of strong-field ionization (SFI) since the all-optical approach probes the system while it is being ionised. Using XUV spectrometers with high spectral resolution, absorption lines can be investigated not only with respect to their energy and line/oscillator strength, but also their specific shape. The continuous transition from a symmetric Lorentzian to an asymmetric Fano line is the result of a change in the phase of the underlying dipole [1].

In this contribution, we perform a systematic analysis of the line shape of an ionic core-to-valence transition in xenon using ATAS at different NIR pump intensities [2]. We extract the dipole phase from the measured/simulated line-shape and identify an indirect ionization pathway. Strong-field ionization of neutral xenon from an XUV core-excited virtual state interferes with the direct pathway of valence-shell strong-field ionization. This interference leads to delay-dependent asymmetry changes of a xenon ion XUV absorption line shape. More specifically, we observe delay-dependent NIR-half-cycle oscillations of the line-shape asymmetry whose amplitude decreases with increasing NIR pump intensity. We attribute this effect to the depletion of the neutral ground state, and hence a weakening of the interfering virtual pathway, which is confirmed by calculating the remaining neutral Xe population [3].

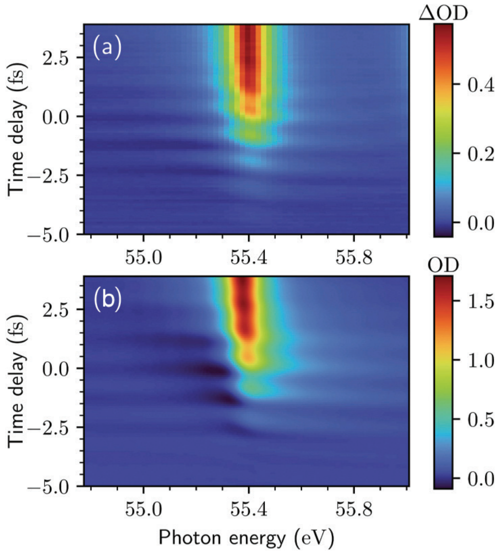

Figure 1. Attosecond transient absorption spectroscopy scan centered on the $5p_{3/2}^{-1} \rightarrow 4d_{5/2}^{-1}$ transition in the time-delay overlap region at an NIR intensity of $1.9 \pm 0.21 \times 10^{14}$ Wcm^{-2}. (a) Measured and (b) simulated optical density, computed with the *ab initio* RMT approach. Delay of probe with respect to pump, pump centered at zero.

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Calculating antihydrogen formation via excited positronium-antiproton scattering

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Synopsis Using the combination of Classical Trajectory Monte-Carlo (CTMC) and fully quantal Convergent Close-Coupling (CCC) theories we establish benchmark cross sections for antihydrogen formation cross sections via the collision process of excited positronium and antiprotons.

The motivation for undertaking the experimental challenge of creating antihydrogen includes tests of symmetry as searches for departures from the Standard Model of Particle Physics, and antimatter tests of the Weak Equivalence Principle of General Relativity [1]. Furthermore, experiments at CERN's "Antimatter Factory" intend to study the gravitational behaviour of antihydrogen. The challenge is to make as many antihydrogen atoms as possible to enable the experiments to be performed.

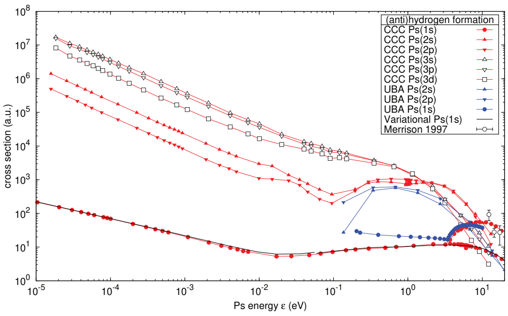

Figure 1. Antihydrogen formation cross sections in Ps(nl)-antiproton scattering, from Ref. [2].

From the theoretical stand point, one pathway to antihydrogen formation is via positronium Ps(nl) scattering on antiprotons, where n and l are the principal and orbital angular momentum quantum numbers, respectively. This is equivalent to Ps(nl) scattering on protons, which can be calculated simultaneously with Ps(nl) formation in positron scattering on atomic hydrogen. Applying CCC to such calculations we showed that the cross section for antihydrogen formation increases very rapidly with increasing n [2], see figure.

Once the importance of large n was established we created the collaboration with CTMC [3, 4] to test the correspondence principle [5], scaling with n, and various threshold laws. As the CTMC calculations become reasonably accurate for $n > 3$ their utility comes to the fore due to their lower computational cost and the capacity to include electro-magnetic fields in the calculations.

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Fundamental studies of positronium using a high-quality energy-tunable positronium beam

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Synopsis A high-quality energy-tunable positronium beam was applied for the observation of the Ps hyperfine resonance in the ground state and the measurement of the photodetachment threshold of positronium negative ions. A Ps transmission experiment through graphene is currently underway for the observation of Ps diffraction.

Positronium (Ps), the bound state of an electron and its antiparticle positron, is hydrogen-like, but because of its reduced mass and the positron spin, the energy levels are much different from hydrogen. The interactions between Ps and materials are also different and, hence, Ps has attracted a lot of interest so far.

In order to study the interaction between Ps and gases, a Ps beam with an energy from 1 eV to 400 eV was developed by the University College London group by using the electron capture process of slow positrons passing through a gas cell. The Ps beam was applied to the measurements of the cross sections of Ps scattering from various gas molecules and electron-like scattering was found [1].

As another method to generate energy tunable Ps beams, at Tokyo University of Science we use the photodetachment of accelerated positronium negative ions (Ps^-), bound states of one positron and two electrons [2]. This was made possible by the discovery that Ps^- is efficiently produced by the bombardment of an alkali metal-deposited tungsten surface with slow positrons [3]. The kinetic energy of the Ps beam is tuned from 0.2 keV to 3.3 keV by changing the Ps^- acceleration voltage. The energy width is determined by the recoil of the photodetached electrons and is around a few percent.

We used this beam to observe the Ps hyperfine resonance by using a static periodic magnetic field [4]. The field was generated by a multi-layered magnetic grating. The grating was a stack of iron and copper foils and had slot holes. As Ps atoms passed though the slots of the grating, they felt a time-dependent oscillating magnetic field in their center-of-mass system. When the field frequency coincided with the Ps hyperfine transition frequency of ~200 GHz, the resonance was observed.

The photodetachment threshold of Ps^-, corresponding to the electron affinity of Ps was also measured by using a tunable optical parametric oscillator and amplifier laser [5]. The threshold energy was experimentally determined for the first time to be 326.88 ± 0.09 (stat) $\pm$ 0.10(syst) meV.

Furthermore, we are trying to observe the diffraction or interference of Ps, which has not been observed so far. Ps diffraction would be a neutral and non-destructive new method to analyse a surface structure by diffraction. The Ps interference is also expected to be used for the measurement of the gravitational force of antimatter [6]. To observe the Ps diffraction, we make the Ps beam pass through a graphene sample and obtain a Ps beam transmission profile. The pattern of the Ps profile will be discussed.

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Many-body theory of positron interactions with molecules

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Synopsis I will present the many-body theory of low-energy positron-molecule interactions and its computational implementation in our `EXCITON+` code. The method takes accurate account of strong positron-molecule correlations. It provided the first *ab initio* calculations of positron binding energies in agreement with experiment [*Nature* **606**, 688 (2022)]. These, and new calculations for molecules including heterocyclics and polyaromatic hydrocarbons will be detailed, as will the extension to scattering and annihilation rates and γ-ray spectra.

Positrons are unique probes of matter, with applications in materials science (as ultra-sensitive diagnostic studies of surfaces, defects and porosity), medical imaging (PET), astrophysics, fundamental AMO physics and molecular spectroscopy, and tests of symmetries and gravity, see e.g., [1, 2, 3] and references therein. The proper interpretation of the AMO experiments and materials science techniques, and the development of antimatter-based technologies and applications requires fundamental knowledge of positron-atom/molecule interactions.

Low-energy positron interactions with atoms and molecules are characterised by strong correlations including polarisation, screening of the electron-positron Coulomb interaction and virtual-positronium formation (temporary tunnelling of the electron to the positron). They significantly modify scattering, and enhance annihilation rates by orders of magnitudes, and even cause positron binding [1, 2, 3]. They also make the theoretical description of positron-atom/molecule interactions a challenging many-body problem (made more formidable for molecules that bind the positron due to vibrational Feshbach resonances that spectacularly enhance annihilation rates [2]).

Focussing on the correlation part of the problem, we have developed a diagrammatic many-body theory of positron-molecule interactions and its state-of-the-art computational implementation (via our Gaussian-orbital-based `EXCITON+` code) that takes *ab initio* account of the dominant correlations. As a first application, we calculated binding energies for a range of polar and non-polar molecules, focusing chiefly on the molecules for which both theory and experiment exist, but also making predictions, e.g., of positron binding to DNA nucleobases [3]. This work gave the first accurate *ab initio* calculations in agreement with the decades of pioneering measurements [2]; quantified the effects of the correlations, e.g., showing that virtual-positronium formation significantly enhances binding in polar molecules and is essential to support binding in non-polar molecules; and elucidated the importance of the anisotropic nature of the potential and the individual roles of molecular orbitals. I will discuss these, and new calculations of positron binding energies in molecules including chlorinated and fluorinated hydrocarbons [4], heterocyclics, and polyaromatic hydrocarbons [5]. Time permitting, I will also present the recent extension of the method to positron scattering and annihilation rates in small molecules [6] and to annihilation γ-ray spectra [5].

*Performed in collaboration with C. H. Patterson (Trinity College Dublin), and my Queen's University Belfast group members J. Hofierka, B. Cunningham, C. M. Rawlins, A. R. Swann, J. P. Cassidy and S. K. Gregg. It was funded by the ERC, grant 804383.

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R-Matrix investigations of low-energy positron scattering from biomolecules

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Synopsis When modelling low energy lepton scattering from biomolecules, accurately describing polarization effects is very important. In positron scattering, this description is particularly crucial, since exchange effects are not present. Conventional scattering approaches struggle to model the interaction targets with high polarizability. Here, improvements to this description are investigated.

Modelling low energy lepton scattering from molecules has applications in many areas. Specifically, PET scans used in medicine to provide highly detailed images of biological matter involve the production inside the body. The focus of the work presented here is to provide data on low energy positron collisions which can be used in combination with higher energy data to model positron interactions with biological matter.

We use the R-Matrix method as implemented in the UKRmol+ suite [1]. In this method, the low energy lepton scattering problem is separated into an inner region, where the projectile-target molecule interaction is accurately described, and an outer region, where correlation and exchange can be neglected. Within the R-Matrix method, polarization effects are modelled by including configurations in the expansion of the inner region target + projectile wave function that correspond to excitations from the ground state configuration. These effects are particularly crucial at low scattering energy, when the projectile spends more time in the interaction region of the molecule. For positron scattering, there is no exchange and, as a result, the accuracy of the polarization and correlation/anti-correlation description become crucial.

We have investigated methods for improving the polarization description in R-matrix calculations of positron and electron scattering from highly polarizable biomolecules. These include using the Polarization Consistent Coupled Hartree-Fock method [2] and enhancing the electron-positron attraction integrals [3].

The effect from these methods can be seen in Figure 1 that presents positron scattering from furan which has a spherical polarizability of 48.79 Å. It can be seen that the Static plus Polarization (SP) calculations, with or without the enhancement factor, as well as the PCCHF approach underestimate the size of the cross section. Inclusion of a Born correction is unlikely to resolve this discrepancy. Note that the step-like shape of the experimental cross section is due to different acceptance angles at different scattering energies.

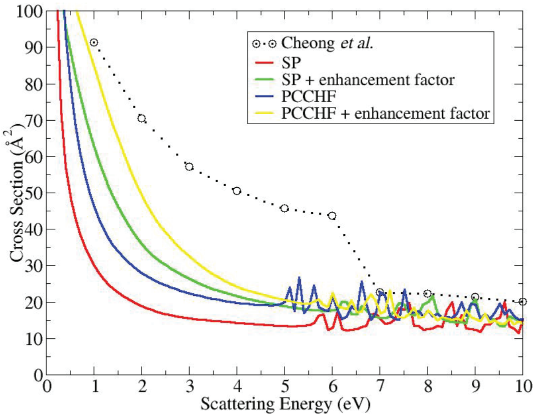

Figure 1. Elastic cross section for positron scattering from furan calculated using different models and compared with experimental results [4]. No Born correction is included in the calculations shown. The spikes in the ross sections are pseudoresonances.

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Ultra-high precision laser spectroscopy of anti-hydrogen

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Synopsis To study fundamental symmetries between matter and antimatter, we aim to improve the precision of 1S-2S frequency measurement in antihydrogen, exploiting recent advances in antihydrogen accumulation and laser cooling. Therefore, we have implemented an active hydrogen maser and a Cs fountain clock as a local realization of the SI second. This will advance our frequency determination capability towards a fractional uncertainty as low as 10^{-15}.

One of the big open questions in modern-day physics is the discrepancy between the matter-antimatter imbalance that is observed in the universe, and the balance required by the theoretical foundations that underpin the Standard Model. Hydrogen plays a fundamental role in the development of our understanding of quantum physics, which requires hydrogen to have the same energy levels as its antimatter counterpart, the antihydrogen atom. The 1S-2S transition in hydrogen has been measured to a fractional uncertainty of $4.2 \cdot 10^{-15}$ [1], while our previous measurement in antihydrogen yields a relative precision of $2 \cdot 10^{-12}$ [2]. Very recent advances have demonstrated that antihydrogen can now be accumulated and directly laser cooled [3]. Here, recent results and progress to improve the metrology capability of our laser system that will enable more accurate frequency determinations.

The Antihydrogen Laser Physics Apparatus (ALPHA) collaboration at CERN traps slow antiprotons in a Penning trap and combines the antiproton plasma with positrons to form antihydrogen. Antiatoms with a kinetic energy of less than 0.54 K are magnetically trapped and illuminated with a cavity-enhanced laser beam of 243 nm, exciting the forbidden 1S-2S transition. Absorption of a third photon leads to ionization and subsequent detection of the annihilating antiproton by a silicon vertex detector.

The optical frequency of the 243 nm laser system is counted via a frequency comb, which was previously referenced by a GPS-disciplined quartz oscillator. To improve on this, we recently implemented an active hydrogen maser, which is compared to other masers in national metrology labs via GNSS common-view frequency transfer. To correct the maser independently of long-baseline links and obtain a local realization of the SI second, we are currently implementing a Cs fountain clock, which has been built at NPL [4]. The maser alone already led to an improvement of our frequency determination capability by an order of magnitude, while the implementation of the Cs fountain and fiber pathlength stabilization will enable fractional frequency uncertainties of 10^{-15} or better.

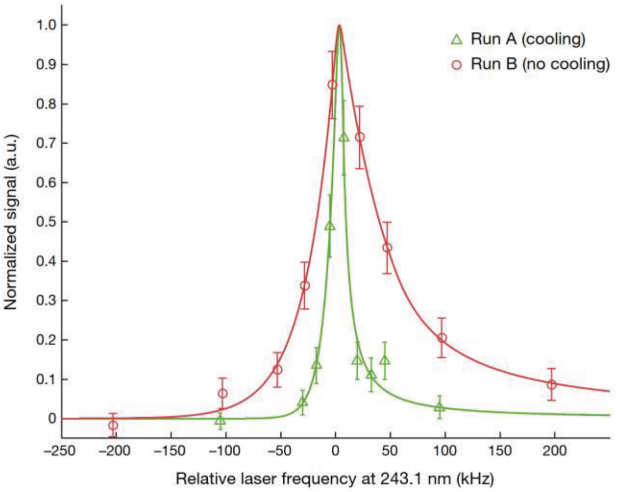

Figure 1. Demonstration of the effect of laser cooling on the linewidth of the 1S-2S transition in antihydrogen. [3]

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Ultrafast imaging of molecular dynamics with electron diffraction

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Synopsis Ultrafast electron diffraction has recently become an established method to investigate structural dynamics in photoexcited molecules, revealing new details about the motion of nuclear wavepackets and reaction dynamics. Here we go beyond the current state-of-the-art to study more complex molecules with multiple reaction channels and to probe reactions triggered by photoionization.

Many important chemical and biological reactions are driven by the conversion of light into chemical and mechanical energy at the level of single molecules. These reactions are characterized by changes in the nuclear geometry that take place on femtosecond time scales. Observing the reactions as they take place is important to understand and eventually control the dynamics and reaction products.

Capturing structural changes in real time is challenging due to the extremely high requirements on the combined spatial and temporal resolution of sub-Angstrom and femtoseconds.

Recent advances have enabled ultrafast electron diffraction (UED) to successfully capture coherent nuclear motions on the relevant time scales [1]. UED has been applied to spatially resolve a wavepacket traversing a conical intersection [2] and to capture ring opening and dissociation reactions [2,3]. So far, UED has been limited mostly to investigate small photoexcited molecules with few reaction channels. Here, we describe two recent extensions of UED: investigating more complex molecules with multiple reaction products, and probing reactions triggered by ionization [4].

We have investigated the dynamics of Cyclo-octadiene excited by femtosecond laser pulses with a wavelength of 200 nm. The experiments are supported by quantum chemical calculations of the reaction dynamics [5]. We have found good agreement between experiment and theory by calculating the UED signal (the observable) from the trajectory simulations. After photoexcitation, the molecule traverses a conical intersection to reach the ground state, where multiple products are formed. In particular, we have identified the main structural changes in the excited state and observed the formation of multiple products soon after reaching the ground state.

We have also extended the capabilities of UED to investigate reactions trigger by ionization. This presents additional challenges because the ionized gas sample can distort the electron beam, and because the once the molecule is ionized the widely used independent atom model no longer accurately describes the diffraction signal. We have found that for short time delays of up to a few picoseconds, the distortion is minimal even for the case of strong-field ionization. Additionally, we have found that the diffraction signal can be accurately modeled using ab-initio scattering methods where the independent atom model fails. We will show an example where UED is used in combination with other experimental methods and ab-initio scattering to determine the products formed by strong field ionization of toluene [6].

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Ultrafast molecular imaging with intense femtosecond laser fields

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Synopsis We experimentally and theoretically investigate the two-dimensional photoelectron momentum spectra of aligned diatomic molecules in an intense femtosecond laser field. By analyzing the interference patterns in the photoelectron spectra of N_2, we successfully reconstruct the highest occupied molecular orbital (HOMO) and extract the molecular internuclear separation. Our work demonstrates that photoelectron spectroscopy in intense laser fields still has unexplored potential for imaging molecular structure and dynamics.

Imaging the structure and ultrafast dynamics of gas-phase molecules poses a major challenge in physics, chemistry and biology. Advances in intense femtosecond laser technology have offered new opportunities in this research area. In the process of intense laser-molecule interaction, the outermost electron of a molecule will be tunnel ionized through the laser field-suppressed barrier. The tunnel-ionized electron carries the information of the molecular orbital, which can be retrieved with photoelectron spectroscopy. Moreover, the tunnel-ionized electron may recollide with the multi-atomic core and form distinct interference structures in the final photoelectron momentum distribution from which the molecular structure can be reconstructed [1].

In this talk, we will report our recent progress in molecular imaging with intense laser fields. We propose a novel method based on laser-induced electron tunneling spectroscopy (LETS) with aligned molecules to retrieve the phase information of the ionizing molecular orbital [2]. By analyzing the interference pattern in the low enery part of the photoelectron spectrum, the weighted coefficients and the relative phases of the constituent atomic orbitals for a molecular orbital can be extracted. With this information we reconstruct the highest occupied molecular orbital of N_2, which is well consistent with the ab initio orbital calculation (see Fig.1). Moreover, our measurement shows a prominent valley structure in the alignment dependence of the high-energy photoelectron spectra along the laser polarization direction. In the framework of the molecular strong-field approximation (MSFA) theory, this novel valley structure is well reproduced and further, simple semiclassical analysis reveals its origin as a direct evidence of the destructive two center interference from the rescattered electrons. Based on this two-center interference, we show that detailed information about the molecular structure, i.e., the internuclear separation, can be extracted directly from the alignment dependent photoelectron spectra [3].

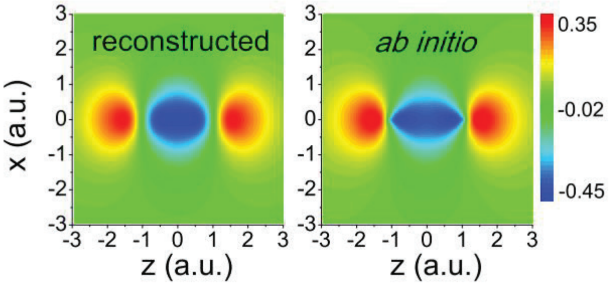

Figure 1. The reconstructed and *ab initio* calculated molecular orbital wavefunction of N_2.

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Attosecond pump-probe spectroscopy: XUV and X-ray induced ultrafast electron dynamics in gas-phase targets

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Synopsis We pursue an accurate theoretical description of the ultrafast dynamics in molecules triggered and traced using different attosecond pump-probe spectroscopic approaches. First, recent applications using HHG sources will be discussed, specifically employing RABBIT techniques, which have shown their great potential to extract time-resolved information on the molecular landscape felt by the ejected electrons. Second, unexplored non-linear phenomena that arise in similar pump-prome schemes when using the more intense ultrashort and highly coherent pulses produced in free electron laseres will be presented.

We explore and exploit the new capabilities of coherent light sources producing sub-femtosecond pulses to manipulate electronic dynamics in atoms and molecules with attosecond resolution.

Attosecond pump-probe spectroscopy using high-order harmonic generation has made it possible to retrieve time-resolved images of molecular excitation and ionization processes [1], at the heart of electron and charge transfer reactions of multidisciplinary interest. In the last years, a wide range of XUV-IR pump-probe protocols have been employed and shown their suitability to retrieve and manipulate electron dynamics in atoms and, more recently, in molecules. Among the variety of schemes, the RABBIT (reconstruction of attosecond beating by interference of two-photon transitions) technique has become particularly successful, e.g., in the retrieval of the so-called photoionization time delays. For molecular targets, an accurate description of the coupled electron-nuclear motion is a requirement when light atoms are involved as proven in recent joint experimental-theoretical in the hydrogen molecule [2,3]. These studies show that the variations of the photoionization time delays with the nuclear kinetic energy can be as large as variations with the electron kinetic energy. Recent applications of this scheme to polyatomic molecules will be discussed [4].

Despite the success of the XUV-IR schemes, it is known that one typically finds that the IR field dominates the dynamics and/or distorts the atomic or molecular potential. We thus have also explored the use of one and two-color pump-probe schemes with attosecond resolution employing ultrashort pulses with XUV frequencies in molecules, and ranging up to the soft X-ray frequency region, as those currently available in free-electron laseres (FELs).

The high intensities and brilliance of light pulses produced in FELs and X-ray FELs give access to a manifold of non-linear phenomena that have remained experimentally unexplored until now [5,6], e.g., time-resolved images of Auger decay or a wide range of highly coherent multiphoton ionization processes in molecules. We will discuss our recent theoretical developments to describe non-linear phenomena induced in atomic and small molecular targets, in experiments performed at FEL facilities, as well as briefly review the new progresses to explore ultrafast charge migration proceses in large molecules using these facilities.

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An ultrafast stopwatch to clock and manipulate molecular dynamics

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Synopsis Light-molecule interactions play a crucial role in photochemistry, at the heart of which is the breaking and formation of chemical bonds. Our ultrafast stopwatch scheme aims to clock the stretching of chemical bonds, explore fundamental physical mechanisms, and further manipulate light-induced molecular dynamics.

For molecules exposed in strong laser fields, valence electrons absorb photons and escape from the ionic potential, while the remaining cation interacts with the strong field and dissociates as nuclear fragments. In this respect, if we construct an ultrafast strong laser pulse characterized by time-dependent polarizations, the time information of ejected electrons and nuclear fragments can be recorded experimentally, and full-dimensional molecular dynamics are explored in principle.

In this presentation, we propose the scheme of an ultrafast stopwatch by constructing a polarization-skewed (PS) laser pulse and demonstrate its powerful applications in clocking and manipulating molecular dynamics in experiments. The PS laser pulses have unique characteristic of resolving ultrafast dynamics within neighboring optical cycles compared to linearly or circularly polarized ones.

First, we demonstrate a straightforward method on clocking the dissociative above-threshold double ionization of H_2 [1], where two electrons and two protons are measured in coincidence. As illustrated in Fig. 1(a), the instants of the first and second ionization steps are encoded in the emission directions of two released electrons, forming an X-shaped momentum distribution. The time interval between the two ionization steps can be extracted from their crossing angle.

Second, we propose a universal approach to time the bond-stretching process during the strong-field dissociation of H_2 from molecular-frame electron angular distributions [2]. The time-energy-resolved proton-electron coincidence measurements reveal the participation of high vibrational states beyond resonant one-photon or net-two-photon dissociation pathways [3].

Third, we discover the parallel and perpendicular multiphoton transitions in dissociative ionization of H_2. Our results demonstrate the ability of the waveform-shaped PS pulses to control reaction pathways through the manipulation of hybrid parallel and perpendicular transitions, as depicted in Fig. 1(b).

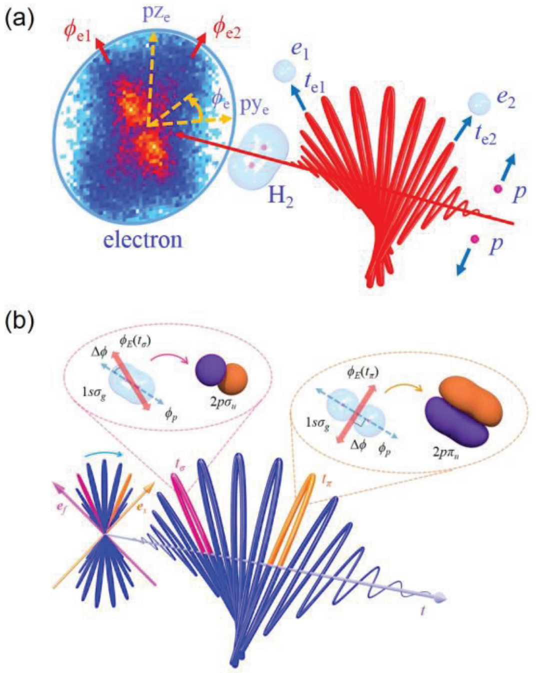

Figure 1. Schematic illustrations of the ultrafast stopwatch using a multicycle PS laser pulse to (a) clock the dissociative above-threshold double ionization and (b) manipulate parallel and perpendicular transitions and thus reaction pathways of H_2 molecules.

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Clocking ultrafast relaxation of Rydberg hollow atoms at surfaces by x-rays

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Synopsis Ultrafast relaxation of Rydberg hollow atoms (n ~ 30), formed in collions of slow highly charged Xe^{q+} ions (q ~ 30) with Be surface, was studied by observing the x-ray emission. The measured spectra of Paschen series, dominated by fast (nf→3d) electric dipole x-ray transitions, exhibit a cut-off at high $n_{cut} \sim 20$ indicating a domination of faster interatomic Coulombic decay (ICD) process for higher n-states. Using the measured fluorescence yields we demonstrate that relaxation of RHA proceeds in a femtosecond time scale.

In slow collisions of highly charged ions Xe^{q+} ions ($q >> 1$) with surfaces the highly excited Rydberg ($n \approx q$) hollow atoms (RHA) are formed [1]. They rapid relaxation to the ground state in solids was a subject of intese debates in last years. In particular, in the experiments with monoatomic layers [2,3] it was demonstrated that relaxation of RHA preceeds in a femotosecond time scale [2] and it was proposed [3] that ICD process [4] is responsible for a successive deexcitation of RHA, but only between the highest Rydberg states. Consequently, further relaxation of RHA down to ground state needs more investigations.

In the present experiment we have studied x-ray emission from collisions of slow, highly charged Xe^{q+} ions (q=23-36) with metallic Be foil in order to access more details on relaxation of RHA in solids. The pulsed beams of Xe^{q+} ions were produced in the EBIS facility and the dominating M-X-rays (nf→3d) emitted in radiative relaxation of highly excited Xe were measured by a Si drift detector.

The measured x-ray spectra, which were interpreted in terms of the MCDF calculations, clearly demonstrate, despite of the radiative and Auger deexcitation, the importance of more exotic two-electron relaxation processes in RHA, namely, the internal dielectronic excitation (IDE) [5], the interatomic Coulombic decay (ICD) and the two-electron-one photon (TEOP) transitions. By interpreting the x-ray spectra measured for different charge states, relative contributions of discussed processes were extracted and the decay rates were estimated using known decay rates of radiative transitions as "internal clock". In particular, by observing a cut-off of x-ray emission in the measured Paschen series at $n_{cut} \approx 23$ for Xe^{35+} ions, it was demonstrated *experimentally* that ICD plays dominating role in early stage ($n > n_{cut}$) of nonradiative relaxation of RHA in solids. Further ($n < n_{cut}$) fast deexcitation of hollow atoms by Auger and IDE processes, as estimated from the measured x-ray fluorescence yields, makes the full relaxation to the ground state an ultrafast process with estimated lifetime of about 1.8 femtosecond.

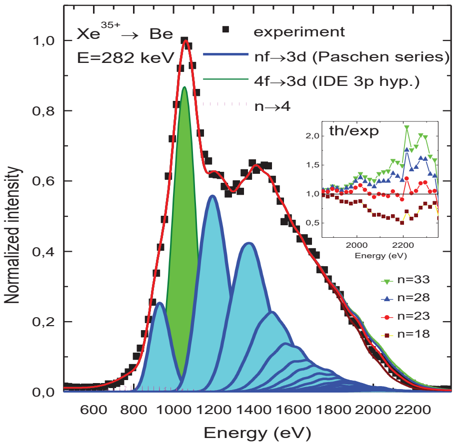

Figure 1. Measured spectrum of M-x-ray nf→3d transitions (Paschen series) in collisions of Xe^{35+} ions with Be. Contributions of IDE (3p-hypersatellite) and ICD cut-off for $n_{cut} \approx 23$ are shown in the figure.

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Spectroscopy of interstellar complex organic molecules

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Synopsis We study the photolysis and signatures of interstellar Polycyclic Aromatic Hydrocarbons (PAHs) using Resonant Enhanced MultiPhoton Ionisation (REMPI), Infrared Multiple Photon Dissociation (IRMPD), and IR-UV double resonance spectroscopy combined with calculations. Our studies reveal vibrational [1,2] and electronic [3] coupling effects to be much stronger in PAHs than expected, photolysis processes leading to isomerisation [4,5,6], and unexpected (F)IR [7,8] and electronic [3] signatures.

Interstellar chemistry constitutes rich organic photochemistry with a large part of the cosmic carbon locked up in Polycyclic Aromatic Hydrocarbons (PAHs). We study the spectral and fragmentation behavior of neutral and ionic PAH species, ranging from symmetric to irregular and small to large using IR-UV double resonance spectroscopy, Resonant Enhanced MultiPhoton Ionisation (REMPI), and Infrared Multiple Photon Dissociation (IRMPD) combined with quantum chemical calculations.

The electronic studies of neutral PAHs reveal irregular species to exhibit strong coupling between electronic states, leading to enhanced transitions in the visible spectral range where the Diffuse Interstellar Bands (DIBs) are observed [3]. The electronic spectra typically exhibit narrow features for the first excited state accompanied by broad features when the second excited-state enters. In combination with calculation, molecular structure was found to induce large spectral shifts, attaining the visible spectral region already for smaller neutral species.

The vibrational behaviour studies of ionic PAHs reveal interesting excited-state dynamics and subsequent fragmentation behaviour. Photolysis of phenylium leads to isomerization of the carbon skeleton before dissociation [4]. Upon photoadsorption, facile ring opening prevents direct H loss and, instead, induces small hydrocarbon fragments. Upon photolysis of deuteronated PAHs, D and H scramble across the PAH perimeter at different rates, resulting in the D atom(s) securing aromatic position(s) and H atoms being more prone to fragment. The mid- to far-IR spectroscopic studies of deuteronated anthracene and phenenthrene demonstrate the ability of PAHs to thus act as a sink for interstellar deuterium [6]. At high excitation energies, H-PAH photodissociation leads to five-ring formation [5]. Further studies in the FIR reveal PAHs to exhibit some surprisingly strong and narow bands [7,8] and little to no spectral congestion. This makes these FIR fingerprints useful candidates for benchmarking and for the search for individual large PAHs in the ISM. Moreover, the irregularly shaped dibenzo[a,l]pyrene cation loses hydrogen alone upon irradiation, despite its 'exposed' pendant rings. The armchair edges could facilitate hydrogen loss while resisting hydrocarbon loss.

These studies illuminate the necessity of experiment to advance theory and unravel the evolving interstellar carbon chemistry.

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Ion and Photon Processing of Astrophysical Ice Analogues

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Infrared absorption spectroscopy was used at various GANIL beamlines and ultraviolet irradiation experiments to examine the interaction of heavy ions and photons with astrophysical model ices. This made possible to simulate the physico-chemical changes caused in astrophysical icy objects exposed to radiation fields such the solar wind and interstellar cosmic rays. The synthesis of organic and inorganic molecules are all briefly covered. The question of the early circumstances for the emergence of life is connected to the latter subject.

The evolution of matter within the star-life cycle in our galaxy is governed by a variety of astrophysical processes, including radiation field processing and astrochemical processes, such as radiation effects, reactions at gas-grain surfaces, ice photochemistry, and so on. After dense molecular clouds collapse, interstellar dust particles are integrated into protoplanetary systems. Therefore, the so-called primitive matter can be influenced by interstellar stuff. Later, planets like the early Earth may get this material from asteroids and comets (made of ice and dust and circling in the Oort cloud, Kuiper belt, or Jupiter family). Laboratory astrochemistry has demonstrated that under interstellar and circumstellar conditions, complex molecules, such as polycyclic aromatic hydrocarbons (PAH), amino acids and nucleobases, can be formed by vacuum UV irradiation, electron and ion bombardment of interstellar ice analogs containing small molecules (H_2O, CO, CO_2, CH_3OH, NH_3, HCOOH), which are the fundamental constituents of organic matter (H, C, N, O, and others). As a result, irradiation processing of ice mixtures may be connected to the issue of how organic matter came to be on Earth by supplying potential precur-sors to the advent of life here and maybe on other bodies in the solar system.

In this work, we conduct an experimental investigation of the impact of heavy ion radiation at intensities that are more comparable to real cosmic rays and ultraviolet (UV) photon radiation (Fig.1). The GANIL accelerator[1] provides high-energy ion in the MeV to GeV range. UV photolysis experiments were performed at NASA Ames Research Center[2] in conjunction with in-situ infrared spectroscopic monitoring of ice mantles. It is common knowledge that a photon or a fast heavy ion's interaction with an ice target is a compli-cated one. By taking into account the phenomenon's many characteristics in succession, partial scenarios are created. In an ion-solid interaction, the projectile and the target atoms repeatedly collide, causing an ongoing transfer of energy from the projectile to the solid. Our research at GANIL [1,3] has demonstrated that heavy cosmic rays—as opposed to other ionizing radiations like protons and UV photons [2,4]—play a dominant role in electronic sputtering, as well as destruction and fragmentation (radiolysis).

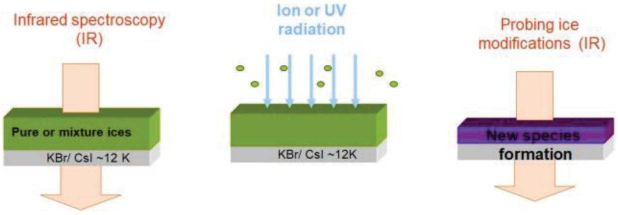

Figure 1. An illustration of the experimental process. The thin ice coating that has been deposited on a KBr or CsI crystal is impinged upon perpendicularly by the ion beam.

We will present some results that can help to answer some questions such as: 1) How to compare processes in complex ice? Are they intrinsically different? 2) Can we build reliable solid state astrochemistry data? 3) Can we lift some of the IR limitations to securely interpret astrophysical data? 4) What does the presence of ice in different astrophysical media tells us?

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Experimental approaches towards understanding the surface physics and chemistry of interstellar dust and atmospheric aerosols

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Synopsis This talk provides an overview of the current level of understanding of physicochemical surface processes on interstellar dust at low temperatures around 10 K, with emphasis on experimental investigations about adsorption, diffusion, and quantum-tunneling reactions of H atoms. I also present our recent laboratory studies for understanding of the photochemistry of liquid fatty acids to elucidate their impact on the troposphere in the Earth.

Astronomical observations have revealed that interstellar clouds, the birthplaces of stars, are chemically rich despite their low-temperature (around 10 K) and low-pressure environments (10^4 cm^{-3}). Around 280 molecules have been discovered in interstellar space. In interstellar clouds, the surface of dust grains is covered by the solid forms of molecules such as H_2O, CO_2, NH_3, CH_4, H_2CO, and CH_3OH. This icy dust is a dominant solid component of interstellar clouds and has played a critical role as a building block for the formation of, for example, the gas and icy giants and comets in the early solar system. For understanding the formation of the solar system, laboratory study of the surface chemistry on interstellar dust is thus highly desirable.

In this talk, we describe our recent experimental studies about surface diffusion and quantum tunneling reaction of H atoms on the ice surface around 10 K [1-4]. At 10 K, even volatile species such as H atoms can barrierlessly adsorb on the dust surface through van der Waals forces (physisorption). In addition, chemical reactions having a barrier can proceed on surfaces through quantum tunneling. These tunneling reactions are crucial in explaining the abundances of molecules such as H_2CO and CH_3OH in interstellar clouds, where thermally activated reactions rarely occur.

If time allows, we also present our recent study for development of a new experimental apparatus for the ultraviolet laser photolysis of liquids by laser-induced fluorescence. Our new approach enables direct detection of OH radicals photodesorbed from the surface of a liquid organic sample.

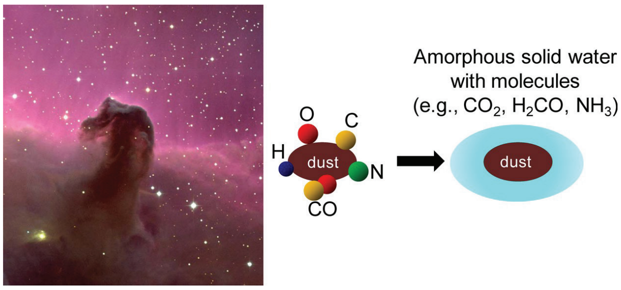

Figure 1. (Left) Part of the Orion molecular cloud containing the Horse Head Nebula. (Credit and copyright: N. A. Sharp/NOAO/AURA/NSF.) (Right) Schematic description of the morphological and chemical structure of dust grains [2].

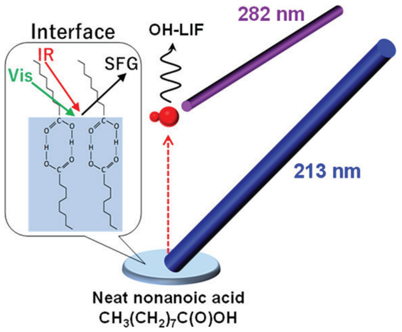

Figure 2. Schematic diagrams of 213 nm photolysis of liquid organic molecules and OH radical probing [5].

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Electron-induced reactivity of molecular cations relevant for astrochemistry and cold plasmas

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Synopsis The major features of the electron/molecular cation reactive collisions at extreme energies are displayed and explained, in the case of recently studied species (including isotopologues): H_2^+, CH^+, ArH^+, BeH^+, NeH^+, CF^+ and some polyatomic ions.

The shape of the cross sections characterizing the dissociative recombination and the rovibrational excitation depends strongly on the energy of the incident electron.

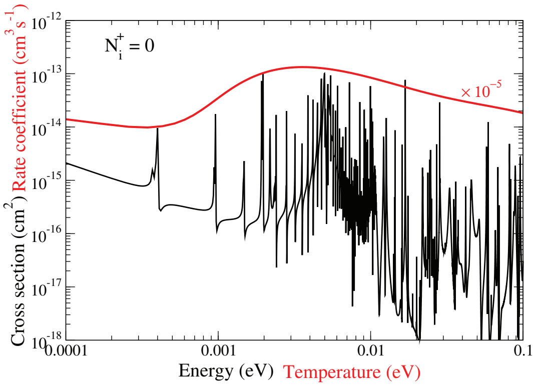

Figure 1. Cross section and thermal rate coefficient of dissociative recombination of ground state D_2^+ (X $^2\Sigma_g^+$, $N_i^+ = 0, v_i^+ = 0$). The thermal rate coefficient is scaled by 10^{-5}.

At energies of the order of few vibrational quantas, most of the ionization channels are closed, which implies a huge number of resonances corresponding to temporary captures of the electron into Rydberg bound states of ground electronic core. This complex behavior is very well modeled by our method based on the Multichannel Quantum Defect Theory (MQDT) [1], which we have applied in the case of H_2^+ and isotopologues [1] - Figure 1 - CH^+ [2], BeH^+ [3] and ArH^+ [4]. At higher energy, the incoming electron can be captured into core-excited Rydberg states, generating broader and more complex resonances [5].

Above the dissociation threshold of the target the number of dissociative states of the neutral increases, the Rydberg resonances disappear, and a further process, the dissociative excitation, competes the dissociative recombination and the ro-vibrational excitation. We studied this latter process in the case of ArH^+ [4] and of BeH^+.

Recently, we addressed the low-energy electronic collisions on NeH^+ - governed by non-adiabatic interactions rather than Rydberg-valence ones as for the previously mentioned species - and we re-visited the collisions with CF^+, using a new approach based on the combination between the MQDT and the direct determination of the reaction matrix using the UK R-matrix based Quantemol-N programme suite [6].

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Detailed Program

Thursday, July 27

9:00 – 10:00	**Plenary Session II** • *Ionization in intense laser fields beyond the electric dipole approximation* • *Room 214* Ursula Keller (ETH Zürich, Switzerland) Chair: Dominique Vernhet (Sorbonne Université, France)
10:00 – 10:30	**Coffee Break** • *Trillium Ballroom*
10:30 – 12:30	**Parallel Session III A: Studies at Free-Electron Lasers** • *Room 214* Chair: Kenichi Ishikawa (The University of Tokyo, Japan)
10:30	*PR: Ultrafast electron-ion coincidence spectroscopy with XUV FEL* Akiyoshi Hishikawa (Nagoya University, Japan)
11:00	*PR: Phase-controlled multiple pulse experiments with atoms and molecules* Carlo Callegari (Elettra – Sincrotone Trieste, Italy)
11:30	*PR: Enhancing elastic x-ray scattering by control of transient electronic populations* Nina Rohringer (Universität Hamburg, Germany)
12:00	*PR: Studying coherent light-matter interaction with a seeded free-electron laser* Saikat Nandi (Institut Lumière Matière, CNRS, France)
10:30 – 12:30	**Parallel Session III B: Biomolecules** • *Room 213/215* Chair: Lucas Sigaud (Universidade Federal Fluminense, Brazil)
10:30	*PR: Spectroscopy of biological molecular ions* Lars Henrik Andersen (Aarhus University, Denmark)
11:00	*PR: Heavy ion interactions with biological and biomimetic systems* Patrick Rousseau (UNICAEN – CIMAP, France)
11:30	*PR: Electron collisions with systems of increasing complexity* Jaroslav Kočišek (J. Heyrovský Institute of Physical Chemistry, Czech Republic)
12:00	*PR: Electron induced bond breaking in radiosensitizing compounds* Ana Isabel Lozano (Consejo Superior de Investigaciones Científicas/Universidade NOVA de Lisboa, Spain/Portugal)
12:30 – 14:00	**Free Time**
14:00 – 16:00	**Parallel Session IV A: Cold Matter I** • *Room 214* Chair: Joseph Thywissen (University of Toronto, Canada)
14:00	*PR: Quantum collisions of cold molecular ions in traps* Roland Wester (Universität Innsbruck, Austria)
14:30	*PR: Measuring the tunneling time for ultracold atoms, and the unexpected emergence of spin textures via collisions between incident and reflected atoms* Aephraim Steinberg (University of Toronto, Canada)

15:00	*PR: Recent progress towards positronium Bose-Einstein condensation* Akira Ishida (The University of Tokyo, Japan)
15:30	*SR: Resonant processes and their impact in many-body dynamics* Robin Côté (University of Massachusetts Boston, USA)
15:45	*SR: Two-photon optical shielding of collisions between ultracold polar molecules* Nadia Bouloufa-Maafa (Université Paris-Saclay, France)
14:00 – 16:00	**Parallel Session IV B: Exotic Methods** • *Room 213/215* Chair: Jian Wu (East China Normal University, China)
14:00	*PR: Strong-field ionization of atoms with sculptured laser fields* Yunquan Liu (Peking University, China)
14:30	*PR: Ionization studies of water molecules using twisted electron beams* Rakesh Choubisa (BITS Pilani, India)
15:00	*PR: Atomic photoionization by attosecond pulses: discovery of reversible spirals* Marcel Ngoko Djiokap (University of Nebraska-Lincoln, USA)
15:30	*SR: Exploring electron-nuclear entangled dynamics in hydrogen molecular ions using quantum computer* Chihiro Osaku (The University of Tokyo, Japan)
15:45	*SR: Realtime tracking of ultrafast dynamics in liquid water* Gaia Giovannetti (Deutsches Elektronen-Synchrotron DESY, Germany)
16:00 – 18:30	**Poster Session II and Exhibition** • *Trillium Ballroom*
20:00 – 21:30	**Public Lecture II** • *A brighter future or the robot apocalypse? The challenges of AI governance* • *Room 214* Teresa Scassa (University of Ottawa, Canada) Chair: TBD

Ionization in intense laser fields beyond the electric dipole approximation

Ursula Keller

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Synopsis

I will review our work for which the dipole approximation is not valid but a fully relativistic description is not required and would like to dedicate this talk to Howard Reiss who died last year (25. Aug. 2022).

The electric dipole approximation is widely used in atomic, molecular and optical physics and is typically related to a regime for which the wavelength is much larger than the atomic structure. However, studies have shown that in strong laser fields another regime exists where the dipole approximation breaks down. Figure 1 shows the green area (the dipole oasis), for which the dipole approximation and the tunneling ionization theory is valid, according to Howard Reiss [1].

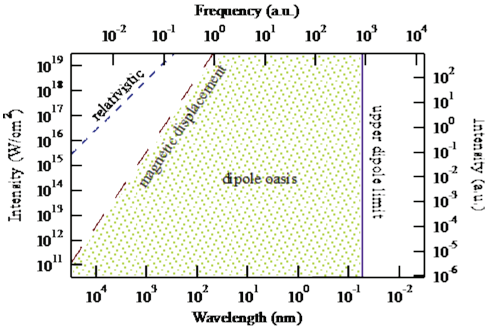

Figure 1. Illustration of the validity range of the dipole approximation, as published in our review article 2021 [2] and according to Reiss [1].

Many experiments have confirmed that the dipole approximation breaks down when moving to either high intensities or to longer wavelengths as shown in Fig. 1. During the ionization process in intense laser fields and at long wavelengths the photoelectrons can reach higher velocities such that the magnetic field component of the laser field becomes significant. The ionization dynamics and the final momentum of the electron is therefore modified by the entire Lorentz force. In contrast the magnetic field interaction is neglected in the dipole approximation.

This talk will review how the breakdown of the dipole approximation is affecting strong laser field interactions and how attosecond time resolution can provide a better understanding.

In the regime of strong field ionization for example the maximum of the photoelectron distribution is shifted opposite to the laser beam propagation direction, which is counter-intuitive within the framework of the radiation pressure [3]. More detailed studies as a function of ellipticities [4-5] also shows how the attoclock measurement [6-7] is affected. We also addressed the question how the transfer of linear momentum of the involved photons are transferred to the photoelectron and used the attoclock technique to resolve a time delay between the minimum of the linear momentum transfer and the maximum of the ionization rate [7].

With further developments in ultrafast lasers at high intensities and long wavelength such experiments with attosecond time resolution will continue to reveal a better understanding of light matter interactions.

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Ultrafast electron-ion coincidence spectroscopy with XUV FEL

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Synopsis Electron-ion coincidence spectroscopy using a magnetic bottle-type spectrometer is utilized to study the ultrafast multiphoton ionization dynamics of Xe and Kr in strong XUV FEL fields, where signatures of transient core-to-core resonances are identified. The application to UV/VIS pump - XUV probe spectroscopy will be also presented.

Responses of matter to strong extreme ultraviolet (XUV) and x-ray laser fields have attracted considerable attention in recent years, for their importance in various applications of free-electron lasers (FELs). The photoabsorption in such high frequency laser fields proceeds in various pathways consisting of different sequences of photoabsorption and core-hole decay. Vacancies created in valence and core orbitals pave additional pathways for photoabsorption, known as “hidden” resonance, which would enhance multiple ionization by orders of magnitude. Understanding of nonlinear processes in XUV and X-ray laser fields has been challenging due to the complicated nature.

Photoelectron spectroscopy is powerful in resolving the contributions from different ionization pathways, as intermediate states populated in the multiple ionization can be determined from the kinetic energies of ejected electrons. However, in some cases, careful analysis is necessary to discriminate particular responses of interest from other signals. To circumvent the difficulty, we employed coincidence spectroscopy with counterpart ions, which allows direct characterization of electrons emitted in a specific ionization pathway.

We studied multiphoton ionization of Xe [1] and Kr [2] in strong XUV-FEL fields at SACLA by using a magnetic bottle-type spectrometer equipped with ion extracting electrodes [3] (Fig.1). For Xe, the electron-electron-ion coincidence spectroscopy allows us to observe an ionization pathway via the $4d^{-2}$ double core-hole (DCH) states at $h\nu = 91$ eV. Interestingly, the photoionization cross section of Xe to Xe^{2+} ($4d^{-2}$) was found to be up to three times larger than the typical cross section of $4d$ inner-shell ionization, indicating an additional contribution to the well-known $4d$ giant resonance.

To explain this large cross section, core-to-core resonant transitions from $4d^{-1}$ to $4p^{-1}$ states in Xe^{+} were proposed. Clear signatures of such hidden core-to-core transitions were identified recently with Kr [2]. The optical transitions $3p - 3d$ are characterized with two distinct spectral lines around $h\nu = 120$ eV. The $3p$ core-hole state formed in Kr^{+} is detected by the $3p$ Auger electrons. The observed core-to-core resonance manifested the significance in multiple ionization to highly charged states.

Combined with pump-probe scheme, the electron-ion coincidence spectroscopy can also be used to elucidate the details of photoreaction dynamics of molecules [4], which will advance our understanding of ultrafast imaging by ultrashort intense XUV and x-ray pulses.

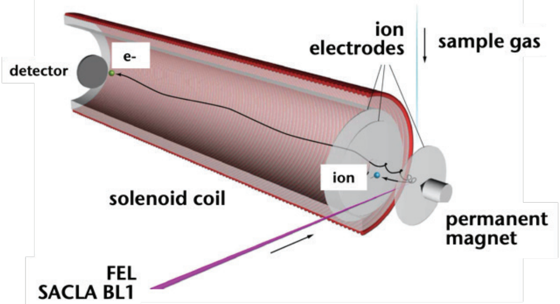

Figure 1. Schematic of the magnetic bottle-type electron-ion coincidence spectrometer used in the present study [3].

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Phase-controlled Multiple Pulse Experiments with Atoms and Molecules

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Synopsis Free Electron Lasers are the most powerful light source presently available in the EUV and x-ray range; they allow the time-resolved study of atoms, molecules, and condensed matter, with chemical sensitivity. The attainment of longitudinal coherence and its control, made possible by a seeded design, greatly expand the range of possible applications, as the phase of the pulse field can be tuned with sub-attosecond resolution. Several schemes have been successfully used at the at the FERMI FEL in Trieste, and will be presented.

In the last decade, Free Electron Lasers (FELs) have firmly established themselves as powerful instruments to produce intense, ultra-short light pulses at short wavelengths. Most of the existing FELs are based on the Self Amplified Spontaneous Emission (SASE) process, in which case only a passive control of the longitudinal coherence properties of the pulses is possible. The Free Electron Laser FERMI in Trieste is based on a seeded design [1] where the coherence properties of the seed laser are imprinted onto the emitting electrons, and transferred to the emitted pulse at a multiple harmonic of the seed. The radiator section of FERMI consists of a set of modules whose resonant wavelength, phase, and polarization, can be set independently, realizing *de facto* a harmonic synthesizer. As well, the electron bunch can accommodate a pair of phase -locked seed pulses. In the framework of Atomic and Molecular Science, these possibilities have been exploited in a number of experiments [2] performed at the Low Density Matter beamline (LDM) [3, 4]. In this work I will survey the technical aspects and limitations of generating phase-locked multi-harmonic or multi-pulse light at FERMI, as well as recent applications and future prospects at LDM.

The results originate from the joint effort of many international laboratories and of a large number of researchers, whose work is gratefully acknowledged.

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Enhancing elastic x-ray scattering by control of transient electronic populations

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Synopsis Focusing femtosecond x-ray pulses onto a copper foil transforms the solid into an electronically highly excited non-equilibrium state by inner-shell photoionization and Auger relaxation. Further, the electronic structure is predominantly shaped by inelastic electron collisions, creating electronic vacancies in the 3d shell. Thereby resonant elastic x-ray scattering channels are opened, largely enhancing the x-ray scattering form factor. We present results of transient x-ray absorption and enhanced x-ray scattering of warm-dense copper, interpreted by a kintetic Boltzmann approach.

X-ray free-electron lasers are capable of driving solids into electronically highly excited states at fs time scales. The resulting transient state is electronically far out of equilibrium with the crystal structure still intact. The characterization of this "warm-dense matter" poses intricate experimental and theoretical challenges. In two recent experiments, our team investigated the early stages of formation of warm-dense copper by transient x-ray absorption spectroscopy and resonant elastic x-ray scattering.

X-ray pulses of 15 fs duration are tuned to the Cu L$_3$ edge at 932 eV and focused on a 100-nm thin foil of Cu (B$_4$C/Cu/SiC multilayer in the 2nd experiment, respectively). Ionization followed by Auger decay rapidly creates hot electrons. Subsequent electron collisions produce highly charged ions with vacancies in the Cu 3d shell. Measuring the transmitted x-ray spectra gives a snapshot of the electronic population averaged over the first 15 fs upon pulse arrival. Increasing the XFEL intensity, an absorption peak below the neutral Cu L$_3$ edge appears in the spectra, assigned to 2p-3d resonant excitations of the created 3d vacancies. The total absorption is thereby increased (reverse saturable absorption). Increasing the XFEL pulse-energy further, higher-charged ions are formed, eventually shifting the 2p-3d resonances out of the spectral window of the x-ray pulse and quenching ionization (saturable absorption). This interpretation is corroborated by simulations based on a kinetic Boltzmann approach that follows the interaction with the x-ray pulse and subsequent electron-electron and electron-ion collisions.

Similarly to resonant absorption, the transient 2p-3d resonances are reflected in additional resonant elastic x-ray scattering channels, resulting in an enhanced scattering (see Fig. 1). Prospects to implement this scheme in the hard x-ray spectral region creating transient enhancement of resonant x-ray scattering on Kα transitions of targeted atomic species are discussed. By anaology with multiwavelength anomalous diffraction of conventional crystallography, these transient resonant x-ray scattering channels would allow for reconstructing the phases of the scattering form factor of these transient states of matter.

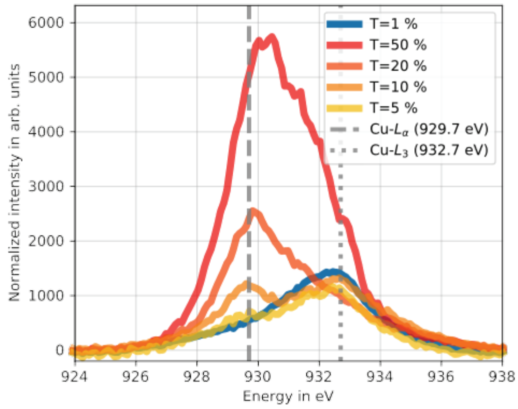

Figure 1. Spectrally resolved x-ray scattering intensity from a B$_4$C/Cu/SiC multilayer for different transmissions of a broad-band XFEL pulse of 15 fs duration and nominal intensity of 7×10^{17} W/cm^2 at 100% transmission

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Studying coherent light-matter interaction with a seeded free-electron laser

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Synopsis A prominent signature of coherent light-matter interaction is the Rabi oscillations in a two-level system. Despite being a cornerstone in quantum mechanics, it is usually studied in the long wavelength region, typically from mid-infrared to visible wavelength. Here, we show that femtosecond extreme ultraviolet (XUV) pulses from a seeded free-electron laser (FEL) can drive Rabi oscillations between two levels in a neutral helium atom across 50 femtoseconds. Our results highlight the relevance of temporally coherent, narrow-band XUV-pulses from a seeded FEL for manipulating quantum matter on an ultrafast timescale.

The periodic interaction of an external electromagnetic field with a two-level system can lead to cyclic transfer of population between the levels if the rate of energy transfer from the field to the system is faster than the spontaneous decay of the excited state. Such oscillations, known as Rabi oscillations [1] in coherent light-matter interactions, are ubiquitous in many branches of physics. Here, we show that intense extreme ultraviolet (XUV) pulses in the femtosecond domain can be used to drive Rabi oscillations between the two levels $1s^2$ and 1s4p in neutral helium atoms in the gas phase.

We took advantage of the high temporal coherence and the narrow photon bandwidth of XUV pulses delivered from the seeded free-electron laser (FEL), FERMI, [2] to probe the Rabi oscillations *in-situ*. The measured photoelectron spectra from two-photon ionization of helium atoms contain a symmetric splitting: an Autler-Townes (AT) doublet. The experimental Rabi period (~52 fs) falls within 20% of the FEL-pulse duration, signifying a near single-cycle build-up of the AT doublet. By tuning the photon energy of the XUV pulse across the atomic transition, we could observe an avoided crossing (see Fig. 1) in the corresponding photon energy diagram that appeared to be blue-shifted by almost 11 meV from the transition. While the avoided crossing can be described in terms of the well-known "atom + driving photons" dressed-state picture, to explain the observed blue-shift, we developed an analytical model based on perturbation theory on top of the Rabi model. It showed that the measured blue-shift originates from the quantum interference between resonant one-photon and non-resonant two-photon pathways in helium [3]. Our results pave the way to study coherent light-matter interaction in the few- to sub-nanometer wavelength domain using FELs.

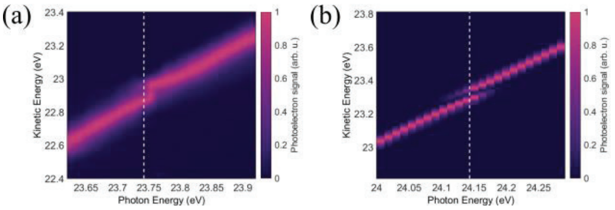

Figure 1. (a) Experimental and (b) theoretical photoelectron spectra as a function of photon energy. In each case, the avoided crossing is blue-shifted compared to the atomic transition (shown as the vertical dashed line) [3].

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Spectroscopy of biological molecular ions

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Synopsis By time-resolved action absorption spectroscopy we studied vibrationally resolved excited-state decay channels and dynamics of cryogenically cooled GFP chromophore anions following excitation at 425-500 nm. We demonstrate how the spectroscopy may be used to shine light on non-adiabatic energy-exchange mechanisms in the photoexcited state.

In this presentation, we shall see the use of a cryogenically cooled RF multi-pole ion trap in combination with the SAPHIRA ion-storage ring at Aarhus University [1]. Buffer-gas cooling in the trap provides fast cooling on the ms timescale and hence a high duty cycle of experiments. In the ion-storage ring, held at room temperature, measurements may be performed before the ions heat up significantly. The performance of the setup was initially tested by cooling OH$^-$, where a rotational temperature of 25 K was acieved [1].

The system is here used in combination with an electrospray ionization ion source for biochromophores. We used time-resolved action spectroscopy to explore the excited-state photophysics of the first electronic band $S_0 \rightarrow S_1$ of the Green Fluorescent Protein (GFP) chromophore. With the time-resolved data of the experiment we differentiate between three types of photo-induced action: Formation of prompt neutral products, delayed neutral photoproducts, and mass-selected negatively charged photofragments.

Based on the vibrationally-resolved spectra, we define four spectral regions with different excite-state photoresponse. The regions are determined by the relative location of the S_1 excited state, the electronic continuum D_0 + e$^-$, and energy barriers in S_1 which prevent internal conversion to the electronic ground state S_0 [2].

With a high energy resolution we determine that the first excited state of the choromophore is electronically bound with respect to autodetachment. The main uncertainty in determining the band origin stems from rotational broadening.

Using a femtosecond laser we may also trace the time evolution of the electronically excited state. The technique has been applied to biochromophores of for example chlorophylls [3], GFP chromophores [2], and protonated Schiff-base retinal [4].

Fluorescence of the GFP chromophore in the gas phase has not been detected so far. We see evidence that cold GFP chromophores may indeed be fluorescent in the gas phase, where excited-state energy barriers determine the rate-limiting decay by internal conversion [2].

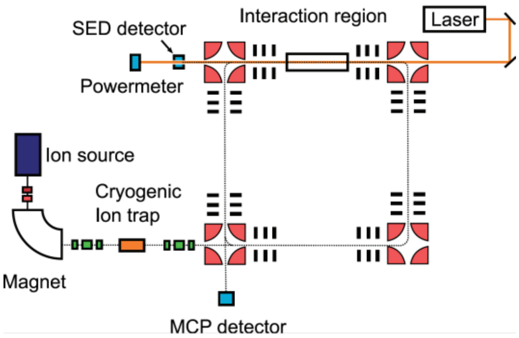

Figure 1. The SAPHIRA ion-storage ring with a cold (6K) ion trap [1]. A secondary-electron detector (SED) allowed detection of ’prompt’ neutral photoproducts. A micro-channel plate detector (MCP) located behind another arm of the ring was used to detect mass-selected photofragments and delayed action.

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Heavy Ion Interactions with Biological and Biomimetic Systems

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Synopsis Here we will focus on the gas phase collisions of low-energy ions with isolated biomolecules and biomolecular clusters.

Complex organic molecules such as amino acids and nucleobases are the building blocks of biomolecular systems like proteins and DNA. Besides the fundamental interest, the study of their interaction with ionising particles such as photons, electrons and ions has applications in radiotherapy and the emergence of life. On the one hand, the primary stage of radiation damage is related to the excitation and ionisation following the interaction of particles with matter, the so-called physical stage. On the other hand, the molecular complexity in the universe may be induced by the interaction of ionising particles with molecular systems.

Using ion beams delivered at GANIL, the French national ion beam facility, we have studied collisions in the gas phase of low-energy multiply charged ions with biomolecules either isolated or embedded in clusters. While collisions with isolated biomolecules allow to probe the intrinsic chemical physical properties of the molecular systems, clusters allow to mimick a simple chemical environment and to address the so-called effects of the environment.

With a coupled experiment-theory approach relying on coincidence time-of-flight spectrometry of the products of the collisions and quantum chemistry calculations, we have been able to determine some fundamental information such as the energy transfer in the collision [1] or the fragmentation dynamics [2, 3].

Considering ion collisions with biomolecular clusters, the aggregate acts as a buffer and we observe a reduced fragmentation, the cleavage of weak intermolecular bonds dissipating the excess of energy [4]. However the intermolecular bonds can also weaken covalent bonds and new fragmentation channels can be observed [4]. Finally neighbouring molecules in the cluster are a reservoir of matter and following the collision the formation of reactive species inside of the cluster may trigger reactivity and new covalent bonds can be formed [5].

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Electron collisions with systems of increasing complexity

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Synopsis The talk shortly overviews our recent progress in studies of electron interactions with matter, from molecules isolated in vacuum through clusters to radiolysis in bulk solutions.

Collisions of balistic electrons with isolated molecules in vacuum are interesting particularly at low collision energies due to the long range character of the electron – dipole interaction and long lifetime of the formed transient negative ions. Electron attachment to isolated molecules is therefore interesting benchmark for theory [1,2].

Direct interaction of electrons with isolated molecules is important in electron rich environments with large electron mean free paths such as outer space or nonthermal plasma [3,4].

However, many important electron-molecule interactions occur in more complex environments. A notorious example is the interaction of ionizing radiation with living tissue, where electrons are formed as secondary species. The seminal works of Leon Sanche on DNA damage triggered a wave of detailed studies on interaction of low-energy electrons with DNA and its components. In such studies, microhydrated molecules [5] can be used to reveal environmental effects on reaction dynamics.

However, the palette of phenomenon, where interactions of electrons with molecules play an important role is more diverse. Molecular clusters allow for mimicking complex chemistry, energy and charge transfer processes occurring on atmospheric aerosols and interstellar dust particles [6]. Clusters are also ideal for studies of fundamental processes in applications such as energy storage [7], localized surface plasmon enhanced chemistry [8] and during charged particle beam deposition [9].

While clusters provide a good model for environmental and complexation effects, they are not able to reproduce realistic biomolecular systems, where reaction dynamics is influenced by presence of buffer solution components or secondary structure of macromolecules. Therefore, we recently expand our experimental portfolio of two new techniques. The first, DNA origami as an unique substrate to study precisely defined DNA sequences. [10] The second, liquid microjet, which aims for studies in fully realistic bulk solutions.

We acknowledge the support from Czech Science Foundation project number 21-26601X (EXPRO).

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Electron induced bond breaking in radiosensitizing compounds

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Synopsis In this contribution, I will present our recent investigation on electron scattering from 1-methyl-5-nitroimidazole (a model radiosensitizer). Absolute total cross sections (TCSs) have been measured with a state-of-the-art experimental setup, and ab-initio scattering and bound state calculations have been performed. Besides providing several new physical insights about the DEA mechanisms, our key finding concerns the observation of several unexpected transient negative ions, whose existence could not be inferred in previous DEA experiments.

Radiosensitizer compounds used in radiotherapy treatments allow to reduce the doses delivered, thus minimizing the damage induced in the nearby healthy tissues [1]. While the fundamental mechanisms behind the efficiency of certain classes of radiosensitizers still remain poorly understood, the production and subsequent chemistry mediated by free radicals certainly plays a key role [2]. In particular, a huge amount of low-energy electrons (LEEs) are generated along the track of the primary ionizing radiation, which are known to induce molecular dissociation, thus implying the formation of one or more free radicals. Despite the well-know role played by dissociative electron attachment (DEA), other electron-induced reactions, specially in the context of radiosensitivity, remain less explored

Here, I will discuss our recent experimental and theoretical investigation [3] with an important model radiosensitizer, 1-methyl-5-nitromidazole. The measured total electron scattering cross sectitions have revealed many signatures related to the formation of transient negative ions (TNIs). With support from theory, novel insight about DEA reactions related to the lower-lying resonances are provided. Surprisingly, the TNIs found at higher energies have no parallel to DEA experiments [4,5], which points to alternative and effective decay mechanisms for these states. While non-dissociative channels cannot be ruled out, we claim neutral dissociation through a catalytic electron [6,7] as a likely relaxation mechanism for these higher-lying TNIs. Even though DEA represents a key component for understanding radiosensitivity, our finding suggests that neutral dissociation probably plays a more important role than previously anticipated.

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Quantum Collisions of Cold Molecular Ions in Traps

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Synopsis Cryogenic ion traps are well suited to study cold collisions and reactions of molecular ions. In this contribution, quantum state-changing inelastic collisions and quantum mechanical tunneling reactions will be discussed.

Cryo-cooled radiofrequency ion traps have become a widespread tool for spectroscopic and collisional studies of a wide range of molecular and cluster ions at low temperatures. In particular multipole radiofrequency ion traps are well suited to cool translational and internal degrees of freedom of trapped molecular ions in a cryogenically cooled buffer gas [1, 2]. In recent years negatively charged molecular ions have drawn a lot of attention, because several negative ions have been detected in different interstellar molecular clouds [3]. Cold negative ions have also been suggested as possible cooling agent for trapped antiprotons.

We have developed photodetachment spectroscopy near the detachment threshold into a tool to probe rotational and vibrational quantum states of cold negative ions. We have used this to study rotational state-changing collisions of $OH^-(J = 1 \rightarrow 0)$ with neutral helium atoms at low temperature [4] and to perform rotational terahertz spectroscopy and infrared overtone spectroscopy. We have also studied photodetachment of the interstellar anions CN^- and C_3N^- near threshold and used these data to improve the accuracies of the respective electronic affinities, including the identification of a dipole bound state in the latter ion [5].

Furthermore, we investigated the homonuclear anion C_2^-, a possible candidate for negative ion laser-cooling. We have carried out a precise spectroscopic characterization of a suitable laser-cooling transition in this ion [6] and have measured the rate coefficient for vibrational state-changing collisions $v = 1 \rightarrow 0$. For this work we used a newly developed cryogenic 16-pole wire trap [7].

We also study reactive collisions of negative ions at low temperatures. By improving the already high sensitivity of ion trap-based reaction kinetics experiments, we could observe the extremely low reaction rate coefficient of the proton transfer reaction $H_2 + D^- \rightarrow H^- + HD$ [8], which only takes place in about 1 out of 10^{11} close encounters. At low temperatures this reaction only occurs by quantum tunneling. Our measured value agrees with accurate quantum scattering calculations [9] and provides a benchmark for molecular theory. Furthermore, we could identify previously unobserved heating dynamics in radiofrequency ion traps.

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Measuring the tunneling time for ultracold atoms, and the unexpected emergence of spin textures via collisions between incident and reflected atoms

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The question of how long particles spend while traversing a tunnel barrier has been controversial for quite nearly a century, and we have now directly measured it, using an analog of Larmor precession as a clock, for Bose-condensed ^{87}Rb atoms interacting with a repulsive, tightly focussed, laser beam.

I will introduce the controversy and the principle of this experiment, along with our early results. Theory suggests that regardless of the thickness of a (symmetric) barrier, reflected atoms will on average spend the same amount of time within it as transmitted ones. In a follow-up experiment intended to test this prediction, we instead found entirely unexpected behaviour, in which collisions between reflected atoms and incident ones led to spin exchange and spin textures. This is in spite of the nearly spin-independent scattering amplitudes for Rubidium, and was hence a surprise. We now understand it as an indistinguishable-particle effect, similar in that sense to the well-known “ISRE”, but different in that the latter is widely understood to occur only in thermal (non-condensed) gases, while our effect requires no bunching and arises even in a condensate. We believe this raises subtle points about spin-changing collisions in degenerate gases in general.

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Recent progress towards positronium Bose-Einstein condensation

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Synopsis Positronium (Ps) is one of the candidates for the first Bose-Einstein condensate (BEC) of any system containing antimatter. We proposed a new scheme to realize Ps-BEC by a positron focusing system and fast Ps cooling which is a combination of thermalization and laser cooling. Our target density and temperature for Ps-BEC transition is 10^{18} cm^{-3} at 10 K. We will summarize our recent experimental progress towards Ps-BEC.

Positronium (Ps), the bound state of an electron and its antiparticle positron, is a purely leptonic system containing antimatter. It is useful to study fundamental physics, including antimatter studies to solve the mystery of the matter dominant Universe.

Recently, we proposed a new method to realize a Bose-Einstein condensate (BEC) of Ps (Ps-BEC) [1,2]. Ps-BEC can be used to measure antimatter gravity using an atomic interferometer. It can also be used as a source for a 511-keV gamma-ray laser. Figure 1 shows the conceptual diagram of our method. We create dense Ps of 10^{18} cm^{-3} by focused positrons, and rapidly cool Ps to 10 K by a combination of thermalization [3] and laser cooling of Ps [4]. We will present our recent progress towards Ps-BEC.

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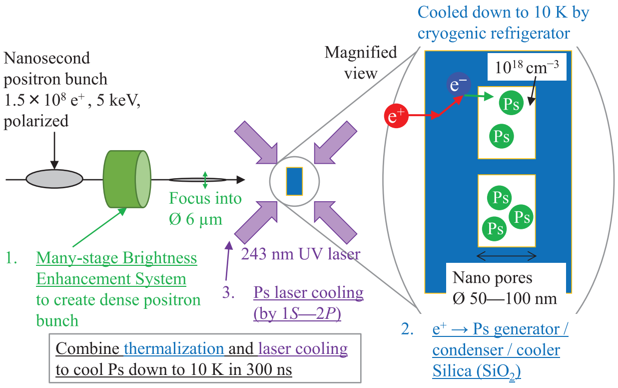

Figure 1. Conceptual diagram of our method to realize Ps-BEC. Positrons are focused by (1) many-stage brightness enhancement system. The dense positrons bombard (2) Ps generator/condenser/cooler material and form dense Ps. We rapidly cool Ps by a combination of thermalization and (3) laser cooling to realize Ps-BEC.

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Resonant processes and their impact in many-body dynamics

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Synopsis We discuss a general process, resonant exchange, that occurs in several atomic and molecular systems. We show that a simple approximation accounts for the exchange cross section over wide range of collision energy.

Resonant exchange is a general process playing a key role in many-body dynamics and transport phenomena, such as spin, charge, or excitation diffusion. The underlying process is described by the resonant exchange cross section $\sigma_{\rm exc}$. A prime example is the diffusion of an ion A^+ in its parent neutral gas A. In fact, the charge actually behaves as a hole (h) at ultralow temperatures, hopping from atom to atom instead of staying on its heavy center (the ion) [1]. We have predicted a faster diffusion coefficient for the hole (D_h) than if the charge was diffusing via collision ($D_{\rm coll}$).

In this work, we show that the exchange symmetry for identical (homonuclear) atom-ion system leads to special outcomes for ion transport in ultracold experiments. We compute the two body charge hopping probabilities and rates, which are used to model charge hopping in the dynamics of an ultracold $^{6/7}$Li$^+$ ion immersed within an ultracold gas of $^{6/7}$Li atoms at micro-Kelvin temperatures [2]. We show that the charge hopping and collisional diffusion compete, giving unique results leading to charge trapping in regions of high atomic density gradient, leading to a region of "negative" diffusion.

As mentioned above, the dynamics is dictated by $\sigma_{\rm exc}$. In previous work [3], we showed that the locking of s-wave phase shifts could be used to explain the behavior of $\sigma_{\rm exc}$ at ultracold temperatures. Moreover, we found an unexpected consequence of phase-shift locking; namely, the behavior of the resonant-exchange cross section over a broad range of energies is largely dictated by s-wave scattering, whose influence extends high above the s-wave Wigner regime. We now generalize our treatment to higher energies and derive an analytical expression for the resonant-exchange cross section which accounts not only for the locking of phase shifts, but also for their gradual unlocking as the energy increases. We find good agreement between the computed (fully quantal) cross section and our newly obtained result, which we illustrate for resonant charge-transfer in ion–atom collisions (see Fig.1 for ^{174}Yb).

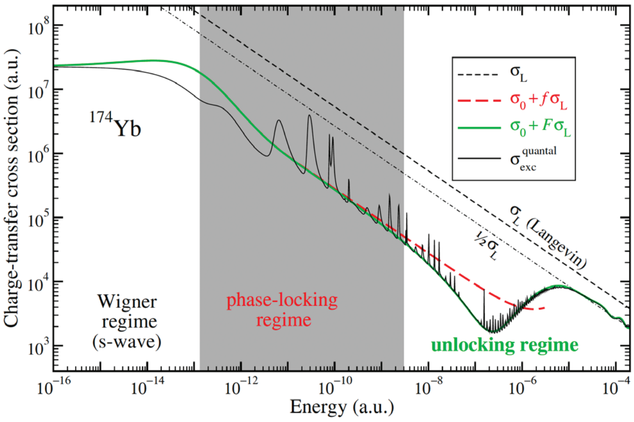

Figure 1. Exchange cross section.

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Two-photon optical shielding of collisions between ultracold polar molecules

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Synopsis We propose a method to engineer repulsive long-range interactions between ultracold ground-state molecules using optical fields, thus preventing short-range collisional losses. It maps the microwave coupling recently used for collisional shielding onto a two-photon transition, and takes advantage of optical control techniques. In contrast to one-photon optical shielding [5], this scheme avoids heating of the molecular gas due to photon scattering. The proposed protocol, exemplified for ^{23}Na^{39}K, should be applicable to a large class of polar diatomic molecules.

The growing availability of quantum gases of ultracold polar molecules in several labs revealed a very peculiar situation in the context of few-body physics: at ultracold energies, two such molecules in their absolute ground level collide with a universal collisional rate, even if they have no inelastic or reactive energetically allowed channels, so that they leave the molecular trap with a short characteristic time. Instead of attempting to fully describe this four-body system, with the aim of identifying the exact cause of the universal loss rate, one can design protocols where molecules would simply not reach short distances in the course of their collision. Several options have been proposed and experimentally demonstrated, based on the modification of the long-range interaction (LRI) between molecules using static electric fields [1] or microwave (mw) fields [2-4], in order to ”shield” their collisions.

In a previous work [5] we proposed an alternative way to engineer LRIs using a laser with a frequency blue detuned from the one of a suitable molecular rovibronic transition. Such a one-photon optical shielding (1-OS), inspired from previous works on cold atoms, results in the laser-induced coupling of the attractive collisional entrance channel to a repulsive one, thus preventing the molecules from reaching short distances, and from creating a sticky complex. One limitation of the 1-OS could be the heating of the molecular quantum gas due to the continuous scattering of off-resonant photons of the 1-OS laser.

In this work we propose a two-photon optical shielding (2-OS) scheme, aiming at overcoming the above limitation, while mapping the case of the microwave shielding [2-4]. Such a scheme combines the best features of the 1-OS (no restriction for the field polarization, convenient laser power, tunability, geometrical versatility, broad compatibility) and mw shielding (no spontaneous emission or photon scattering). The scheme relies on coupling three molecular states $|g_1\rangle$, $|q\rangle$ and $|g_2\rangle$ where $|g_1\rangle$ is the entrance channel and $|q\rangle$ and $|g_2\rangle$ are well chosen states of the collisional complex via a two-photon transition from $|g_1\rangle$ to $|g_2\rangle$. In the dressed state picture, this maps the mw shielding scheme onto an effective optical coupling of the dressed states.

The proposed protocol, exemplified for ^{23}Na^{39}K, should be applicable to a large class of polar diatomic molecules.

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Strong-field ionization of atoms with Sculptured laser fields

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Synopsis In strong-field physics, the fundamental Gaussian beam is widely employed both experimentally and theoretically, since it is the routine spatial mode from the lasers. And thus, the plane wave approximation is usually adopted in analysing SFI and HHG with such laser fields. Recently, the non-trivial spatial and temporal phase structures have been introduced in strong-field ionization (SFI) and high harmonic generation (HHG). The structured lights, such as the optical vortex beams and vector beams, allow to introduce new degrees of freedom for the interaction between the intense light fields and matters. To date, such the spatially and temporeally sculptured laser laser fields has provided new opportunities for strong-field physics with auspicious applications in ultrafast science.

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Laser-induced atomic dynamics, triggering a broad range of ultrafast phenomena such as the generation of attosecond light pulses, photoelectron diffraction and holography, has laid the foundation of strong-field physics and attosecond science. Using the attoclock constructed by single-color elliptically polarized laser fields, previous experiments have measured the tunneling rates, exit positions, exit velocities and delay times for some specific electron trajectories, which are mostly born at the field peak instant where the laser electric field and the formed potential barrier are stationary in terms of the derivative versus time. From the view of the wave-particle dualism, the electron phase under a classically forbidden, tunneling barrier has not been measured, which is at the heart of quantum tunneling physics. Here we present a robust measurement of tunneling dynamics including the electron sub-barrier phase and amplitude using temporal sculptured laser fields. We combine attoclock technique with sculptured circular fields to accurately calibrate the angular streaking relation and to probe the non-stationary tunneling dynamics by manipulating a rapidly changing potential barrier. The sculptured laser fields provides a general time-resolved approach to access the underlying quantum dynamics in intense-light-matter interactions. In the end, I will discuss high harmonic generation with the structured lights, such as the optical vortex beams and vector beams. That allows to introduce new degrees of freedom for the interaction between the intense light fields and matters.

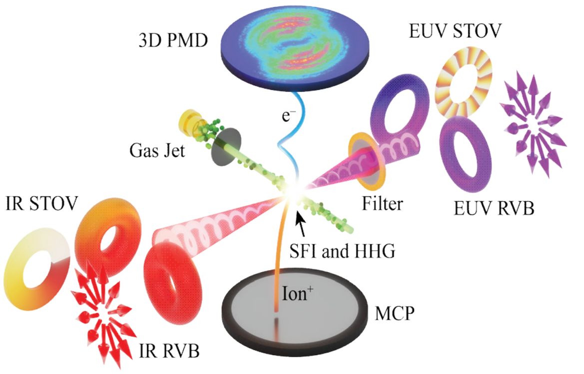

Figure 1. Illustration of strong-field ionization (SFI) and high harmonic generation (HHG) experiments with various optical vortices. The products of HHG and SFI are the extreme ultraviolet (EUV) photons and photoelectrons, respectively. IR, infrared; STOV, spatiotemporal optical vortex; RVB, radial vector beam; PMD, photoelectron momentum distribution; MCP, microchannel plate.

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Ionization studies of water molecules using twisted electron beams

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Synopsis In this talk, we present the results of the triple differential cross-section (TDCS) for the (e, 2e) process on water molecule for the twisted electron impact to explore the effect of opening angle θ_p and orbital angular momentum number m on the TDCS.

One of the most important collision processes in atomic and molecular physics is the ionization of a given target by an electron impact The generation of electron vortex (or twisted) beams (EVBs) has received a lot of attention from both theoretical and experimental perspectives. These electron beams possess a helical wave-front and non-zero projection of the orbital angular momentum (OAM) m onto their propagation direction [1]. The water molecule plays a crucial role in biological matters. We explore the role of the twisted electron beam parameters (OAM number m and opening angle) on the (e, 2e) process for the water molecule. We investigate the angular profiles of the TDCS for an incident electron vortex beam in co-planar asymmetric geometry for the outer orbitals $1b_1$, $3a_1$, $1b_2$ and $2a_1$ of the water molecule [2]. We develop the theoretical formalism in the first-Born approximation (FBA). In addition, we also investigate the average over impact parameter cross-section ($(\text{TDCS})_{av}$) to explore the influence of the opening angle of the twisted electron beam on the TDCS. The angular profiles for averaged cross-section show the dependence of TDCS on the opening angles. For $\theta_p = \theta_s$ (opening angle of the beam equals the scattering angle), we observed a substantial deviation of the angular profile of the $(\text{TDCS})_{av}$ from the plane wave TDCS. At the conference, we intend to report the effects of the twisted electron beam parameters (opening angle and OAM) on the angular profile of TDCS for the water molecule. We will also report our results for the CH_4 and NH_3 molecules.

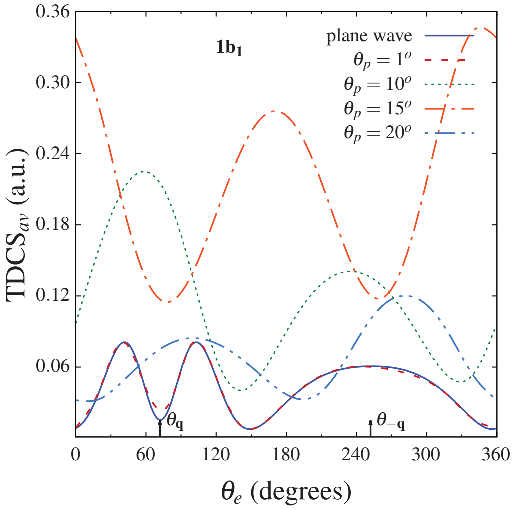

Figure 1. $(\text{TDCS})_{av}$ plotted as a function of the ejected electron angle θ_e for the plane wave (solid line) and twisted electron beam for different opening angles as shown in the frames of each sub-figure. The kinematical conditions are $E_i = 250$ eV, $E_e = 10$ eV and $\theta_p = \theta_s = 15°$.

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Atomic Photoionization by Attosecond Pulses: Discovery of reversible spirals

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Synopsis We study the linear process of single-photon ionization of S-state atoms by a pair of synchronous opposite circularly polarized attopulses linearly chirped within the rotating wave approximation and discovered in the photoelectron momentum distribution a new class of spiral phenomena, termed reversible spirals because of their energy-dependent handedness. The astrophysical concept of spiral arm pitch angle is borrowed to gain a better insight into this electron phenomenon, to determine the attochirp difference as well as the binding energy characteristic of an atomic target. Our results indicate potential applications in attochirpmetry and polarimetry.

A significant area of concern regarding the groundbreaking role of attopulses in achieving the ultimate goals of attoscience is the compensation of their intrinsic chirp (known as attochirp). Current techniques for synthetizing attopulses within the XUV or soft x-ray spectral region from high-order harmonic generation or free-electron lasers always introduce a chirp, i.e., a time-dependent carrier frequency; this broadens their duration and decreases their intensity, delaying thus the realization of the holy grail of attophysics. Therefore, for better control of electron motion it is crucial to study whether this attopulse imperfection can influence the photoelectron momentum distributions (PMDs). Chirp as a control knob and its applications have been the subject of various theoretical and experimental ionization studies in atoms, molecules, and condensed matter, but mostly in the femto than in the attosecond regime. All these studies, however, are for nonlinear processes, not for a linear process such as the fundamental process of one-photon single ionization (dubbed photoionization) from a state where chirp of a laser pulse within the rotating wave approximation (RWA) is meaningless.

In this talk, I will discuss how attochirp can affect dramatically the PMD from photoionization within the RWA of S-state atoms by two laser pulses (not a single pulse) oppositely circularly polarized (OCP). For two identically chirped pulses, the PMDs at any time delay coincide with those from transform limited pulses [1], meaning that attochirp has no effect. The situation changes dramatically when the two pulses with equal but opposite chirp rates reach the target simultaneously. Instead of a dipole pattern, a reversible two-arm spiral with energy-dependent sense of rotation emerges in the PMD [2], see Figure. Perturbation theory analysis of our TDSE results reveals that the two pulses with opposite chirps impart the photoelectron a spectral phase with linear and quadratic components of opposite sign, fully explaining this new electron effect. Varying the amount of chirp rates arbitrarily and introducing nonzero time delays into the game allow an exquisite control of the reversible spirals by manipulation of the linear and quadratic spectral phases [3]. The concept of pitch angle borrowed from astrophysics is introduced here in attoscience to gain a better insight into the origin of this uncharted pattern, determine the attochirp difference as well as the binding energy characteristic of the atomic target under investigation.

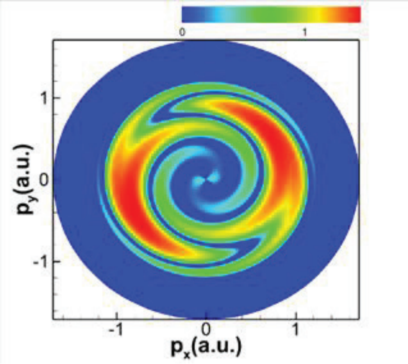

Figure 1. Reversible spiral created by a pair of synchronous opposite circularly polarized linearly chirped attopulses following one-photon single ionization of He.

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Exploring Electron-Nuclear Entangled Dynamics in Hydrogen Molecular Ions using Quantum Computer

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Synopsis We have developed a non-adiabatic simulation method for hydrogen molecular ions under an intense laser field using a quantum computer and succeeded in calculating with high accuracy using an actual quantum computer.

The interaction between matter and intense laser fields is of great interest in contemporary physics, with many applications in areas such as plasma physics, materials science, and chemistry. When subjected to intense laser fields, matter can exhibit fascinating and unexpected phenomena. Understanding these phenomena is crucial for designing and controlling material properties. While we have developed first-principles methods for studying molecules in intense laser fields [1], they suffer from the problem of exponentially increasing computational cost with the number of particles.

Therefore, quantum chemical calculations using quantum computers, which can be calculated in polynomial time instead of exponential time, have attracted much attention [2]. In our laboratory, we have developed a quantum-classical hybrid method, the time-dependent optimized unitary coupled cluster method (TD-OUCC), which can incorporate particle correlations using time-dependent orbital functions. However, the application of this technique was limited to electronic systems only.

In this study, we extend the TD-OUCC method to multicomponent systems and use it to calculate the real-space dynamics of one-dimensional molecular hydrogen ions under an intense laser field.

Figure 1 shows the time evolution of the electron and nuclear density when a 1D molecular hydrogen ion model is irradiated by a high-intensity laser. Figure 1(a)(c) was calculated on a classical computer using a quantum circuit simulator, and (b)(d) was obtained using the reduced density matrix calculated on the quantum computer ibm_kawasaki, which was installed in Kawasaki, Japan in 2021. The tunneling ionization and subsequent dissociation, which cannot be described without incorporating the electron-nucleus correlation [3], could be reproduced. It should be emphasized that the results obtained by the quantum computer with noise [Fig. 1(b)(d)] excellently agree with ideal results [Fig. 1(a)(c)] on noiseless classical computers.

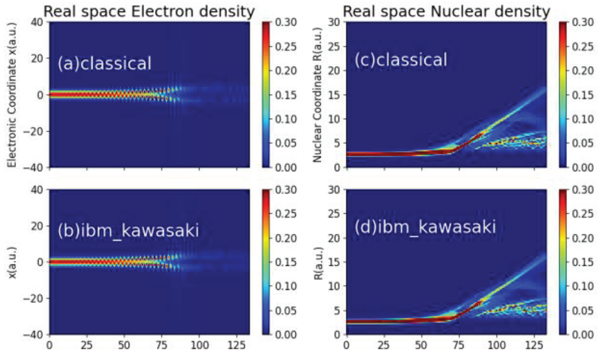

Figure 1. Time evolution of the electron(a)(b) and nuclear(c)(d) density of one-dimensional H_2^+ irradiated by a laser pulse with a wavelength of 800 nm, an intensity of 2×10^{14}W/cm^2, and the duration of about 50 fs. Comparison of the results of a quantum circuit simulator (a)(c) and ibm_kawasaki (b)(d).

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Realtime tracking of ultrafast dynamics in liquid water

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Synopsis The ultrafast vibrational dynamics of liquid water, initiated via Impulsive Stimulated Raman Scattering (ISRS) by a sub-4 fs NIR pump pulse in the ground state of the molecule, is revealed with unprecedented time resolution via transient absorption of sub-2 fs UV pulses. The coherent signal is dominated by the O-H stretching mode and decays in 25 fs, revealing an extremely fast dephasing of this mode.

Understanding the properties of aqueous solutions is a key first step in determining the effects of the liquid environment on the chemical reactions occurring in biological systems, for this reason vibrational relaxation and therefore energy dissipation in liquid water have been intensely investigated [1, 2].

Pump-probe spectroscopy is a powerful technique allowing the realtime investigation of the combined electronic and vibrational dynamics occurring in photoexcited water. So far, pump-probe measurements performed in liquid water have been limited to a time resolution of a few tens of femtoseconds [3].

Here, we present a time-resolved investigation of the vibrational dynamics initiated in liquid water by a sub-4 fs near-infrared (NIR) pump pulse. The rapid evolution of the vibrational wave packet, created by impulsive stimulated Raman excitation in the ground state of the molecule, is then probed with unprecedented time resolution by monitoring the transient absorption using sub-2 fs UV probe pulses [4]. In our experiment, the NIR pump and UV probe pulses are focused on a thin liquid jet operating in vacuum. The transmitted UV probe pulse is recorded as a function of the pump-probe delay.

A preliminary analysis of our data shows an oscillatory transient signal with a period of 10 fs and a decay time of 25 fs. These values match the ones expected for the O-H stretching mode in the ground electronic state of liquid bulk water [5], here measured for the first time in the time domain. The large bandwidth of our UV pulses allows to probe the dynamics in different spectral regions. In particular, the blue and red sides of the transient absorption exhibit out-of-phase oscillations between positive and negative values.

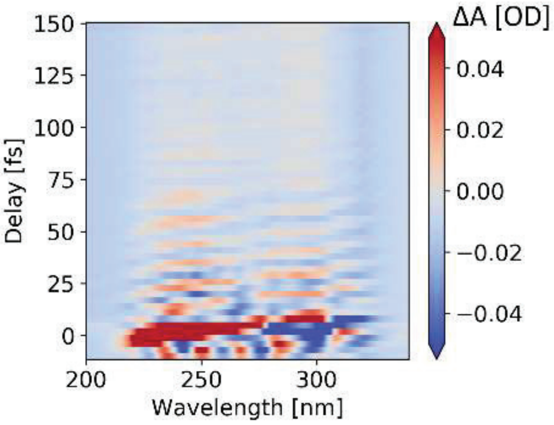

Figure 1. Colormap of the measured transient absorption signal as a function of the UV probe wavelength and the pump-probe time delay.

Further theoretical insights will allow us to assign specific contributions from the ground, excited and ionized states.

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Detailed Program

Friday, July 28

8:30 – 9:30	**Plenary Session III** • *A glimpse into the world of ICD and ETMD* • *Room 214* Lorenz S. Cederbaum (University of Heidelberg, Germany) Chair: Kiyoshi Ueda (Tohoku University, Japan)
9:30 – 10:00	**IUPAP Early Career Scientist Prize Talk** • *Unraveling the electronic quantum coherence in photosynthetic protein complexes* • *Room 214* Hong-Guang Duan (Ningbo University, China) Chair: Rosario González-Férez (Universidad de Granada, Spain)
10:00 – 10:30	**Coffee Break** • *Trillium Ballroom*
10:30 – 12:30	**Parallel Session V A: Attosecond Physics II** • *Room 214* Chair: Diego Arbó (CONICET-UBA, Argentina)
10:30	*PR: Polarization control in two-color atomic ionization* Diego Boll (CONICET-UNR, Argentina)
11:00	*PR: Scaling of the fractional angular momenta of a light polarization Möbius strip in extreme nonlinear optics* Thierry Ruchon (Université Paris-Saclay, CEA, CNRS, LIDYL, France)
11:30	*PR: Phase retrieval from angular streaking of XUV atomic ionization* Anatoli S. Kheifets (The Australian National University, Australia)
12:00	*SR: Optical tunnelling without a barrier?* Anne Weber (King's College London, UK)
12:15	*SR: Time-resolving molecular tunneling dynamics with free-electron-laser-pump and high-harmonics-generated-probe transient absorption spectroscopy* Alexander Magunia (Max Planck Institute for Nuclear Physics, Germany)
10:30 – 12:30	**Parallel Session V B: Electron-Molecule Interactions** • *Room 213/215* Chair: Oddur Ingólfsson (University of Iceland, Iceland)
10:30	*PR: Dissociative electron attachment and electron-impact vibrational excitation of molecules* Karel Houfek (Charles University, Czech Republic)
11:00	*SR: Dynamics of Dissociative Electron Attachment to Acetylacetone* Surbhi Sinha (Tata Institute of Fundamental Research, India)
11:15	*SR: Symmetry breaking in dissociative ionization of symmetric molecules by electron impact* Noboru Watanabe (Tohoku University, Japan)
11:30	*PR: Electron-induced fragmentation of biologically relevant molecules* Janina Kopyra (Siedlce University, Poland)
12:00	*SR: Production of O_2^+ following the double ionization of CO_2* Ana Beatriz Monteiro-Carvalho (Universidade Federal Fluminense, Brazil)
12:15	*SR: Charge-state distributions after beta decay of ^{6}He to form ^{6}Li* Aaron Bondy (University of Windsor, Canada)

12:30 – 14:00	**Free Time**
14:00 – 16:00	**Parallel Session VI A: Imaging** • *Room 214* Chair: Joshua Williams (University of Nevada, USA)
14:00	*PR: Dynamics of weakly-bound molecules* Doerte Blume (The University of Oklahoma, USA)
14:30	*PR: Directly imaging excited state-resolved transient structures of water induced by valence and inner-shell ionization* Chuncheng Wang (Jilin University, China)
15:00	*PR: Soft x-ray multi-photon absorption for transient spectroscopy and Coulomb explosion imaging* Rebecca Boll (European XFEL, Germany)
15:30	*SR: The big, the small & the shoulder: controlling OCS post-ionization dynamics* Heide Ibrahim (Advanced Laser Light Source at Institut national de la recherche scientifique, Canada)
15:45	*SR: Differentiating molecular structures using laser-induced Coulomb explosion imaging* Huynh Van Sa Lam (Kansas State University, USA)
14:00 – 16:00	**Parallel Session VI B: Spectroscopy** • *Room 213/215* Chair: Stephan Fritzsche (Helmholtz-Institut Jena, Germany)
14:00	*PR: High-resolution spectroscopy of electronic K x-rays from muonic atoms using transition-edge sensor microcalorimeters* Takuma Okumura (Tokyo Metropolitan University, Japan)
14:30	*PR: High precision spectroscopy of pionic helium atoms* Masaki Hori (Imperial College London/Johannes-Gutenberg University Mainz/Max Planck Institute of Quantum Optics, UK/Germany)
15:00	*PR: New test of bound-state QED: High-resolution measurement of an intra-shell transition in He-like U* Robert Loetzsch (Friedrich Schiller Universität Jena, Germany)
15:30	*SR: Precision x-ray spectroscopy of He-like uranium employing metallic magnetic calorimeter detectors* Philip Pfäfflein (Helmholtz Institute Jena, Germany)
15:45	*SR: Cold molecular dynamics and chemical reactions of H_2 (D_2) in strong laser fields* Lianrong Zhou (East China Normal University, China)
16:00 – 18:30	**Poster Session III and Exhibition** • *Trillium Ballroom*

A glimpse into the world of ICD and ETMD

Lorenz S Cederbaum

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How does a microscopic system like an atom or a small molecule get rid of the excess electronic (or vibrational) energy it has acquired, for instance, by absorbing a photon or by impact with an ion or electron? If this microscopic system is isolated, the issue has been much investigated and the answer to this question is more or less well known. But what happens if our system has neighbors as is usually the case in nature or in the laboratory? In a human society, if our stress is large, we would like to pass it over to our neighbors. Indeed, this is in brief what happens also to the sufficiently excited microscopic system. A mechanism of energy transfer named ICD (Interatomic/Intermolecular Coulombic Decay) has been theoretically predicted and verified in by now many exciting experiments. This mechanism seems to prevail "everywhere" from the extreme quantum system of the He dimer to water, to systems in cavity, and even to quantum dots. The transfer is ultrafast and typically dominates other relaxation pathways.

ICD is often accompanied by ETMD (Electron Transfer Mediated Decay). As charge transfer is usually much slower than energy transfer, ICD dominates. However, ETMD can be widely operative when our microscopic system itself does not possess excess energy, i.e., when ICD is inactive. The energy needed is created by the ETMD itself. ICD and ETMD are introduced and discussed. Examples and arguments are presented which make clear that the processes in question play a substantial role in nature and laboratory.

Experimental and theoretical work on ICD, ETMD and related processes can be found in the Bibliography: `http://www.pci.uni-heidelberg.de/tc/usr/icd/ICD.refbase.html`

A recent review: Jahnke T *et al.* 2020, Interatomic and Intermolecular Coulombic Decay, *Chem. Rev.* **120** 11295

Unraveling the Electronic Quantum Coherence in Photosynthetic Protein Complexes

Hong-Guang Duan[1]*, Ajay Jha[2,3], Lipeng Chen[4], Vandana Tiwari[5], Pan-Pan Zhang[1], Michael Thorwart[6,7] and R. J. Dwayne Miller[8]

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Synopsis In this work, we employed the two-dimensional electronic spectroscopy to study the ultrafast energy transfer in FMO and other photosynthetic protein complexes. We measured the 2D electronic spectra of the FMO complex at 20 K (Fig. 1(b) to (e)) to capture a clear evidence of coherent energy transfer. Moreover, we also examined the coherent dynamics in PSII reaction center at low temperature. The lifetime and the role of electronic and vibrational coherences are discussed.

Deciphering the nature's secrets of efficient primary steps of energy and charge transfer processes in photosynthesis is one of the long standing issues in understanding structure-function relationships in biological systems. In this work, we employed the two-dimensional electronic spectroscopy (2DES) to study the ultrafast energy transfer in FMO and other photosynthetic protein complexes. We measured the 2D electronic spectra of the FMO complex at 20 K (Fig. 1(b) to (e)) to capture a clear evidence of coherent energy transfer [1]. We also examined the coherent energy transfers in FMO by extending the temperature range our measurements from 20 K to 150 K, which could give us a consistent conclusion [3] along with results from our pervious measurement at room temperature [2]. Our advanced data analysis and theoretical calculations unravel the lifetime of electronic quantum coherences in different blocks of pigments (identified by the strength of electronic couplings) in FMO protein complex at different temperature (Fig. 1(a)). Recently, we have also probed PSII reaction center at 20 K using 2DES [4]. The coherent effects in the energy and charge transfer processes in reaction center will be discussed.

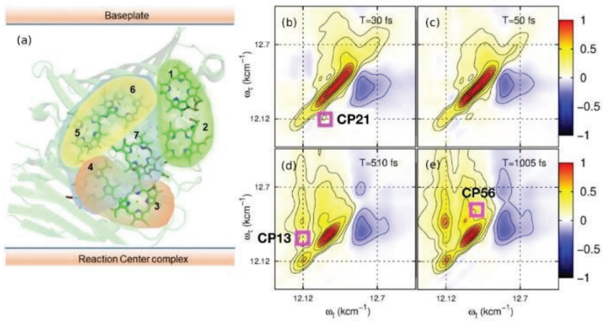

Figure 1. The protein structure of FMO complex is shown in (a). The measured 2D electronic spectra of FMO complex are presented with selected waiting times, which has been marked from (b) to (e).

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Polarization control in two-color atomic ionization

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Synopsis The polarization control on two-color experiments provides a route to steer photoionization reactions, acting directly on the angular degrees of freedom. Here, we show that using short wavelength photon energies below the ionization threshold leads to a degree of control exceeding the one achieved in the above-threshold case. Additionally, we demonstrate that the combined action of the polarization control and the reconstruction of attosecond beatings by interference in two-photon transitions induces the emergence of interference patterns frustrated when laser pulses are collinearly polarized.

Pump-probe two-color experiments constitute the building blocks for ultrafast science. In that class of experiments, ultrashort extreme ultraviolet laser pulses trigger excitation or ionization electron dynamics subsequently probed by an infrared laser pulse. So far, most theoretical and experimental studies on these phenomena employed pump and probe lasers with a collinear polarization direction, while the relative delay between pulses may act as a control knob for the reaction. However, there is another method to steer the outcome of two-color processes. The relative polarization direction of the pump and probe laser fields may pave the way to a selective population of different partial waves on the final electron state. This scheme, known as polarization control, has led to the identification of dichroic effects revealing variations of relative contributions of partial waves with different angular momenta [1].

Here, we will present our recent progress in the theoretical study of ultrafast two-color polarization control processes. Firstly, and bearing in mind the high spectral resolution and fine-tunability in frequency that Free Electron Lasers (FEL) can achieve, we show that the below-threshold polarization control scheme may be a valuable tool to identify interference minima in partial waves populated upon two-photon transitions from the ground state to final continuum states. Emphasis will be placed on identifying the interference mechanism leading to these minima and its dependence on the pulse duration [2].

On the other hand, one of the methods of choice to access the phase of complex-valued transition matrix amplitudes is the reconstruction of attosecond beatings by interference in two-photon transitions (RABBITT). This method originated as a characterization procedure for attosecond pulse trains. Now it is one of the most successful approaches to retrieving the total time delay in photoionization processes. For nonresonant, angle-integrated measurements, the total time delay results from the addition of electron delays induced on the pump and the probe stages [3]. More interestingly, the angularly-resolved total time delay may exhibit steep variations for some emission angles [4]. Previous studies linked these variations with the spherical harmonics describing the angular dependence of photoemission [4] and their interplay with the transition matrix amplitudes [5]. However, most previous studies on time delay using RABBITT configurations rely on a collinear polarization of the fields. Here, we combine RABBITT and polarization control approaches to show that qualitative variations of angularly-resolved time delays stem from interference channels latent in the parallel case [6, 7].

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Scaling of the fractional angular momenta of a light polarization Möbius strip in extreme non linear optics

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Synopsis The rotational symmetries of a light beam are linked with angular momenta. Thus, the spin and orbital angular momentum are respectively related to the rotational invariance of the polarization vector and of the spatial distribution of the light field. They may take values which are integer multiple of $\hbar$. In some cases, a generalized angular momentum, linear combination of the first two and taking fractional values, appears naturally. We have shown theoretically and experimentally that it is conserved during high harmonics generation, yielding beams with half integer units of $\hbar$ angular momenta.

The use of standard decomposition basis, such as the Hermite-Gaussian or the Laguerre-Gaussian modes, with left and right polarization, are most often suited to the description of any light beam. These modes are eigen modes of both the Spin and Orbital Angular Momenta (SAM and OAM) operators, yielding quantified values of the helicity as $\pm\hbar$, and of the OAM as $\ell\hbar$, with $\ell \in \mathbb{Z}$. Recently, Ballantine *et al.* [4] observed that in some specific conditions, light beams may be neither an eigen vector of the SAM (S_z) nor OAM (L_z) operators, but rather of a linear combination of them, reading $J_{\gamma,z} = L_z + \gamma S_z$, with γ a rational value determined by the symmetries of the beam. Although the discovery of this "Generalized Angular Momentum" (GAM) offered new possibilities for fundamental tests, beam shaping, quantum optics, data transfer. . . , it received little attention ever since. In particular, it was predicted to be nicely behaved in extreme non linear optics [5], but this was never experimentally tested.

The challenge to investigate the behavior of this GAM in non linear optics is to find a non linear medium that simultaneously does not alter the polarization state, and yields wavelengths for which GAM measurements is possible. In previous works, we had shown that High Harmonic Generation (HHG) is a perfect testbed for the studies of the conservation laws of OAM [2, 3]. Here we report on the development of experimental methods to measure the GAM of a light beam in the eXtreme UltraViolet spectral range [1]. We observed that the GAM is indeed scaling linearly with the harmonic order in HHG [1].

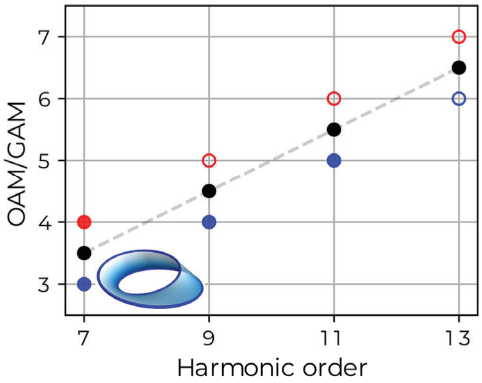

Figure 1. Experimental observation of the scaling of angular momentum in HHG. Each odd harmonic frequency is made of two underlying beams with opposite SAM (red and blue dots) carrying different OAM. Conversely, the GAM is single valued (black dots), with half integer values, and scales linearly with the harmonic order.

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Phase retrieval from angular streaking of XUV atomic ionization

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Synopsis We achieve an accurate phase retrieval of XUV atomic ionization by streaking the photoelectron in a circularly polarized IR laser field. The streaking phase can then be converted to the atomic time delay which opens access to atomic and molecular photoionization on the attosecond time scale. This novel technique will find its use in XFEL facilities and will be instrumental for studying inner shell atomic and molecular ionization.

Angular streaking of XUV atomic ionization with a circularly polarized IR laser radiation has become a powerful tool for a shot-to-shot characterization of isolated attosecond pulses from free-electron laser sources [1, 2]. This technique is analogous to the attosecond streak camera [3] in that XUV pulses are the primary source of ionization while it is common to the attoclock [4] in that the ionized electrons interact with a circularly polarized laser field which alters the photoelectron momentum distribution. Both the streak camera and the attoclock are senitive to the ionization phase that can be converted to the atomic time delay and the tunneling time, respectively. Here [5] we demonstrate, for the first time, an accurate phase retrieval of XUV atomic ionization by angular streaking.

In our numerical simulations, we solve the time-dependent Schrödinger equation for an atom ionized by a short XUV pulse in the presence of circularly polarized laser radiation. Our qualitative analysis is based on the strong field approximation [6] and the lowest order perturbation theory [8]. The two alternative techniques suggest the phase retrieval methods that can be applied both to the simulated and experimental data. In simulations, the XUV/IR delay is systematically varied. In an experiment, a second ionization feature in the same target or a mixed target could be used as a reference.

We test the proposed technique by comparing the XUV ionization phase of the hydrogen atom delivered by angular streaking with the analogous set of data returned by a well established RABBITT (reconstruction of attosecond beating by interference of two-photon transitions) technique [9]. The two sets of data agree very well in a wide range of XUV photon energies.

An analogous investigation conducted on the H_2 molecule [10] demonstrates sensitivity of the proposed technique to the molecular axis orientation and two-center interference effects.

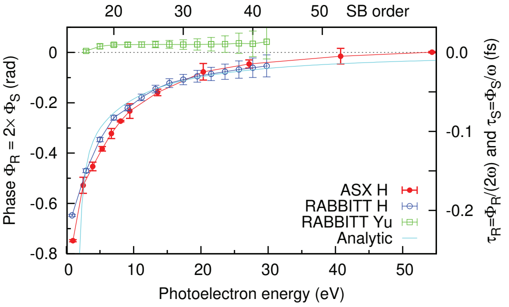

Figure 1. Left axis: RABBITT phase Φ_R is compared with the twice the streaking phase $2\Phi_s$ obtained from the isochrone ansatz of [6]. Right axis: the RABBITT time delay $\tau_a = \Phi_R/(2\omega)$ is compared with the analytic model [7].

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Optical tunnelling without a barrier?

A Weber[1 *], **and E Pisanty**[1]

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Synopsis We study tunnel ionization by a bichromatic strong-field driver in which the ω-field is gradually replaced by the 2ω-field. We show that there is a tunnelling event contributing to the spectrum of ATI for which the electric field at the time of ionization is zero. This represents a purely nonadiabatic optical tunnelling ionization event which cannot be modelled within the semi-classical picture of optical tunnel ionization.

Tunnel ionization is a central phenomenon of strong-field physics involved in essentially all intense laser-matter interactions. Strong-field ionization in the tunnelling regime takes place as discrete events which the strong-field approximation describes via saddle points that give rise to the well-established formalism of quantum orbits.

In this work we consider the nonadiabatic above-threshold ionization of a 1D model atom by a bichromatic field. We pose the question of what happens to these ionization events (i.e., saddle points of the action) when we gradually replace a monochromatic beam with its second harmonic (Figs. 1(a) through (d)). Over this replacement, the number of ionization events per cycle of the fundamental changes from two to four. We therefore ask: Which ones are new? And, how did they get there?

The transition comprises two interesting features. Firstly, we identify configurations in which the saddle points describing ionization events coalesce in a caustic (triangle in Fig. 1(b)) and form a branch point. Here, continuous labelling of saddle points becomes impossible, the saddle point approximation breaks down and instead uniform approximations have to be employed.

More remarkably, we find that the new saddle points start contributing to the ionization yield long before the field changes sign (Fig. 1(c)). In other words, we present a tunnelling ionization event which occurs when the instantaneous electric field is zero, and hence at a time when there is no barrier. This results purely from a nonadiabatic picture of tunnelling, and presents a situation which cannot be modelled within the semi-classical picture of optical tunnel ionization.

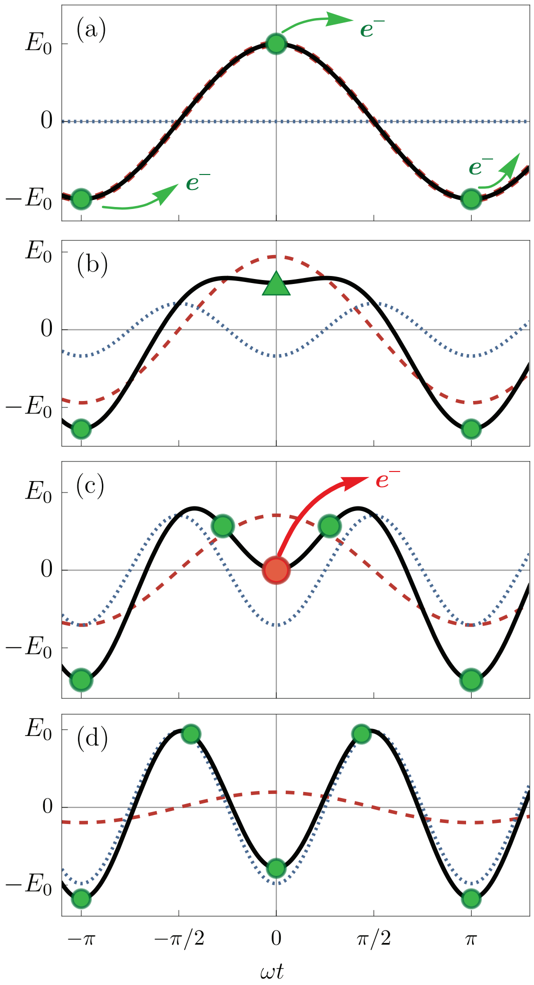

Figure 1. Total electric field formed by superposing a fundamental with its second harmonic. Green disks represent ionization events and the triangle marks the coalescence of solutions. The red disk in (c) shows a tunnelling ionization event when the electric field is zero and there is therefore no tunnelling barrier.

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Time-resolving molecular tunneling dynamics with Free-Electron-Laser-pump and High-Harmonics-Generated-probe transient absorption spectroscopy

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We combine XUV-FEL-pump with XUV-HHG-probe pulses in a transient absorption spectroscopy experiment to investigate the dissociation of molecular oxygen. We time-resolve the tunneling of the O_2^+ ($c^4\Sigma_u^-$ v=0) state into two channels within picoseconds by identifying absorption resonances of the neutral and ionic fragments.

We introduce an all-XUV FEL-pump—HHG-probe transient absorption spectroscopy scheme (see Fig. 1a), which allows to investigate XUV-initiated molecular dynamics with electronic-state-resolved sensitivity to neutral and ionic fragments. For a first benchmark of this new measurement scheme, we consider the tunneling and pre-dissociation dynamics in oxygen molecules from a specific FEL-excited state by measuring the broadband HHG-probe absorption spectra, covering 10s of characteristic absorption lines from 23 to 35 eV. The FEL-excited O_2^+ ($c^4\Sigma_u^-$ v=0) state, which exhibits a local potential-energy minimum in the Franck-Condon region, can dissociate along two parallel pathways, with the rates $R_{1,2}$, respectively, 1st: the $O(^3P)$ + $O^+(^4S^o)$ channel or 2nd: the $O(^1D)$ + $O^+(^4S^o)$ channel including the electronically excited state $O(^1D)$ (see Fig. 1c). We identify these fragments in the time-resolved absorption spectrum (ΔOD, Fig. 1b) from well-known resonant atomic transitions and find, in agreement with a rate equation model and theoretical expectations [1–4], all fragements to appear with a common 280 ps time constant.

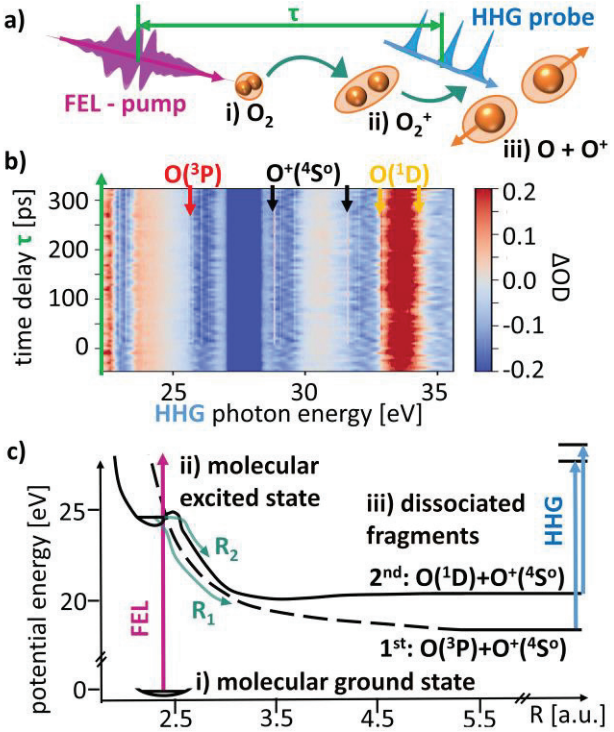

Figure 1. a) experimental scheme, **b)** time-resolved absorption spectrum, **c)** relevant O_2 potential-energy curves

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Dissociative electron attachment and electron-impact vibrational excitation of molecules

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Synopsis We report on the recent development of the nonlocal theory of nuclear dynamics in electron-molecule collisions at low energies and its successful application to dissociative electron attachment and vibrational excitation of diatomic and especially polyatomic molecules for which the constructed models were used to interpret previously unexplained features in the cross sections and electron energy-loss spectra.

Inelastic processes such as dissociative electron attachment and vibrational excitation that appear in low-energy resonant electron-molecule collisions have been studied both theoretically and experimentally for several decades. The theoretical description of these collisions consists of three steps, calculation of potential energy surfaces for both target molecules and corresponding negative molecular ions, construction of a model for nuclear dynamics based on fixed-nuclei electron scattering calculations, and final determination of the cross sections from nuclear dynamics calculations.

As the application of the theory moves from diatomic to polyatomic molecules, the nuclear dynamics calculations become quite demanding, especially when treated within the nonlocal theory of the discrete state in the electronic continuum which is necessary for a proper description of threshold effects, virtual states, etc. Recently, advancements in computational methods and resources together with the construction of the nonlocal models based on symmetry considerations enabled us to perform the first such calculations for molecule CO_2 including all vibrational degrees of freedom as a prototype for other polyatomic molecules. In the talk, we summarize these recent developments in the theory and present the application to several systems.

The detailed study of electron collisions with molecular oxygen O_2 provided an interpretation of an unusual oscillatory structure just above the threshold of dissociative electron attachment [1].

The one-dimensional (NH bond stretching) nonlocal resonance model for isocyanic acid HNCO successfully explained features in the measured cross sections of dissociative electron attachment [2] and vibrational excitation [3].

The main breakthrough in the development of the nonlocal theory was achieved by the construction of the full-dimensional model for carbon dioxide CO_2 [4] using which we were able to explain most features appearing in the 2D electron energy-loss spectrum, shown in the figure, which were observed in the experiment [5, 6].

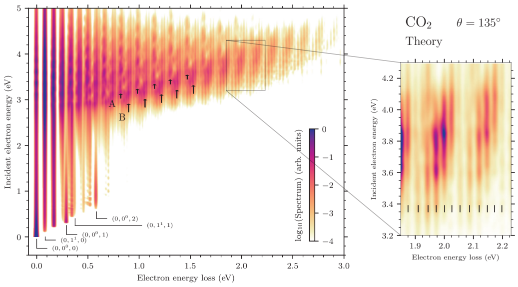

Figure 1. Calculated 2D electron energy-loss spectrum for CO_2.

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Dynamics of Dissociative Electron Attachment to Acetylacetone

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Synopsis We have studied the dissociation dynamics of acetylacetone (AcAc) on attachment of low energy electrons and identified the negative ion fragments formed and their respective resonances. We also compare the dissociative electron attachment (DEA) mechanism to photodissociation of AcAc and comment on the similarities in the two processes. We have used Velocity Slice Imaging technique to obtain momentum images of the two major fragments H- and OH-.

Low energy electrons (0-15 eV), when interacting with molecules, can form a negative ion resonance state (NIR). This NIR state can decay by autodetachment of the excess electron, or if it survives long enough, the molecule can undergo dissociation into a negative ion and one or more neutral fragments. The latter process is called DEA. We have studied DEA to acetylacetone (AcAc) molecule in the gas phase. AcAc is an interesting organic molecule that exists in two tautomeric forms, keto and enol. In the gas phase, most molecules stay in the enolic form. This leads to the presence of multiple functional groups in the molecule, like alkene, polyene, carbonyl and enol. We have studied the dissociation dynamics of this molecule and recorded the negative ion fragments formed by varying the electron energy. The major negative ion fragments observed are H^- and OH^-, followed by O^-, CH_3^- and higher masses of 41 & 43, which we assign to be $HCCO^-$ & H_2CCOH^- respectively, and 57 & 59, which we assign to be $CH_2COCH_3^-$ & $CH_3CHOCH_3^-$, respectively. All the ions are observed to have a resonance near 8.5 eV.

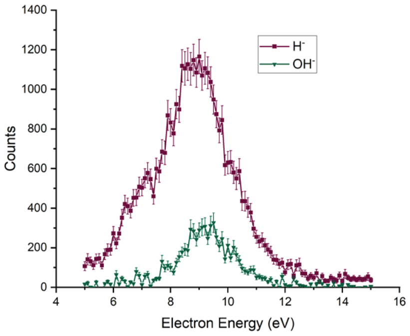

Figure 1. Excitation function of H– and OH– ion with varying electron energy.

This has two interesting implications. Firstly, based on functional group site selectivity [2], H– from the enolic site should peak around 6.5 eV, and that from the alkyl site should peak around 8.5 eV. Even though ground state AcAc is in the enolic form, we see no 6.5 eV peak. Secondly, 8.5 eV is very close to the photodissociation energy of AcAc, as recently studied by Antonov et al. [1]. Also, the DEA fragments at this energy are similar to photodissociation products. This suggests that the parent state for NIR in DEA is close to the excited dissociating state. We have compared the absolute cross-section of the formation of H–, OH–, and O– with acetone [3] and acetaldehyde.

Table 1. Absolute cross-sections of respective anions for Acetaldehyde, Acetylacetone and Acetone (in 10^{-18} cm^2).

	Acetaldehyde	Acetylacetone	Acetone
H^-	0.28 (8.9 eV)	1.01 (8.5 eV)	0.25 (8.4 eV)
O^-	0.11 (10 eV)	0.02 (9 eV)	0.04 (8.8 eV)
OH^-	0.07 (10 eV)	0.23 (9 eV)	0.01 (7.8 eV)

We have also taken momentum images of H– and OH– ions at 8.5 eV. The images show low kinetic energy release for both of these fragments which suggests that the dissociation is a multibody fragmentation process.

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Symmetry breaking in dissociative ionization of symmetric molecules by electron impact

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Synopsis We report experimental evidence of symmetry breaking in electron-impact dissociative ionization of inversion-symmetric molecules. Electron-ion coincidence experiments of CO_2 and N_2 reveal that symmetry breaking appears in the angular distribution of fragment ions. If ionization and dissociation are two separate processes, such asymmetry cannot occur. It follows that electron localization in the molecular ion is induced by the interaction with the slow ejected electron.

Symmetry plays a crucial role in photon- and electron-induced processes in molecules; it provides fundamental insights into the spectroscopic properties and gives strict rules for the angular distributions of the dissociation fragments. For instance, in dissociative ionization (DI) of an inversion-symmetric molecule, such as H_2, the fragment ion is generally emitted into both directions along the molecular axis with equal probability. However, we have recently found that under some conditions, asymmetric ion emission occurs in electron-impact DI even for symmetric molecules [1]. In this contribution, we provide experimental evidence of the symmetry breaking in electron-impact DI of CO_2 and N_2, and discuss the underlying mechanism.

Scattered electron-fragment ion coincidence experiments were carried out using an (e, e+ion) apparatus [2]. An incident electron energy of ~1.4 keV was used in the measurements. From the results, we obtained the angular distributions of the fragment ions with respect to the direction of the momentum transfer vector $\boldsymbol{K}$.

Here we show the results of CO_2. Figure 1 depicts the angular distributions of CO^+ with kinetic energy of 1.4-2.3 eV, which are plotted as a function of angle between $\boldsymbol{K}$ and the recoil direction of CO^+, $\phi_{\boldsymbol{K}}$. It has generally been assumed that DI consists of two independent steps: firstly, the ionized electron quickly escapes to infinity and subsequently, the molecular ion dissociates. Within this assumption, the probability of CO^+ emission in the direction of $\boldsymbol{K}$ should be the same as that in the opposite direction due to the inversion symmetry of CO_2^+. Indeed, the result at the electron energy loss of E = 34-36 eV is forward-backward symmetric. Nevertheless, unexpected asymmetry has been observed at E = 28-30 eV: the intensity at $\phi_{\boldsymbol{K}} \sim 0°$ is noticeably higher than that around 180°. To get a clue to the origin of this phenomenon, we consider ionization channels associated with the 28-30 eV region. Three channels, 3 $^2\Pi_u$, 2 $^2\Pi_g$, and 4 $^2\Pi_u$, can contribute to the production of CO^+ with KE ≥ 1.4 eV, and their ionization potentials (27.3, 29.7, and 30.5 eV) are close to each other. One may conceive that the Coulomb interaction between the slow ejected electron and CO_2^+ causes mixing of the close-lying $^2\Pi_u$ and $^2\Pi_g$ states. The superposition of the gerade and ungerade states leads to asymmetric electron localization in CO_2^+ and therefore breaks symmetry. Such an electron-localization effect should be general in electron-impact DI reactions over a wide impact energy range.

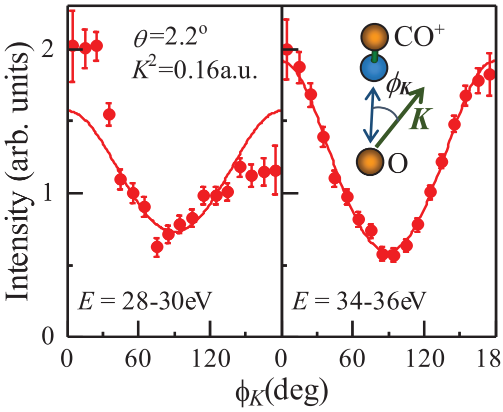

Figure 1. Angular distributions of CO^+ at scattering angle of θ=2.2°.

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Electron-Induced Fragmentation of Biologically Relevant Molecules

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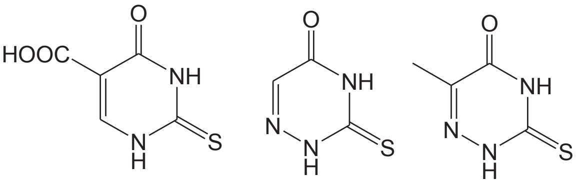
Synopsis In this work, we report on the interaction of derivatives of pyrimidines, the compounds that apart from the sulphur atom contain an additional (N) heteroatom within the six-membered ring or an electron-affinic side group -COOH, with low energy (< 12 eV) electrons in the gas phase. We observe the production of several various negatively charged species arising from low lying resonances. These data will be discussed in the context of reported results from DEA to native pyrimidine nuclobases as well as thio-analogues of bases.

Reactions induced by electron capture to molecules, including those which result in molecular dissociation, drive many of the important processes in many fundamental areas of physics, astrochemistry, material science, (nano)technology, chemical engineering, radiation physics and chemistry, and radiation therapy [1,2].

In the last decades, we have experienced a remarkable increase in research interest in studying the low-energy electron interactions with biologically relevant molecules. Among them, a large number of experimental and theoretical studies have been dedicated to DNA macromolecules and their subunits [3-5] to unravel the molecular mechanism by which LEEs damage macromolecules. More recently, much research has been devoted to compounds that can act as potential radiosensitizers in the treatment of tumors. This group of compounds contains, e.g., modified bases and nucleosides by introducing halogen atom(s) into the molecular structure. Some of these compounds exhibit a supra-additive cytotoxic effect when combined with radiation, that is, the reduction of tumor tissues is more efficient in combination than the sum of the individual effects from chemotherapy and radiotherapy.

In the present contribution, I will present experimental gas phase studies on dissociative electron attachment to six-membered rings with two or more heteroatoms and fused carbocyclic derivatives, namely 5-carboxy-2-thiouracil, 6-azauracil, and 6-aza-2-thiothymine. Such chemicals are frequently used to mimic the behaviour of (aza)pyrimidine nucleobases under reductive conditions and may be considered as potential radiosensitizers.

In particular, emphasis will be placed on the description of the formation of the transient negative ions and on the comparison of the fragmentation patterns for a series of (aza)pyrimidines.



(A) (B) (C)

Figure 1. Structure of 5-carboxy-2-thiouracil (A), 6-azauracil (B), and 6-aza-2-tiothymine (C).

Acknowledgements: This work has been supported by the Polish Ministry of Science and Higher Education,

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Production of O_2^+ following the double ionization of CO_2

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Synopsis Although CO_2 ionization and fragmentation have been the object of many studies, so far the production of O_2^+ had not been reported. In this work, absolute cross sections for the production of O_2^+ following ionization of CO_2 by electron impact is reported for the first time. We guarantee that the O_2^+ is produced by the CO_2 fragmentation by measuring its kinetic energy distribution with the DETOF technique.

The removal of one or more electrons from molecules opens up a myriad of post-collisional pathways for the system, either through stabilization of fragmentation. Furthermore, when a molecule is ionized, it is usually taken, along the Franck-Condon region, to an excited vibrational state of the new electronic configuration. This creates the possibility for new bonds to be formed between nuclei that were not originally bound to one another in the parent molecule. One such example is the well-known pathways leading to the formation of (vibrationally excited) H_2 in the fragmentation of the water molecule [1].

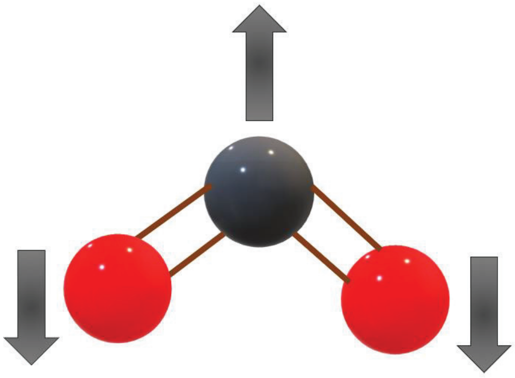

Figure 1. Illustration of the bending vibrational mode of the CO_2 molecule that leads, after the removal of two electrons, to the $C^+ + O_2^+$ fragments formation. Black and red represent the carbon and oxygen nuclei, respectively.

On the other hand, such a pathway has never been reported for carbon dioxide so far [2,3]. Differently from water, where the hydrogen nuclei stand at a ~104º angle with respect to the oxygen nucleus in the fundamental state of the molecule, carbon dioxide presents a linear structure. Nevertheless, there are well-know vibrational states of the molecule [4], including stretching and bending modes (see figure 1). In addition, the removal of more than one electron from a molecule has been shown to produce strong geometrical rearrangements in more complex compounds such as benzene [5], making it reasonable to expect that it can lead to moieties containing elements not originally bound.

The breakup of the CO_2 following ionization was studied by means of a pulsed electron gun in the 30 to 800 eV energy range, a gas cell with monitored pressure and a time-of-flight mass spectrometer. Along with all other known ionic fragments coming from CO_2 ionization [2,3], we report here the observation of the O_2^+ ion. The DETOF technique, which allows one to determine the kinetic energy distributions presents for each produced fragment [5], was employed to ascertain that the detected O_2^+ did not com from air contamination – if its parent molecule were O_2, then the resulting ion would have a Maxwell-Boltzmann thermal distribution, since it wouldn't have come from fragmentation and therefore would not acquire velocity, which happens in the breakup process. That was not the case here – the observed O_2^+ has a kinetic energy distribution centered at 1.4 eV for all measured impact energies above 40 eV.

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Charge-state distributions after beta decay of ^{6}He to form ^{6}Li$^+$

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Synopsis Projection operators have been developed to treat the double ionization of ^{6}Li$^+$ following the beta decay of ^{6}He.

The electron-antineutrino angular correlation coefficient characterizing the beta decay of ^{6}He has long been studied in searching for physics beyond the Standard Model [1]. At present, there exists a major discrepancy in the amount of double ionization predicted [2] after this beta decay compared with what is observed experimentally [3].

In Ref. [4], we partially resolve this discrepancy; the results are shown in Table 1. The difficulty encountered in previous theoretical works is shown in Figure 1, where the $E > 0$ region contains overlapping continua where single and double ionization can occur. In order to partition these two outgoing channels of ionization, we have developed projection operators by forming configuration-interaction-like products of one-electron Sturmian functions. These projection operators are then applied to the $E > 0$ region of the Li$^+$ pseudospectrum shown in Figure 1, which is formed variationally using Hylleraas wave functions and is assumed to describe the state of the ^{6}He system after beta decay in the sudden approximation.

In this poster, we will describe these methods along with their benefits and shortcomings, and offer ideas for the future resolution of this problem within the framework described here.

Table 1. ^{6}Li^{3+} charge-state fractions (in %) for each initial state following beta decay.

	Previous[2]	Present[4]	Exp't.
$1\,^1S_0$	1.2(1)	0.35(5)	0.018(15) [1]
$2\,^3S_1$	1.86(7)	0.53(7)	<0.01 [3]

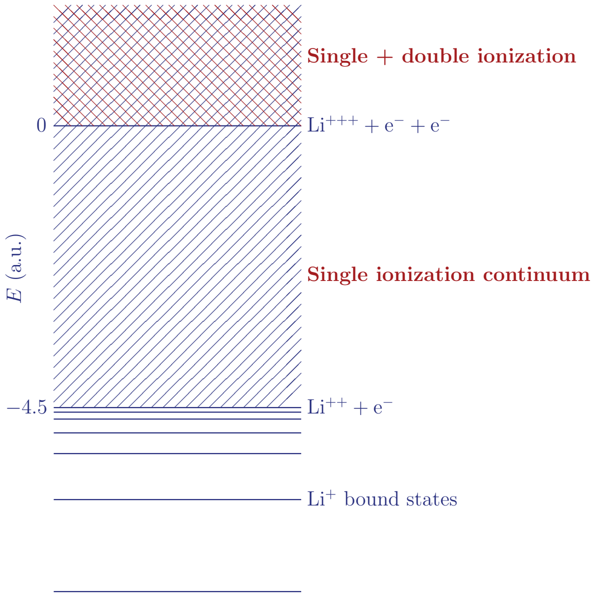

Figure 1. Energy level diagram of ^{6}Li$^+$ following beta decay. The single and double continua overlap for $E > 0$.

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Dynamics of weakly-bound molecules

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Synopsis This talk will discuss the helium dimer and trimer dynamics that ensues in response to a short laser kick.

The helium dimer is extremely weakly bound. Specifically, two bosonic helium-4 atoms support a single bound state with binding energy of approximately 1.5mK; no rotationally excited states are supported. The mixed isotope dimer (one helium-4 atom and one helium-3 atom), in contrast, does not support a bound state at all. In the trimer sector, three helium-4 atoms support two bound states. The ground state is about 100 times more strongly bound than the dimer while the excited Efimov state has a binding energy that is comparable to that of the dimer. The excited trimer state disappears upon isotope substitution. The system consisting of two helium-4 atoms and one helium-3 atom supports only a single bound state. The extremely weakly bound nature of small helium molecules makes them intriguing candidates for dynamical studies. This talk discusses the dynamics of the helium dimer [1] and the helium trimer that ensues in response to a short laser kick. The dynamics will be contrasted with those for heavier molecules that are known to feature rotational revivals.

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Directly imaging excited state-resolved transient structures of water induced by valence and inner-shell ionization

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Synopsis Real-time imaging of transient structure of the electronic excited state is fundamentally critical to understand and control ultrafast molecular dynamics. The ejection of electron from the inner-shell and valence level can lead to the population of different excited states, which trigger manifold ultrafast relaxation processes, however, the accurate imaging of such electronic state-dependent structural evolutions is lacking. Based on the three-body Coulomb explosion imaging driven by the femtosecond laser and electron beam, we revealed the ultrafast nuclear relaxation along the ground and excited states of cation and dication, and retrieved the accurate geometry of neutral D_2O.

Capturing the transient position of nuclei with sub-Angstrom and femtosecond spatiotemporal resolution for a specific electronic state can visualise the ultrafast structural dynamics of polyatomic molecules, which is a key step towards a better understanding and controlling of the chemical reaction. The CEI was developed decades ago to study the molecular structure by ionising the target to a highly charged state upon various radiation sources. The molecular structure prior to Coulomb explosion (CE) can be reconstructed from the momentum information of all the fragments in the molecular frame of reference. Benefited from the ion momentum imaging technique, CEI has equal sensitivity for the probing of light and heavy atoms.

However, retrieval the accurate electronic-state resolved structure of molecules with CEI is still elusive. A direct comparison study of the CEI induced by the ionisation of intense laser field and electron impact can provide solid experimental evidence to reveal the electronic state-resolved ultrafast nuclear relaxation dynamics of polyatomic molecules.

By developing the laser-induced electron recollision-assisted Coulomb explosion imaging approach and molecular dynamics simulations, snapshots of the vibrational wave-packets of the excited (A) and ground states (X) of D_2O are captured simultaneously with sub-10 picometer and few-femtosecond spatiotemporal precision. We visualised that bond length and angle are significantly increased by around 50° and 10 pm, respectively, within 8 fs after initial ionisation for the A state of cation, and the R_{OD} further extends 9 pm within 2 fs along the ground state of the dication.

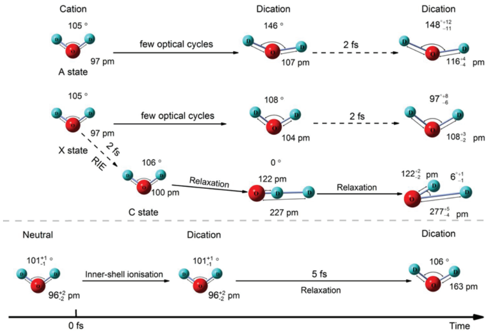

Figure 1. The summary of the time-resolved structural evolutions for different electronic states.

Moreover, the ultrafast nuclear relaxation along the autoionisation state of dication has been studied, where the R_{OD} can stretch more than 50 pm within 5 fs after double inner-shell ionisation induced by electron impact.

These results provide comprehensive structural information for studying the fascinating molecular dynamics of water, and show rich electronic states-resolved nuclei dynamics triggered by the inner-shell and valence level ionisation. Our studies pave the way towards to make a movie of excited state-resolved ultrafast molecular dynamics and light-induced chemical reaction.

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Soft x-ray multi-photon absorption for transient spectroscopy and Coulomb explosion imaging

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Synopsis Understanding the interaction of intense, femtosecond X-ray pulses with atoms and molecules and the mechanism of creating (transient) ionic states is crucial to gain insight into the structure and dynamics of matter. The fully tuneable photon energy at the European XFEL facilitates a new type of resonance spectroscopy which reveals transient species in heavy atoms, featuring, for example, up to six simulataneous core holes. X-ray induced Coulomb explosion using a reaction microscope/COLTRIMS is used to image structure and dynamics of complex molecules with unprecedented clarity.

X-ray free electron lasers (XFELs) featuring ultrashort (few femtoseconds) and ultraintense (several millijoules) pulses have opened up a variety of new science areas in the last decade. Higher repetition rates and freely tuneable photon energies have recently become available at the European XFEL. The energy tuneability over an unprecedented range (~1 keV) facilitates a new type of multiple-core-hole ion spectroscopy [1]. The very intense pulses drive many ion charge states into saturation, such that their yield becomes independent of the fluence. This facilitates the extraction of fluence-independent ion spectra mapping out transient resonant structures. Up to six simultaneous core holes are observed during X-ray ionization of xenon atoms.

The short and intense X-ray pulses are furthermore an exquisite tool for Coulomb explosion imaging (CEI) of complex molecules [2–4]. Snapshot images of the complete structure of molecules with eleven atoms, including all hydrogens can be captured, see Fig. 1. Contrary to previous expectations, this does not require to record all ions in coincidence, but three particles prove to be sufficient. The very rapid charge-up leads to a violent Coulomb explosion that preserves the information about the molecular structure at the instant of ionization.

The sensitivity of CEI to the molecular structure allows studying processes such as the influence of transient molecular resonances [5], intramolecular charge rearrangement [2] and molecular fragmentation dynamics [4]. The sensitivity of the fragmentation pattern to the molecular structure at the instant of ionization, in combination with the femtosecond pulse duration, holds the promise of monitoring the temporal evolution of the molecular structure with this method in a time-resolved experiment [3], and we have taken first steps in this direction already. Together with the prospect of even higher repetition rates at upcoming continuous XFELs, this brings the dream of recording molecular movies of photochemical reactions very close to realization.

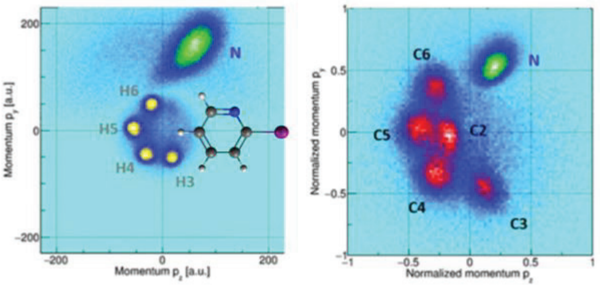

Figure 1. Molecular-frame momentum maps of iodopyridine (C_5H_4NI) molecules. Nitrogen ions (green), hydrogen ions (yellow, left), and carbon ions (red, right) are clearly distinguishable. All ions are singly charged.

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The Big, the Small & the Shoulder: Controlling OCS post-Ionization Dynamics

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Synopsis Using phase-locked two-color laser fields, we demonstrate control of the fragment ejection direction and selective bond scission in the heavy polar molecule OCS. Detected with Coulomb explosion imaging (CEI) we analyse different break-up channels with different dynamics in a major channel, a minor one and a shoulder peak. In addition to the expected direct ionization effects from these asymmetric laser fields, we also see important post-ionization contributions, which are usually not visible in heavy polar molecules.

Photo-chemical reactions can be coherently controlled in various ways. Simple pulse shaping techniques using asymmetric electric field such as carrier-envelope-phase (CEP) stabilized few-cycle pulses or phase-locked two-color laser fields have been employed to investigate the underlying mechanisms of such reaction control.

The importance of post-ionization interactions, e.g. population transfer or potential deformation in the cation to control the fragment ejection direction has been discussed for many *non-polar molecules* such as H_2, C_2H_2, and CO_2. On the contrary, the fragment ejection direction in asymmetric laser fields of *polar molecules* has been exclusively explained by the anisotropy of the tunneling ionization rate, which is determined by the shape of the ionizing molecular orbital (usually the highest occupied molecular orbital) and the molecule's permanent dipole moment rather than by post-ionization interactions. Here, we investigated the break-up processes of the prototypical polar molecule OCS in phase-locked two-color intense laser fields and identified post-ionization interaction effects [1].

To obtain these asymmetric fields, a fundamental beam is superimposed with its second harmonic while controlling the relative phase between both of them.

Dissociation into the two break-up channels of the dication, $OCS^{2+} \rightarrow O^{+}+CS^{+}$ (minor channel) and $OC^{+}+S^{+}$ (major channel) was studied and controlled. The branching ratio of the breaking of the C–O and C–S bonds followed a pronounced 2π-oscillation, depending on the relative phase of the two-color laser fields.

The fragment ejection direction of the main peak of both break-up channels reflects the anisotropy of the tunneling ionization rate, following a 2π-periodicity, as well.

Besides the main peak, the major channel also shows a shoulder peak that was not previously observed. These two dissociation pathways in the C–S bond breaking channel show different phase dependencies of the fragment ejection direction, which are assigned to post-ionization dynamics. These observations, resulting from the excitation with asymmetric two-color intense laser fields, supported by state-of-the-art theoretical simulations, reveal the importance of post-ionization population transfer in addition to tunneling ionization in the molecular fragmentation processes, even for heavy polar molecules.

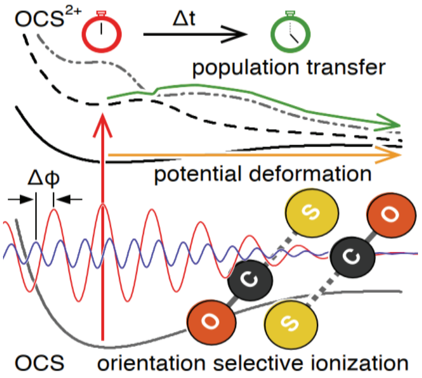

Figure 1. Scheme of post-ionization dynamics in OCS.

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Differentiating Molecular Structures using Laser-induced Coulomb Explosion Imaging

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Synopsis We show that laser-induced Coulomb explosion imaging can serve as a robust method for differentiating molecular structures and holds great promise for following structural changes, such as ring opening, with atomic resolution in pump-probe experiments.

Coulomb explosion imaging (CEI) with XFELs has recently been demonstrated as a powerful method for obtaining detailed structural information of gas-phase planar ring molecules with eleven atoms [1]. This opens up the possibility of using time-resolved CEI to directly image structural changes of intermediate-size molecules during photochemical reactions, such as ring-opening processes, with atomic resolution. However, distinguishing different products in a time-resolved measurement remains challenging.

In this work, we investigate the potential of this method in the context of CEI using a tabletop laser. We study the static CEI patterns of planar and nonplanar molecules that resemble the structures of ring-closed, open-chain, and ring-chain products formed in UV-induced ring-opening reactions [2]. As shown in Fig. 1, each molecule fragments into a well-localized and distinctive pattern in 3D momentum space, allowing the differentiation of these structures. These patterns provide direct information about molecular structure and can be qualitatively reproduced using a simple classical Coulomb explosion simulation model.

Our findings suggest that laser-induced CEI can serve as a robust method for differentiating molecular structures. Furthermore, the technique holds great promise for following structural changes at the individual atom level in pump-probe experiments, such as ring-opening reactions.

This work is supported by the Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, Office of Science, U.S. Department of Energy, Grants DE-FG02-86ER13491 and DE-SC0020276 (SB), and by the National Science Foundation Grant PHYS-1753324 (ASV).

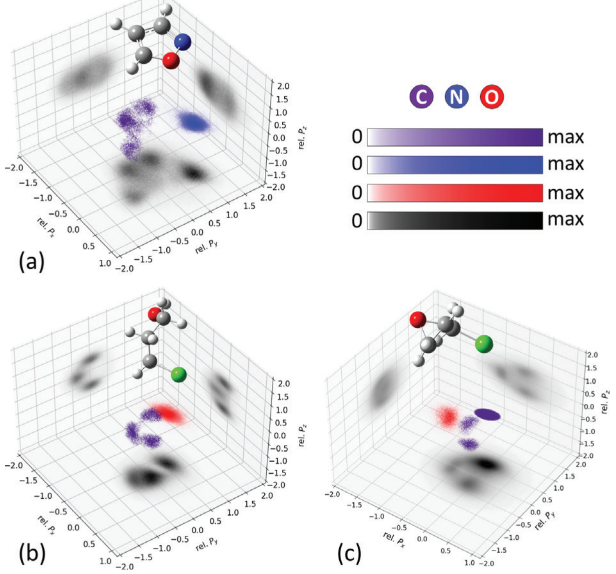

Figure 1. 3D scatter plots showing the normalized measured momenta of individual atoms in (a) isoxazole, (b) 3-chloro-1-propanol, and (c) epichlorohydrin from the 4-body (a) (C^+, C^+, N^+, O^+), and (b-c) (C^+, C^+, O^+, Cl^+) channels. The position of each data point is determined by its normalized momentum, while its color corresponds to the surrounding density. In (a), the recoil frame is rotated and rescaled such that the momentum of O^+ is set as the unit vector along the x-axis (so-called x-reference ion), and the momentum of N^+ is in the xy plane (referred to as xy-reference ion). Momenta of other ions are plotted in this frame of coordinates. The x- and xy-reference ions are Cl^+ and O^+ in (b), and Cl^+ and the first C^+ in (c). The x-reference ion is not plotted in any panels. We also do not plot the $xy-$reference ion in the p_zp_x and p_zp_y projections; they are simply a high-intensity line along $p_z = 0$.

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High-resolution spectroscopy of electronic K x rays from muonic atoms using transition-edge sensor microcalorimeters

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Synopsis We measured high-resolution spectra of electronic K x rays from muonic atoms with state-of-the-art transition-edge sensor microcalorimeters. By using a gas-phase and a metal target, we observed spectra with completely different shapes, which reflects differences in electron dynamics during muon cascade processes.

A muonic atom, where an atomic nucleus bounds a negative muon instead of electrons, has unique properties because the muon is 207 times closer to the nucleus than electrons. When a negative muon encounters an atom, the muon is captured onto a highly excited orbital of the atom and then starts a cascading deexcitation process called a muon cascade. Firstly, the muon deexcites via Auger electron emissions, which leads to the stripping of bound electrons, and then the cascade is followed by x-ray emissions. During the cascade, electron holes formed by the muon-induced Auger processes are immediately filled by the upper-level electrons via characteristic x-ray and Auger electron emissions. The dynamics of the muon cascade can be probed by a high-resolution spectrum of *electronic* K x rays because their energies strongly depend on muon states and electron configurations at the moment of the x-ray emission. However, an insufficient resolution of conventional x-ray detectors prevents detailed study.

We carried out high-resolution measurements of electronic K x rays from muonic atoms at J-PARC using a state-of-the-art x-ray detector, transition-edge sensor microcalorimeters [1]. For muonic Ar (μAr) in a gas phase, we found distinctive three peaks corresponding to electronic $K\alpha$ x rays from He-like and Li-like μAr, which implies only a few electrons remain due to Auger processes during the muon cascade. On the other hand, for muonic Fe (μFe) in a Fe metal, we observed an asymmetric and broad peak starting from the $K\alpha$ x-ray energy of a $Z-1$ atom, i.e., Mn [2]. This broad structure reflects that most of the bound electrons remain in μFe because fast electron-transfer processes from surrounding atoms occur during the cascade in the metal.

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High precision spectroscopy of pionic helium atoms

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Synopsis Laser spectroscopy was carried out on a three-body atom containing a negatively-charged pion, helium nucleus, and electron. This constitutes the first laser spectroscopy of an atom containing a meson.

Laser spectroscopy of atoms containing mesons have not been previously achieved because of the small number of atoms that can be synthesized and their typically short ($<$ 1 ps) lifetimes against the absorption of the mesons into the atomic nuclei. Metastable pionic helium ($\pi^4\mathrm{He}^+ \equiv \pi^- + {}^4\mathrm{He} + e^-$) is a heretofore hypothetical three-body exotic atom [1, 2, 3, 4, 5, 6] composed of a helium nucleus, electron, and negatively-charged pion occupying a highly-excited state with principal and orbital angular momentum quantum numbers of $n \approx \ell - 1 \approx 17$. The atom retains an anomalously long, $\tau \approx 7$ ns lifetime. We recently used the 590 MeV ring cyclotron facility of PSI which provided a high-intensity pion beam to synthesize $\pi^4\mathrm{He}^+$ in a superfluid helium target [7]. The atoms were irradiated with 800 picosecond-long resonant laser pulses of infrared frequency $\nu = 183760$ GHz that induced a pionic transition $(n, \ell) = (17, 16) \rightarrow (17, 15)$. This laser transition triggered an electromagnetic cascade that resulted in the pion being absorbed into the helium nucleus. The nucleus underwent fission and the neutron, proton, and deuteron fragments were detected. This constituted the first laser excitation and spectroscopy of an atom containing a meson. By improving the experimental precision of the $\pi^4\mathrm{He}^+$ transition frequencies and comparing them with the results of three-body quantum electrodynamics (QED) calculations [2, 6], the pion mass may be determined to a high precision. Limits may also be established on exotic forces that arise between pions and nuclei.

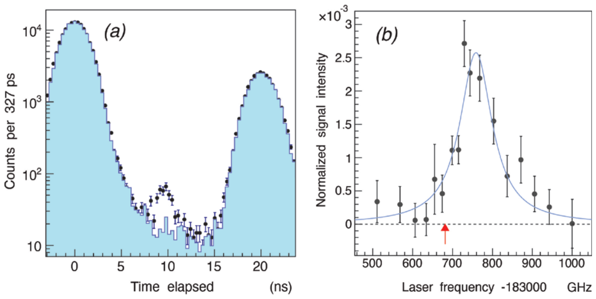

Figure 1. (a): Time spectra of protons, neutrons, and deuterons that emerged from pion absorption by helium nuclei measured with (filled circles) and without (blue histogram) laser irradiation of $\pi^4\mathrm{He}^+$. The peak in the former spectrum at $t = 9$ ns corresponds to the resonance transition $(n, \ell) = (17, 16) \rightarrow (17, 15)$. (b): Spectral profile measured by scanning the laser frequency and plotting the signal counts. The blue line indicates the best fit of a double Lorentzian, the red arrow the transition frequency obtained by a QED calculation [2]. The deviation between the two is approximately equal to the expected collisional shift [4].

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New test of bound-state QED: High-resolution measurement of an intra-shell transition in He-like uranium

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Synopsis We measured the $2p_{3/2} \rightarrow 2s_{1/2}$ transition in He-like uranium, employing a bent crystal Bragg spectrometer and a novel multi-reference method based on Doppler-tuned x-ray emission from stored Uranium ions with different charge states. This allows for an measurement of the transition energy with an unprecedented accuracy of 0.17 eV, enough to be sensitive to two-loop quantum electrodynamics effects and to rule out some of the most recent theoretical predictions.

He-like ions, the simplest multi-body atomic systems, offer the possibility to probe QED correlation and electron interaction effects. The theoretical description of these effects in extreme high electric fields, as for high-Z ions, is still challenging and different approaches leaves to different results. Thus tests by experiments are needed. By measuring the difference in transition energies between He- and Li-like ions, it is additionally possible to disentangle the contribution of electron-electron interaction in heavy bound systems from the one-electron QED contributions and from the uncertainty related to the nuclear radius. Precision spectroscopy of He-like heaviest ions is also experimentally very challenging and the $2p_{3/2} \rightarrow 2s_{1/2}$ transition in uranium was only measured in an pilot experiment [1] at the ESR with limited accuracy.

We report on an experiment conducted at the internal gas jet target of the ESR at GSI. The statistical accuracy for the measured transitions is about 0.06 eV and by comparing the similar transition in two- three- and four-electron Uranium, and an additional stationary reference source, we were able to obtain the absolute energy of the He-like uranium transition with an accuracy of 0.17 eV and the relative energy difference of He- and Li-like transition with an accuracy of 0.05 eV. This allows for the first time to be sensitive to higher order effects in the strong field regime of QED.

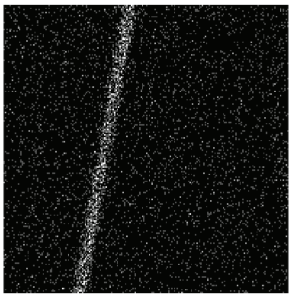

Figure 1. Detector image of the $2p_{3/2} \rightarrow 2s_{1/2}$ transition in He-like uranium. Dispersion is in the horizontal direction. The slant of the line is due to the Doppler shift.

This research has been conducted in the framework of the SPARC collaboration, experiment E125 of FAIR Phase-0 supported by GSI. It is further supported by the Extreme Matter Institute EMMI and by the European Research Council (ERC) under the European Union's Horizon 2020 research as well as by the innovation programme (Grant No 682841 "ASTRUm") and the grant agreement n° 6544002, ENSAR2. We acknowledge substantial support by ErUM-FSP APPA (BMBF n° 05P19SJFAA and 05P21SJFA1) too.

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Precision X-Ray Spectroscopy of He-like Uranium employing Metallic Magnetic Calorimeter Detectors

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Synopsis In a recent experiment, two metallic magnetic calorimeters have been applied for X-ray spectroscopy of helium-like Uranium at CRYRING@ESR at GSI, Darmstadt. The ground state transitions were recorded with a resolution of better than 90 eV at transition energies of around 100 keV. This allowed to resolve the substructure of the Kα_1 and Kα_2 lines for the first time, leading to a substantial improvement in the determination of the transition energies compared to previous studies.

Helium-like ions are the simplest atomic multi-body systems. Their study along the isoelectronic sequence provides a unique testing ground for the interplay of the effects of electron–electron correlation, relativity and quantum electrodynamics. However, for ground-state transitions in ions with nuclear charge $Z > 54$, where photon energies of up to 100 keV are reached, there is currently no data available with sufficient resolution and accuracy to challenge state-of-the-art theory [1]. In this context, the recent development of metallic magnetic calorimeter (MMC) detectors is of particular importance. Their high spectral resolution of a few tens of eV FWHM at 100 keV incident photon energy, in combination with a broad spectral acceptance down to a few keV, will enable new types of precision X-ray experiments [2, 3].

First X-ray spectroscopy studies at the electron cooler of the low-energy storage ring CRYRING@ESR at GSI, Darmstadt have recently been performed for highly-charged ions [4, 5]. We report on the second campaign, where MMC detectors have been used to study X-ray emission associated with the formation of excited helium-like uranium (U^{90+}) as a result of radiative recombination between stored U^{91+} ions and cooler electrons. The achieved spectral resolution of better than 90 eV at X-ray energies close to 100 keV enabled us to resolve the substructure of the Kα_1 and Kα_2 lines. In contrast to former experiments [6, 7], this enables a direct comparison with theoretical predictions for the individual ground-state transitions in He-like uranium without any further assumptions.

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Cold molecular dynamics and chemical reactions of H_2 (D_2) in strong laser fields

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Synopsis Rotational dynamics of D_2 molecules inside helium nanodroplets is investigated. The observations show that the D_2 molecules inside helium nanodroplets essentially rotate as free D_2 molecules. In addition, helium droplets provides the opportunity to capture two D_2 moluecules, where D_3^+ is detected implying the presence of the reaction of $(D_2\text{-}D_2)^+ \rightarrow D_3^+ + D$. We further time and control D_3^+ formation from bimolecular reaction in a D_2-D_2 dimer in gas phase.

Helium (^{4}He) nanodroplets with an extremely cold environment at 0.37 K and a broad transparent spectral range are ideal nanoreactors for light-induced physical and chemical reactions of the embedded atoms and molecules. The in-droplet molecules can rotate freely, manifesting the superfluidity of helium nanodroplets on a microscopic level. By using a non-resonant fs pulse to create rotational wave packets in D_2 molecules embedded in helium nanodroplets and measuring the rotational dynamics through timed strong-field ionization, we find the observed rotational dynamics is essentially the same as that of isolated gas-phase D_2 molecules [1].

As compared to the nuclear motion, the electron acts much faster and thus serves as an ultrafast probe of the condensed environment. More recently, we investigated the above-threshold multiphoton dissociative ionization of H_2 embedded in superfluid He nanodroplets driven by ultraviolet femtosecond laser pulses. We found that the surrounding He atoms enhance the dissociation of in-droplet H_2^+ from lower vibrational states as compared to that of isolated gas-phase molecules [2].

Cold molecular beams permit the formation of unstable moleucular dimers, e.g. H_2-H_2 dimers, achieved by precooling the molecules before its expansion into vacuum. We investigate the ultrafast formation dynamics of D_3^+ from a bimolecular reaction of a gas-phase D_2-D_2 dimer driven by ultrashort laser pulses (Fig. 1a). The formation time varies for different reaction pathways (Fig. 1b). As compared to the fast double ionization pathway, the slow single ionization pathway takes about 139 fs (Fig. 1c). By performing the molecular dynamics simulation, we track the reaction dynamics in time (Fig. 1d). Furthermore, we achieved control over the formation dynamics of D_3^+ ion by manipulating its emission direction using a tailored two-color laser field with unprecedented precision. More details can be found in Ref. [3].

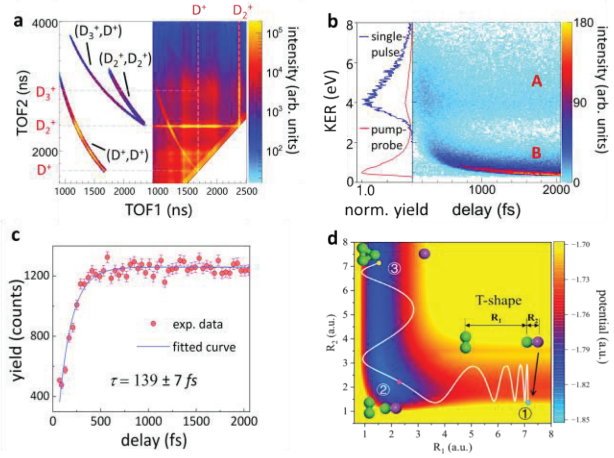

Figure 1. a, Measured photoion-photoion coincidence spectrum. b, Measured time-dependent kinetic energy release spectrum. c, Yield of D_3^+ as a function of pump-probe time delay. d, Nuclear dynamics evolving along the white curve to form D_3^+.

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Detailed Program

Monday, July 31

9:00 – 11:30	**Poster Session IV and Exhibition** • *Trillium Ballroom*
11:30 – 12:30	**Plenary Session IV** • *Electron impact ionization as a fundamental few-body reaction and a tool to study molecular dynamics* • *Room 214* Alexander Dorn (Max Planck Institute for Nuclear Physics, Germany) Chair: Emma Sokell (University College Dublin, Ireland)
12:30 – 14:00	**Free Time**
14:00 – 16:00	**Parallel Session VII A: Studies at Synchrotrons** • *Room 214* Chair: Paola Bolognesi (CNR-Istituto di Struttura della Materia, Italy)
14:00	*PR: The origin of enhanced* O_2^+ *production from photoionized* CO_2 *clusters* Smita Ganguly (Lund University, Sweden)
14:30	*PR: Synchrotron radiation studies on complex gas-phase molecules and nanoparticles* Aleksandar R. Milosavljevic (Synchrotron SOLEIL, France)
15:00	*PR: Electron attachment to cations in water by interatomic Coulombic electron capture* Nicolas Sisourat (Sorbonne Université, France)
15:30	*SR: Photoexcited polycyclic aromatic hydrocarbon undergoes intermolecular Coulombic decay* Surav Dutta (Indian Institute of Technology, India)
15:45	*SR: Shake-up and shake-off satellites as probe of ultrafast charge delocalization in liquid water* Florian Trinter (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany)
14:00 – 16:00	**Parallel Session VII B: Studies at Storage Rings** • *Room 213/215* Chair: Henning Schmidt (Stockholm University, Sweden)
14:00	*PR: Photodetachment studies with electrostatic ion-beam storage rings* Dag Hanstorp (University of Gothenburg, Sweden)
14:30	*PR: Survival of free-flying polycyclic aromatic hydrocarbon ions* Henning Zettergren (Stockholm University, Sweden)
15:00	*PR: First experiments at the CRYRING@ESR low-energy heavy ion storage ring* Michael Lestinsky (GSI, Germany)
15:30	*SR: Probing the internal dynamics of homonuclear dimer anions via time-dependent electron detachment inside an electrostatic ion trap* Roby Chacko (Weizmann Institute of Science, Israel)

15:45	*SR: Mutual neutralization of $^{1,2}H^-$ with Li^+, O^+, N^+ and C^+ at DESIREE* Alice Frederike Schmidt-May (Stockholm University, Sweden)
16:00 – 16:30	**Coffee Break** • *Rideau Canal Atrium*
16:30 – 18:00	**Parallel Session VIII A: Complex Systems and Dynamics** • *Room 214* Chair: Allison Harris (Illinois State University, USA)
16:30	*PR: Photoelectron circular dichroism: energy dependence and sensitivity to molecular configuration* Markus Schöffler (Goethe-Universität Frankfurt, Germany)
17:00	*PR: Chiral effects in dissociative electron attachment* Marcio Varella (Universidade de São Paulo, Brazil)
17:30	*SR: Observation of ultrafast proton and energy transfer in hydrated pyrrole dimers induced by electron impact* Xueguang Ren (Xi'an Jiaotong University, China)
17:45	*SR: Oscillator model applied to calculations of energy loss in anisotropic 2D materials* Silvina Segui (FAMAF UNC, Córdoba, Argentina)
16:30 – 18:00	**Parallel Session VIII B: Ion Collisions** • *Room 213/215* Chair: Lokesh Tribedi (Tata Institute of Fundamental Research, India)
16:30	*PR: Dissociation mechanisms of multiply ionized small organic molecules by heavy ion impact* Baoren Wei (Fudan University, China)
17:00	*PR: Ionization of water, ammonia, and methane by proton collision: experimental and electronic configuration studies* Wania Wolff (Universidade Federal do Rio de Janeiro, Brazil)
17:30	*SR: Fast heavy-ion-induced anion-molecule reactions on the droplet surface* Takuya Majima (Kyoto University, Japan)
17:45	*SR: Nonradiative electron capture in collisions of fast Xe^{54+} with Kr and Xe* Bian Yang (Institute of Modern Physics, Chinese Academy of Sciences, China)
19:00 – 22:00	**Conference Dinner** • *Trillium Ballroom*

Electron impact ionization as a fundamental few-body reaction and a tool to study molecular dynamics

Alexander Dorn [*]

Max Planck Institute for Nuclear Physics, Heidelberg, 69117, Germany

Synopsis Progress in reaction microscope studies of atomic and molecular ionization by electron impact is discussed. Proceeding from simple atoms to small organic molecular clusters kinematically complete experiments allow to analyse few to many-body reactions which are relevant wherever ionizing radiation interacts with matter.

This talk discusses studies of electron impact ionization of atoms, molecules and clusters in which all momenta of the participating collision partners are specified. The early (e,2e) experiments using electrostatic electron spectrometers provided detailed insight in fundamental few-particle dynamics. Consequently theory advanced tremendously culminating, e.g., in exact solutions of the Coulombic three-body problem.

I will present investigations extending the limits of these conventional instruments by using multi-electron - ion imaging spectrometers (reaction microscopes). These allow accessing the full solid angle of particle emission, small cross sections down to 10^{-21} cm^2, coincident detection of up to five particles as well as usage of low-density targets like cluster beams and weak positron projectile beams.

Our earlier studies of few-body (e,ne) reactions confirmed that the most fundamental atomic systems are well understood in present days while there are open questions and challenges for larger atoms, for the four-body continuum (i.e. double ionization) and for reversing the projectile charge sign by studying positron impact. Proceeding to molecules with a number of more degrees of freedom it is intriguing to analyze the ionization dynamics as function of their spatial alignment. Likewise the binding energy of the ionized orbital determines the molecular fate concerning its dissociation and here molecular dynamics simulations can facilitate the interpretation.

We extended these investigations to molecules embedded in an environment like it is the case in weakly bound clusters where the ionization dynamics is modified and new reaction channels are emerging. On one hand we confirmed that molecular ions can stabilize by dissipating their internal energy to the environment. On the other hand we identified dimers where only the ionization-induced intermolecular vibrations initiate molecular fragmentation [1]. Other phenomena in ionized clusters are the suppression of molecular roaming [2] and the transfer of electronic energy to a neighbor ionizing it and initiating a Coulomb explosion. While this latter so-called inter-molecular Coulombic decay (ICD) process was mostly studied for photoionization, it is likewise important for electron impact. We have found ICD for a number of bio-relevant molecular dimers as hydrated pyridine, hydrated tetrahydrofuran and also for benzene dimers [3]. For these species the accessibility of the ICD channel delicately depends on the energy spectrum of the inner-valence vacancies and the lowest monomer and dimer double ionization energies [4].

From these observations it is expected that ICD is a widespread phenomenon in loosely bound matter and that ICD can initiate the direct damage of hydrated biomolecules such as DNA in the irradiation of biological tissue.

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The origin of enhanced O_2^+ production from photoionized CO_2 clusters

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Synopsis This joint experimental-theoretical study investigates the photoreactions of CO_2 clusters induced by soft X-ray ionization. Using multi-coincidence electron-ion spectroscopy and quantum chemistry calculations, we identify a size-dependent structural transition of the clusters from a covalently bonded arrangement to a weakly bonded polyhedral geometry, resulting in dramatically enhanced production of O_2^+. Our findings demonstrate that the photochemistry of small clusters/particles could significantly impact ion balance in atmospheres, emphasizing the need for a deeper understanding of their photochemistry.

Clusters studies improve our fundamental understanding of the evolution of matter from a single molecule to an infinite solid. Recent quantum chemical calculations predict that pure CO_2 clusters exist at high altitudes in the CO_2-rich Martian atmosphere as cloud precursors [1]. At these high altitudes (60-100 km), ionizing radiation is abundant and can induce dissociation reactions in CO_2 clusters. While the formation of O_2^+ after X-ray ionization of CO_2 clusters has been previously reported [2], we present here a comprehensive experimental and theoretical study on the underlying mechanisms that lead to the production of O_2^+ [3].

We investigate the production of O_2^+ from core-ionized CO_2 clusters, using 3-D momentum coincidence imaging. CO_2 clusters were ionized using soft X-Rays (320 eV) from the MAX-II storage ring in Lund, Sweden. The measured O_2^+ yield from the ionized CO_2 clusters is substantially higher than molecular studies [4] as shown in Figure 1. The dramatic increase in yield is due to the presence of intermolecular interactions in clusters, that opens specific reaction pathways. The ion-momentum analysis shows that O_2^+ ions are produced via two different sequential dissociation processes in the clusters; and these are dependent upon the cluster size. Quantum chemical calculations allow us to propose different reaction pathways. The simulations show that the most efficient photoreaction leading to O_2^+ is when the mother cluster ion has an icosahedral structure.

We believe that these reactions are relevant to the chemistry of the CO_2-rich Martian atmosphere and can contribute to the O_2^+ concentration in the ionosphere.

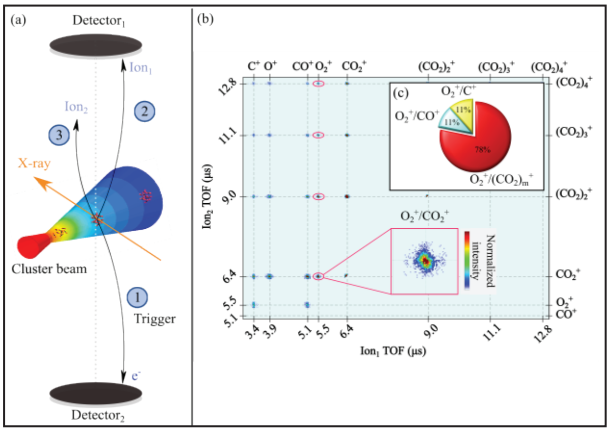

Figure 1. Principle of the experiment. (a) A schematic of the experiment of a typical electron-ion coincidence measurement. (b) 2-D coincidence map of ion time-of-flights (TOFs) produced by CO_2 clusters (20 molecules) ionized by X-ray photons (320 eV). All the cluster dissociation channels producing O_2^+ ions are highlighted in red. (c) Contribution of dissociation channels to the overall O_2^+ production.

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Synchrotron radiation studies on complex gas-phase molecules and nanoparticles

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Synopsis Technical and fundamental challenges in performing synchrotron radiation x-ray photoelectron spectroscopy of increasingly complex targets (biomolecules, clusters and nanoparticles) isolated in the gas phase will be addressed. The example results help understand fundamental properties of weakly bound molecular systems and (functionalized) nanoparticles, with a wide range of potential applications.

X-ray photoelectron spectroscopy (XPS) of targets isolated in the gas-phase, free of any solvent or substrate, allows to investigate both the intrinsic physicochemical properties of the target itself and the interaction between the projectile and the target. Furthermore, the corresponding theoretical results could be more accurately compared against the experiment, therefore providing a better understanding of the desired systems, representing a foundation for understanding the phenomena at large scales.

In this contribution, we will present an experimental setup at the PLEIADES beamline of the SOLEIL synchrotron (France) that allows for XPS of increasingly complex molecular systems isolated in the gas phase: (bio)molecules, (hydrated) clusters, and (functionalized) nanoparticles (NPs). The setup is based on the previously developed multi-purpose source chamber (MPSC) [1] and versatile target sources that can deliver to the gas phase a focused beam of large molecules, clusters [2] and NPs [3]. We will describe the above experimental systems in detail (Figure 1) and address both experimental and fundamental challenges associated with performing photoelectron spectroscopy of such complex isolated targets (binding energy calibration, working function, depth profiling etc.). Perspectives towards on-the-fly photoelectron spectroscopy of mass/charge-selected ionic targets produced by an electrospray ionisation (ESI) source will be briefly discussed as well.

Finally, we will give examples of recent results related to the investigation of clusters and NPs. The weak interactions that play an important role in the structure and dynamics of biomolecular sytems through the XPS of pure or hydrated clusters of small biomolecules [2]. The possibility to probe in situ the electronic structure of ligand-free silver iodobismuthate NPs produced for the first time by aerosol generation [3]. The investigation of localized surface plasmon resonances on noble metal NPs that drive reactions of adsorbed ligand molecules [4].

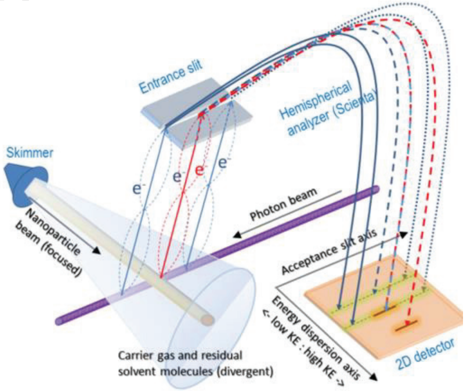

Figure 1. XPS of NPs at PLEIADES, SOLEIL [3].

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Electron attachment to cations in water by Interatomic Coulombic Electron Capture

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Synopsis Interatomic Coulombic Electron Capture (ICEC) is an environment-enabled electron capture process in which a free electron can efficiently attach to a quantum system by transferring the excess energy to a neighbor thus ionizing it. We investigate theoretically the ICEC electron attachment to a cation in the neighborhood of a water molecule.

Interatomic Coulombic Electron Capture (ICEC) is an environment-enabled electron capture: it is a unique inelastic electron scattering process in which a free electron can efficiently attach to a quantum system by transferring the released excess energy to a neighbor which is then ionized [1, 2]. This transfer can take place over large distances and has thus specific physical implications. For instance, it reduces one species (electron attachment) while oxydating another within the environment.

ICEC leads to a strong enhancement of the electron capture cross sections [3, 4]. We will report on the ICEC process in microhydrated cations. Our results show that the presence of water molecules increases significantly the electron attachment cross sections to the cations due to ICEC. Furthermore, we will show that the ICEC cross sections exhibit clear Fano profiles. The latter stem from the interferences between the ICEC final states and resonant states in which the incoming electron temporarily binds to the systems. Due to these interferences, the ICEC cross sections can be substantially enhanced or suppressed.

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Photoexcited Polycyclic Aromatic Hydrocarbon undergoes Intermolecular Coulombic Decay

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Synopsis We report Intermolecular Coulombic Decay using low-intensity UV-Visible light in an unbound system of Polycyclic Aromatic Hydrocarbon.

A system where inner valence vacancy is created by a photon it relaxes either by emitting a photon or losing another electron. This latter is known as Auger Decay. In certain cases the Auger Decay channel is energetically forbidden. However, even in such cases, if the same system is embedded in an environment, the emission of valence electrons from the neighbouring system can relax the excitation. This process is called Interatomic or Intermolecular Coulombic Decay (ICD) [1]. In the case of collective ICD, more than atoms or molecules in a cluster is excited simultaneously. The excited atoms or molecules deexcite and transfer their energies to another excited atomic or molecular system in the same cluster and ionizes it [2]. High-intensity sources are required to simultaneously excite that many atoms/molecules in a cluster. Here we report an efficient collective ICD between unbounded Polycyclic Aromatic Hydrocarbon molecules(PAHs) excited at ambient light intensity [3]. The chemical evolution of the photoexcited PAHs gives parent cations and daughter cations fragments.

The gas phase PAHs were released into the interaction region through a solenoidal pulse valve operated at 10 Hz. An unfocused 266 nm photon beam of width 4ns from the 4th harmonic of Nd: YAG pulsed laser operated at 10Hz with intensity 1×10^5 to 1×10^7 W/cm^2 was employed to photoexcite the molecules. The gas and Laser beam was crossed at this interaction region. The interaction region was the midpoint between the first two plates of the Wiley-McLaren type Time of flight (TOF) mass spectrometer, which mass separated the cations' form after light-matter interaction. The $\pi - \pi*$ excitation of PAH monomers allows them to undergo a covalent bond-forming association in our experimental condition. Two excited monomers on the way of association exchange energy via ICD resulting in ionzation (see Figure 1). The associated dimer cation is unstable and fragments into parent and daughter cations. This observed unusual collective ICD assisted by excited state molecular association implications in environmental chemistry, molecular astrophysics etc. The detailed experiments and results will be presented at the conference.

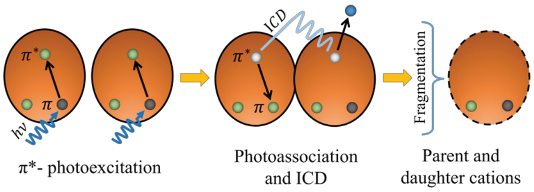

Figure 1. Schematic of the mechanism: The excited PAH monomers followed by associative interaction and ICD. The associated dimer cation formation and relaxation by molecular fragmentation are shown.

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Shake-up and shake-off satellites as probe of ultrafast charge delocalization in liquid water

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Synopsis Employing synchrotron radiation and liquid-jet photoelectron spectroscopy, we study shake-up and shake-off satellites as probe of ultrafast charge delocalization in liquid water.

Probing decays of molecular systems after core ionization, either via Auger electrons from non-radiative decay or via photons in the radiative decay channel, gives insight into nuclear dynamics as well as charge and energy transfers on the timescale of the core-hole lifetime. In particular, Auger studies on liquid water have revealed ultrafast proton dynamics in liquid water, driven via hydrogen bonding [1]. It is well known that core ionization with sufficient energy can be accompanied by the additional promotion of a valence electron into an unoccupied orbital or into the continuum, termed shake-up and shake-off, respectively. The former produces an excited, doubly ionized state, while the latter yields a triply ionized species. While these processes and the resulting spectral satellite structures have been studies intensively since the 1970s, so far, they remain unexplored in the liquid phase. Furthermore, due to the increased computational complexity, the energetics of shake-up processes have been described far less. In the case of the water molecule, early studies on the shake-off satellites exist both for via X-ray [2] and Auger emission [3], but shake-up processes have been only considered in the direct photoemission channel (e.g., [4]). Studying shake-up and shake-off satellites in liquid water promises to give new insight into ultrafast charge- and energy-transfer processes during these alternative decay pathways. For example, electrons residing in the lowest unoccupied orbital (LUMO) are known to have a high probability of delocalizing into the liquid. Also, a triply charged species may have the ability to drive bond elongation and proton transfers much more strongly. Here, it is beneficial to explore both X-ray and Auger emission channels, as the latter channel involves a change in charge state of the remaining ion and is much more sensitive to the different energetics of the shake-up and shake-off processes. Here, we systematically study shake-up satellites in gaseous and liquid water for the first time, and show that satellite states can be used to identify novel charge-transfer channels in the liquid phase. Our results will give new insight into the mechanism of proton-transfer dynamics in liquid water.

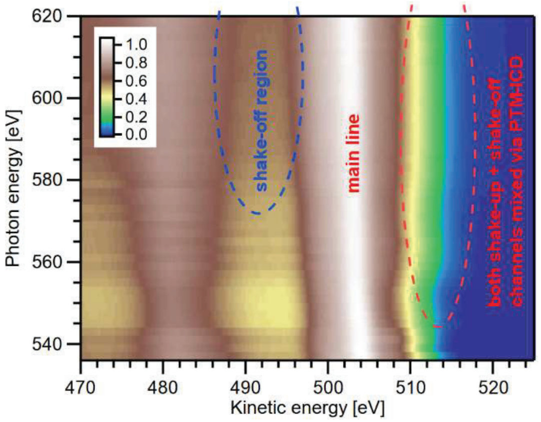

Figure 1. Liquid-water Auger emission spectra measured while scanning the photon energy above ionization; spectra are normalized to the K-$1b_1 1b_1$ Auger line. An increase in intensity at kinetic energies specific to shake-up (above main line) and shake-off (below main line) satellites is observed.

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Photodetachment studies with electrostatic ion-beam storage rings

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Synopsis By means of selective photodetachment in an electrostatic storage ring we have demonstrated that it is possible to produce a beam of pure ground state negative ions. We have used this to measure the electron affinity (EA) of oxygen in the most precise EA measurement of any element, even sufficient to resolve the isotope shift. We have also applied the method of selective photodetchment in studies of mutual neutralization. Finally, results of a systematic investigation of lifetimes of bound excited states in atomic negative ions will be presented.

Negative ions are not bound by a net Coulomb potential, and electron correlation is therefore relatively enhanced compared to neutral atoms and positive ions. Thus, negative ions are ideal systems for benchmarking atomic theories beyond the independent particle model [1].

DESIREE is a double electrostatic storage ring designed to study interactions between positive and negative ions [2]. The low temperatature (13 K) and extremely good vacuum (10^{-14} mbar) yields long storage times and a very small collisional background, making it ideal for detailed studies of negative ions.

By exposing stored negative ions with laser light that has a photon energy slightly smaller than the electron affinity (EA), it is possible to selectively detach ions in excited states while leaving ground state ions unaffected. In this way we can produce a pure ground state beam.

The EA, a key figure for determining the chemical properties of an element, can be mausured by observing the onset of the photodetachment process as negative ions are interacting with light from a tunable laser, as shown in Fig. 1. A limiting factor in such experiments is the background caused by photodetachment from bound excited states, but this background can be eliminated by selectively photdetaching the excited states. We used this method to measure the EA of ^{16}O to be 1.461 112 972(87) eV [4]. This is the most accurate EA measurement of any element, where the resolution is sufficient to resolve the isotope shift (IS) in the EA between the ^{16}O and ^{18}O isotopes. Both experimental and theoretical results of the IS will be presented in my talk. This method is general and can be applied to EA measurements of most atomic and many molecular systems.

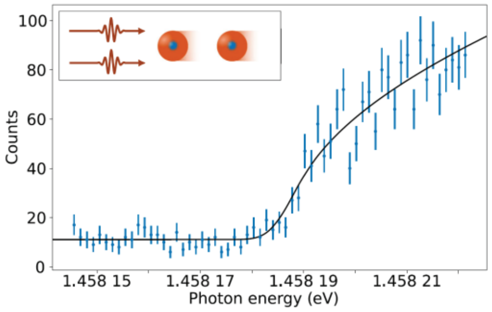

Figure 1. Photodetachment threshold of O^- using counter propagating laser and ion beams. The solid line is a fit to the Wigner law [3] convoluted with a Gaussian function.

We have further used the method of depleting negative ions in excited states in an experiment on mutual neutralization (MN) between Si^- and Na^+ ions. Here, we compared MN using a beam of pure ground state Si^- ions with a beam where both the ground state and the excited states were populated.

Finally, I will present results from a systematic investigation of lifetimes of long-lived bound excited states in atomic negative ions. The lifetime can be investigated by probing the population of the excited states as a function of the time after injection into the ring [5]. The lifetime of an excited state is highly depedent on electron correlation, making our experimental results relevant for comparisons with theoretical investigations.

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Survival of free-flying Polycyclic Aromatic Hydrocarbon ions

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Synopsis We have studied the survival of Polycyclic Aromatic Hydrocarbon (PAH) cations that are internally hot, defected and highly reactive, and after they have captured electrons in sub-eV collisions with atomic anions.

Polycyclic Aromatic Hydrocarbon (PAH) molecules have recently been unambiguously identified in the interstellar medium by radio astronomy observations [1,2]. These findings support the long-held hypothesis that this class of molecules is ubiquitous in space and thus constitutes a significant fraction of the carbon mass in the Universe [3].

Cryogenic electrostatic ion beam storage ring devices offer new opportunities to address key open questions related to how complex molecules, e.g. PAHs, may survive and interact in astrophysical environments [4]. In this progress report, I will present results from such studies of PAH cations at the DESIREE (Double ElectroStatic Ion Ring ExpEriment) infrastructure at Stockholm University. These include studies of radiative cooling processes where we monitor the spontaneous decays of hot ions and use laser probing techniques to determine their cooling rates on timescales ranging from milliseconds to seconds and beyond [5,6]. The present results highlight the importance of recurrent fluorescence for the survival of internally hot PAHs, i.e. inverse internal conversion followed by photon emission from the thermally populated electronically excited state. Small PAHs are therefore much more resilient against fragmentation than previously assumed in astrochemical models, which may have important consequences for their abundances in space [6].

Furthermore, I will present results from DESIREE experiments demonstrating that defect PAHs [7] will survive indefinitely in isolation (see Figure 1). These highly reactive species are formed in collisions typical of those in interstellar shocks and can thus act as important intermediates in the formation of larger molecules from smaller ones [7]. Finally, I will highlight pilot studies of neutralization of PAH cations in sub-eV collisions with atomic anions. In these studies we take full advantage of the unique DESIREE features [8] to monitor their survival and determine the excited states being populated in such reactions as well as the relative reaction rates as a function of center-of-mass collision energy. These results are important to benchmark theory and models for reliable predictions of e.g. the ionization balance in molecular clouds [3].

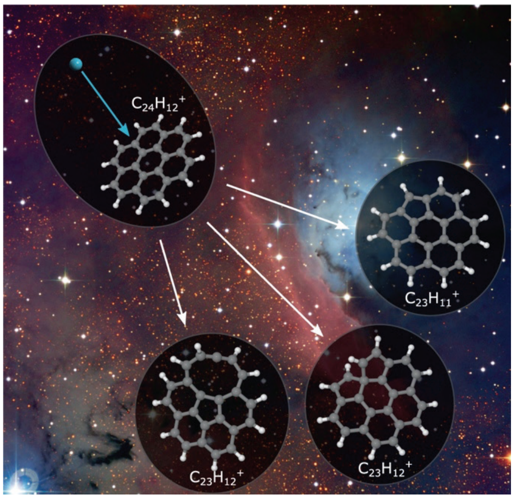

Figure 1. Highly reactive knockout-damaged PAHs are stable on astronomical timescales. In this example they stem from energetic helium atoms colliding with coronene ($C_{24}H_{12}$) [7]. Background image credit: ESO/U. G. Jørgensen.

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First experiments at the CRYRING@ESR low-energy heavy ion storage ring

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Synopsis The heavy-ion storage ring CRYRING@ESR is in operation and experiments with low-energy highly charged ion have commenced. Photonic, electronic and atomic probes are employed for precision spectroscopy in the strong field regime, for collision dynamics in slow collisions and to measure astrophysical reaction rates in the atomic and the nuclear domain. Machine performance and results from the first production runs are reviewed and an outlook for the coming years of this installation will be given.

CRYRING, a formerly Swedish facility, has been integrated into the heavy-ion accelerator topology of GSI and FAIR and is in operation. Downstream from ESR, decelerated beams are transferred to CRYRING@ESR, where the ions can be stored and cooled and probed with a variety of targets. At its new location, access to completely new classes of beam species have become available: from highly charged ions like the ultimate case of bare U^{92+} ions to in-flight produced rare isotopes. For independent operation, also a local ECR ion source with a 300 keV/u RFQ are available and provide a small range of light, stable ion species for testing setups and for some experiments. Moreover, novel experimental instrumentation is in development and some have already been implemented to CRYRING@ESR, to perform precision spectroscopy, study the dynamics of slow collisions, or provide absolute reaction rate measurements in atomic and nuclear collisions. A rich research program for the next decade has been formulated [1] and regular operation for experiment proposed by the SPARC collaboration [2] have started in 2021 [3].

We have prepared experimental installations in four sections of CRYRING@ESR which are indicated in Figure 1: At the electron cooler section merged beams electron-ion recombination can be observed through e.g. x-ray spectroscopy of photons emitted by the recombining ions or through resonant processes like dielectronic recombination. On the opposite site of the ring, a straight section is foreseen for a flexible configuration of experimental installations. Presently, a dense high-energy transverse electron target, a gas-jet target and CARME, the detector setup for nuclear reactions are mounted there and undergo commissioning. Beam extraction is a new function of the ring, where decelerated highly charged ions are deflected out and are available for material science studies with slow heavy highly-charged ions. Finally, and also along the stored-beams axis of the same section, a setup for fluorescence detection in collinear laser spectroscopy was installed.

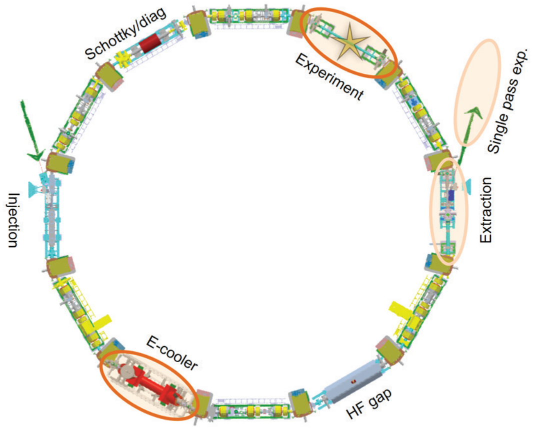

Figure 1. Schematic overview of CRYRING@ESR and its experimental installations

The talk will present the machine status, review the results from our first experiment campaign in comparison with expectations and give a preview on planned experiments in the near future.

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Probing the internal dynamics of homonuclear dimer anions via time-dependent electron detachment inside an electrostatic ion trap

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Synopsis The internal dynamics and relaxation processes within the homonuclear dimer anions of copper (Cu_2^-) and silver (Ag_2^-) are investigated employing a novel experimental technique. The experimental set-up includes electrostatic ion beam trap (EIBT), laser-assisted photodetachment, and velocity map imaging spectrometry of ejected electrons. The study reveals transitions that were not reported earlier. The results give insights into the lifetime and the internal decay processes of the anion dimers of copper and silver.

Understanding the internal energy distribution and the dynamics of energy evolution is crucial in many studies of molecules in the gas phase. Homonuclear dimer anions generally possess only one bound state, and the excited states typically lie in the detachment continuum. This makes them short-lived, and experimentally that can be challenging. We study the internal structure and dynamics of silver and copper dimer anions using a novel technique developed in our lab [1].

A unique experimental setup is fashioned with a combination of laser assist photodetachment, ion beam storage, and electron spectrometry to survey the electron ejection from the molecular anions via photodetachment and autodetachment over long time scales. Anions accelerated to 4.2 keV energy are injected into an Electrostatic Ion beam Trap (EIBT), where they oscillate between the two electrostatic mirrors of the EIBT. A laser-assisted Velocity Map Imaging(VMI) spectrometer integrated into the system records the ejected electrons' position and time-of-flight [2]. The corresponding neutral fragments are recorded separately via a MCP detector mounted after the exit mirrors of the EIBT. The coincidence events between the electrons and neutrals are stored and analyzed as a function of trapping time. The internal energy dynamics can be inferred from the photoelectron spectra obtained at different storage time windows.

The internal decay processes of hot anion clusters of silver and copper over a long time scale has been measured recently [3, 4, 5] with no direct information about the actual internal energy distribution. The present study probes the decay processes of hot anion dimers of copper and silver via electron detachment. We observe new transitions with different angular distributions which were not reported earlier. The temporal analysis allows probing the lifetime of the states. The results from this study will be presented at the conference.

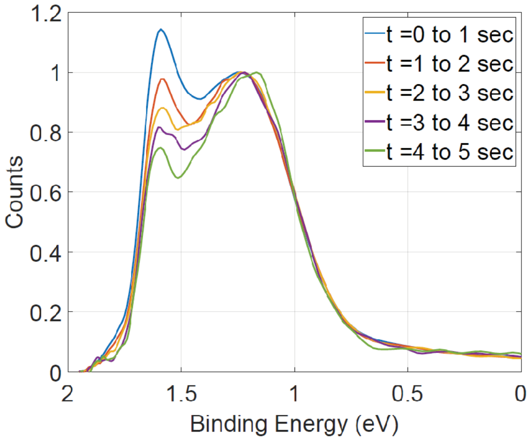

Figure 1. Photoelectron spectra of Ag_2^- at different storage times.

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Mutual neutralization of ^{1,2}H$^-$ with Li$^+$, O$^+$, N$^+$ and C$^+$ at DESIREE

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Synopsis
We present mutual neutralization studies of ^{1,2}H$^-$ with Li$^+$, O$^+$, N$^+$ and C$^+$ at DESIREE. The systems are of astrophysical interest and the collisions take place at sub-electronvolt energies which are typical collision energies in cool stellar photospheres, such as the Sun. For Li$^+$, we find a strong isotope effect on the branching fraction into Li(3s), which constitutes one of the first observations of its kind. We compare our results to theoretical predictions with varying degree of agreement.

Stellar photospheres commonly deviate from thermal equilibrium and inelastic processes influence the population distribution. The impact of collisions with the most abundant element hydrogen on the abundance analysis was studied in detail in the cases of Li, Na and Mg [1, 2, 3, 4]. Charge-transfer reactions such as mutual neutralization, and its reverse process ion-pair production, were found to have a significant influence on the abundance. Cross sections employed in non-LTE modelling are commonly estimated and reliable cross sections are highly sought after. Barklem introduced an asymptotic model based on linear combinations of atomic orbitals (LCAO) for the molecular structure and combined it with a multi-channel Landau–Zener model for the dynamics with the idea of being more widely applicable than full quantum methods [5]. Experimental results on the branching fractions such as ours serve as an important benchmark for these calculations. Specifically when studying hydrogen, the large mass ratio between hydrogen and the collision partner poses a technical challenge and hydrogen is often replaced by deuterium in the experiments. With our measurement of the MN of Li$^+$ + ^{1,2}H, we offer one of the first experimental observations of an isotope effect on the product distribution. The obtained kinetic-energy distributions are displayed in Fig. 1 and show the significant decrease of the Li(3s) product when deuterium replaces hydrogen. Additionally, we present preliminary results on ^{1}H$^-$ + C$^+$, N$^+$ and O$^+$ and compare the experimentally obtained product distributions to the predictions by LCAO.

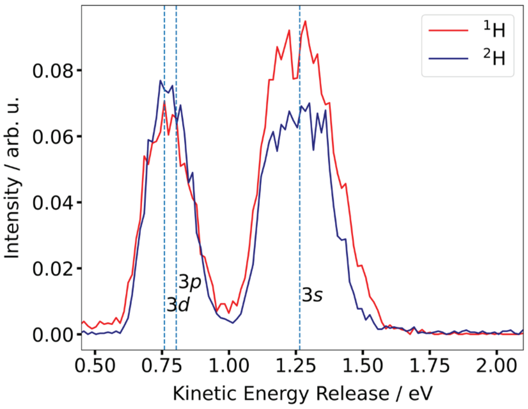

Figure 1. The obtained kinetic-energy-release distributions of MN between ^{7}Li$^+$ and ^{1}H$^-$ in red and ^{2}H$^-$ in blue. The deuterium data are from a previous study at DESIREE [6]. Both distributions are normalized to the counts in the unresolved 3p-3d peak.

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Photoelectron Circular Dichroism: energy dependence and sensitivity to molecular configuration

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Synopsis Photoelectron Circular Dichroism is the the asymmetric answer of a chiral molecule of one specific handedness, which becomes illuminated with right/left circularly polarized light. An overview of recent systematic experiments will be given.

When molecules exceed a minimum number of 4 atoms they could be chiral. This means that the molecules exists in either one of the two mirror symmetric enantiomers. Well-known examples here are sugar-molecules or amino acids. Therefore, the interest in the development of highly sensitive methods for chiral recognition is quite large. For studying single molecules in the gas-phase, several techniques have been developed, but, for example, the direct determination of the handedness of chiral molecules by Coulomb Explosion Imaging is currently restricted to small molecules [1,2]. In the past two decades, photoelectron circular dichroism (PECD) has become a new tool for the recognition. The PECD signals are much stronger (a few percent), especially compared to those of the conventional circular dichroism (CD), which relies on a scalar observable (the helicity-dependent difference in the absorption probability of circularly polarized light by chiral molecules). The PECD, the helicity-dependent emission probability of the photoelectron as a function of its emission angle exists even for randomly oriented molecules. Due to the rather strong signals of PECD, it is especially suitable for accurate examination of dilute gas-phase samples or those with a small enantiomeric excesses.

Here we report on our recent investigations and systematic studies of PECD in the gas-phase. Therefore we used an optimized COLTRIMS Reaction Microscope. The liquid samples, such as methyloxirane and derivatives of it expand with its vapor pressure through a 200 μm nozzle, forming a free super sonic gas jet, which is then skimmed twice. A closed loop recycling with 95 % efficiency per cycle [3] is used, as the samples are rather expensive. The gas jet is at right angle intersected with the synchrotron radiation. A homogeneous electric field projects the electrons and ions onto position and time sensitive detectors, with the ion-detector having a high-efficiency funnel micro channel plates [4].

In this report we will discuss how the molecule redirects the emitted electrons asymmetric in the forward/backward direction. Here the Photoelectron's kinetic energy has a tremendious influence [5,6], but also where the molecules becomes ionized [7]. Furthermore comparisons will be made for closely related molecules, where a constituent of the molecule is changed [5]. Upon the initial inner-shell photoionization, the molecule usually undergoes an Auger decay, which is followed by a Coulomb Explosion of the molecule in at least two charged fragments. This allows investigating PECD als a function of the fragments mass and its orientation in space [5,7,8]. For certain cases, where the molecule can be fixed in 3d, the molecular frame photoelectron angular distributions [9] can be derived and a PECD of fully spatially oriented molecules [10,11].

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Chiral Effects in Dissociative Electron Attachment

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Synopsis We report theoretical results for electron scattering and dissociative attachment to halocamphor molecules. Our results allow for a better understanding of the chiral asymmetry data.

The chirality dependent scattering of electrons with well defined helicity states is usually referred to as Electron Circular Dichroism (ECD)[1]. While chiral asymmetries were observed in electron transmission experiments decades ago [2, 3], asymmetries in dissociative electron attachment (DEA) reactions were reported much more recently [4, 5]. The dissociation asymmetry data for halocamphor molecules called attention because the measurements could not be fully explained based on the well-known mechanisms for ECD [1]. The data could also be viewed as consistent with the Vester-Ulbrich (VU) hypothesis [6] for the homochirality of life, which proposed that chiral unbalance could arise from the interaction with spin polarized photons or electrons.

The DEA asymmetry data could be partly understood from the cross sections calculated for electron scattering by 3-bromo-camphor (3BrC), 3-iodo-camphor (3IC) and 10-iodo-camphor (10IC) molecules [7]. Those recently reported results indicate that low-lying resonances with σ^*_{CX} character, where X denotes the halogen atom, initiate the DEA reactions of interest. While the calculated cross sections do not describe chiral asymmetries, since the spin-orbit interaction was neglected, they provide some insight into the experimental results. The energetics of the resonance states indicate the suppression of the DEA reactions in 3IC, which is consistent with the data, and also rule out couplings to higher lying anion states.

We also proposed a semi-empirical model to obtain the DEA symmetries [8], which employed spin-orbit entry amplitudes estimated from the transmission asymmetry data. The complex potentials describing the σ^*_{CX} resonance states were then built from bound-state and scattering calculations, so the DEA yields could be calculated from wave packet propagation on those potentials. While not quantitative, in view of the poor estimates for the spin-dependent entry amplitudes, our results are consistent with the DEA asymmetry data [4, 5].

Finally, we discuss the implementation of the electron-molecule spin-orbit interaction in the Schwinger Multichannel Method with pseudopotentials [9]. The improved scattering codes will allow for direct estimates of the transmission asymmetries, and hopefully also DEA asymmetries, without resorting to empirical parameters.

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Observation of ultrafast proton and energy transfer in hydrated pyrrole dimers induced by electron impact

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Synopsis Primary processes in hydrogen-bonded networks triggered by electronic ionization play a fundamental role in radiation chemistry and biology. The intermolecular proton and energy transfer processes of hydrated pyrrole dimers can potentially be initiated via a number of competing relaxation channels. By determining the fragmentation ions coincident momentum spectroscopy and the ab initio molecular dynamics (AIMD) simulations, the underlying ionization and subsequent fragmentation mechanisms are expected to be revealed.

The radiolysis of hydrated biomolecules is of great importance to a range of chemical and biological processes. The biomolecules can be excited or even ionized when they are exposed to ionizing radiation and the excited molecules are often unstable tending to dissociate. The presence of weakly bound neighbors, such as water, may substantially reduce the probability for fragmentation of the initially ionized molecules, which can manifest as a protective effect in biomatter. However, the mechanisms of electronic relaxation in hydrated molecules remain, to a large extent, unexplored due to the complex hydrogen bonding networks in these systems.

Recently, we studied the double ionization and fragmentation dynamics of hydrated pyrrole dimer by electron-impact ionization (200 eV). The experiments were performed using a reaction microscope [1], where the two resulting cations from the double ionization of H_2O-C_4H_5N dimer are detected in coincidence and their three-dimensional momentum vectors are determined. The heterocyclic aromatic molecule pyrrole is selected as the prototype since it is an important building block of large biological molecules. The electron-initialed processes were recognized as crucial for understanding an essential part of fundamental science from planetary atmospheres to biological radiation damage.

In the experiment, the sequential ionization (SI), intermolecular Coulombic decay (ICD), and electron transfer-mediated decay (ETMD) will lead to the dissociation channel H_2O^++$C_4H_5N^+$. For SI, the projectile electron successively kicks out one outer-valence electron from H_2O and C_4H_5N. The ICD can be initiated with the removal of a carbon 2s (C2s) or an oxygen 2s (O2s) inner-valence electron. Afterward, an electron from the outer-valence shell of $C_4H_5N^+$ or H_2O^+ fills the inner-valence vacancy, and the energy released ionizes the neighboring molecule [2]. The $C2s^{-1}$ and $O2s^{-1}$ state can also decay through the ETMD, where an electron from the neighboring molecule fills the initial vacancy causing the emission of another electron of the initial ionized unit [3]. While the localized double ionization of the complexes may cause the intermolecular proton transfer from the initial ionized unit to the neutral neighbor forming, e.g. the H_3O^++$C_4H_4N^+$ or HO^++$C_4H_6N^+$ channels.

The competition between these local and nonlocal decay mechanisms, as well as the follow-up ultrafast dynamics is expected to be revealed by our further experiments and *ab initio* molecular dynamics calculations. Details about these results will be presented at the conference.

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SR MONDAY

Oscillator model applied to calculations of energy loss in anisotropic 2D materials

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Synopsis We apply the oscillator model to study the energy loss processes of external charged particles interacting with a two-dimensional (2D) material characterized by an anisotropic conductivity tensor. We model the material as a monolayer of harmonic oscillators, with anisotropic modes for the in-plane electronic vibration. We consider parallel and perpendicular trajectories of the external particle, obtaining analytical expressions in terms of reduced variables. This allows us to analyze in detail the interaction and to adapt the model to the considered material using adequate values for the physical parameters involved.

Anisotropic 2D materials are of interest due to their multiple potential applications in nanoscale optoelectronics. In particular, the anisotropic optical response allows the propagation of the so-called hyperbolic plasmon-polaritons, of interest in waveguides, hyperlenses, focusing, etc. In these 2D materials, the anisotropy arises as a consequence of the atomic structure. Some examples are germanene, silicene, antimonene, and specially phosphorene, which stands out as a reference material.

In the present work we explore the properties of an anisotropic 2D material through its interaction with a beam of charged particles.To this end, we adapt the oscillator model developed previously [1, 2] representing the material as a planar array of anisotropic, non-interacting oscillators (the atomic electrons) harmonically bound to the nuclei. The characteristic frequencies of these oscillators are derived from the material's conductivity tensor. The anisotropy is introduced by allowing different frequencies $\{\omega_x, \omega_y\}$ and effective masses $\{m_x, m_y\}$ along the crystallographic directions $\{x, y\}$. The energy exchange takes place along the incident particle's trajectory, which is considered to be rectilinear, either parallel or perpendicular to the layer.

We obtain several useful analytical expressions for the energy loss as a function of the relevant parameters of the process. Figure 1 shows a polar representation of stopping power S for a particle traveling on a parallel trajectory as a function of its direction with respect to the crystallographic axes $\{x, y\}$, for a fixed velocity. Calculations were made for several values of impact parameter $\bar{b}_0$ (distance from the trajectory to the material plane), and given fixed variables. The anisotropy of the material appears in the elongated shape of the curves, which stretch along the y or x axes depending on the value of $\bar{b}_0$.

This model gives a promising alternative to study 2D materials with their distinctive properties.

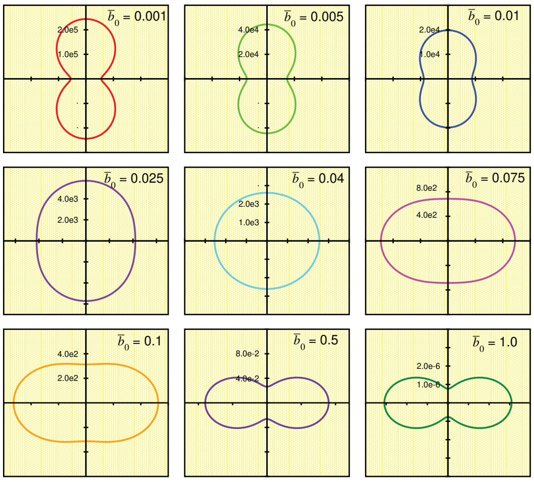

Figure 1. Polar representation of the reduced stopping power for parallel trajectory and different values of impact parameter $\bar{b}_0$. $\beta = v/c = 0.1$, $\omega_y/\omega_x = 1$, $m_x = 0.2m_0$ and $m_y = m_0$ (with m_0 the electron mass).

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Dissociation mechanisms of multiply ionized small organic molecules by heavy ion impact

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Synopsis Understanding molecular dissociation is important for research areas, e.g. interstellar media, radiation damage, and control of chemical reactions and synthesis. We present the experimental and theoretical studies on the fragmentation mechanism of hydrocarbon molecule induced by highly charged ion collisions.

As one of the most important interactions in the nature, collision processes of atoms and molecules induced by charged particles have always been one of the hot spots in the field of atomic and molecular research. Understanding molecular dissociation under energetic particle collisions by means of detecting the resultant reactive products is crucial for a wide spectrum of research areas, e.g. interstellar media, radiation damage, and control of chemical reactions and synthesis [1,2]. During collisions with charged particles, the bound electrons of a molecule could be excited and ionized. The ultrafast electronic migration will trigger nuclear motion, which leads to molecular fragmentation if enough internal energy is available [3]. The parent molecular ion could be decomposed into two or more ionic fragments in various ways, e.g., sequential versus concerted, prompt versus delayed, and "direct" versus "indirect" (whether involving isomerization or not).

The fragmentation dynamics of typical hydrocarbon molecules, i.e. CH_4, C_2H_4 and C_2H_6 [4-7], observed on the 150 kV highly charged ion collision platform at Fudan University in Shanghai, are addressed in this report. Formation mechanism of H_3^+ ions from doubly charged hydrocarbons was investigated by combining charged particle collision experiments and quantum chemical calculations. The kinetic energy release (KER) distribution of each H_3^+ loss process was measured with the cold target recoil ion momentum spectroscopy. For the asymmetric fragmentation channel of $C_2H_6^{2+}$, the reaction pathway involving hydrogen-migration-induced isomerization of $[CH_3\text{-}CH_3]^{2+}$ to $[CH_2\text{-}CH_4]^{2+}$ was confirmed, which can be accessed in the lowest triplet state rather than the ground singlet state of ethane dication. The isomerization channels ($C^+ + CH_2^+$) in C_2H_2, ($CH^+ + CH_3^+$) in C_2H_4 and the three-body fragmentation processes were also studied.

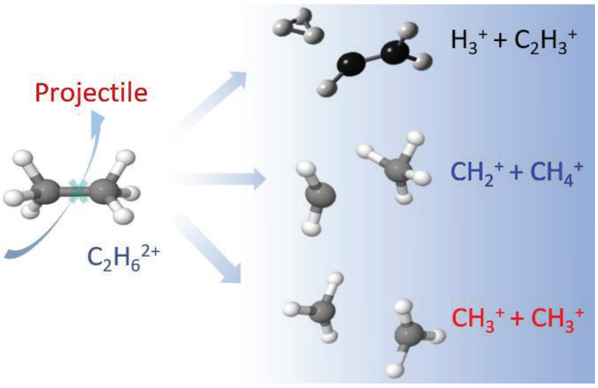

Figure 1. Fragmentation pathways of $C_2H_6^{2+}$ induced by 3 keV/u Ar^{8+} ion collisions.

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Ionization of water, ammonia, and methane by proton collision: experimental and electronic configuration studies

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Synopsis The ionic species of the isoelectronic molecules water, ammonia, and methane are a prolific source for the formation and damage of organic compounds in environments. The single ionization and fragmentation of H_2O, NH_3 and CH_4, induced by 125 to 2700 keV protons are evaluated through experimental and model cross sections. The ion´s formation depend on the selection of which electron is removed by the proton. The molecular states including the satellite states of the molecules play a dominant role in controlling the ionization and fragmentation processes.

Located in the first-row hydrides, water (H_2O), ammonia (NH_3) and methane (CH_4) are among the most important and ubiquitous chemical species. The fragmentation of these molecules by ionizing particles may involve the simultaneous breaking of one or several bonds, rearrangement, and attachment of the radicals with the consequent formation of highly reactive fragment species, ions, and neutrals, which can lead to the formation of complex molecules. These products enrich the chemistry scenario and the inventory of many physicochemical environments subjected to radiation, as planetary atmospheres, ecosystems, cosmic objects, or the human body exposed to radiation therapy.

In the report we focus to discuss some patterns among the single vacancy production of the isoelectronic molecules in the view of the molecular electronic configuration. Theoretical results and experimental data indicate a partial breakdown of the orbital picture of the ionization for the innermost orbital of water, ammonia, and methane [1]. The influence of electron-electron correlation during relaxation following the production of a vacancy need to be included in the ionization process. In the ionization of the valence orbitals many body structures were observed in the ionization spectra for ammonia in the form of a dispersion of the innermost valence ionization intensity [2]. Vertical transitions from the valence orbitals are responsible for most part of the ions production but the formation of atomic ions and ions attached to a single hydrogen are attributed to the ionization to the satellite states prepared by the shake-up process.

The ionization and subsequent dissociation of water, ammonia and methane molecules in a gas phase induced by swift protons is presented with energies varying from 125 to 2700 keV [3-5]. The experimental cross sections were well described by simple model cross sections, which incorporate to the picture of ionization the satellite structures indicating the relevance of valence excited states in the ion formation. Table 1 exemplifies for ammonia the contribution suggested by the model for the ion formation attributed to the ionization to $3a_1^{-1}$, $1e^{-1}$, $2a_1^{-1}$ and to the bands of satellite $2a_1'^{-1}$ states.

Table 1 Attribution of the ionized states to ion´s species of ammonia

	$3a_1^{-1}$	$1e^{-1}$	$2a_1^{-1}$	$2a_1'^{-1}$
NH_3^+	1	.12		
NH_2^+		.88	.07	
NH^+			.21	.1
N^+				.055

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Fast heavy-ion-induced anion–molecule reactions on the droplet surface

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Synopsis We performed a mass spectrometric study of secondary ions emitted from microdroplet surfaces by using MeV-energy heavy ions. We found that a wider variety of negative ions than positive ions were formed. We propose that the primary formation mechanism of complex negative ions is rapid association reactions of anion fragments and neutral fragments. This study provides new insights into the importance of anion–molecule reactions among fragments as the mechanism that generates complex molecular species in fast heavy-ion-induced reactions in condensed matter.

MeV-energy heavy ions deposit a large amount of energy into molecules along their trajectories in condensed matter via ionization and electronic excitation. Various fragment ions and radicals can be produced at high densities. As a result, complex molecules are expected to be produced in secondary reactions among the fragments. Secondary ions emitted from surfaces after fast heavy-ion impacts are powerful probes for obtaining molecular-level understanding of physicochemical reactions in heavy-ion tracks. Recently, we developed a coincidence measurement system for mass spectrometry on liquid surfaces—using microdroplet targets under high vacuum—to investigate complex ion–molecule reactions induced by heavy-ion irradiation [1,2]. In this study, we observed positive and negative secondary ions from droplet surfaces; such as ethanol [1,2], methanol [3], and water–methanol mixtures. In addition, we compared the results of methanol (CH_3OH) with deuterated methanol (CH_3OD) to identify the hydrogen elimination site of the intermediates that are involved in the reactions.

Microdroplets were generated by ultrasonic atomization under 1-atm Ar and then transported to the collision chamber with a differential pumping system. The droplets were irradiated with 2-MeV C^{2+} and 4-MeV C^{3+} beams from a 2-MV Pelletron accelerator. Positive and negative secondary ions were separately analyzed by time-of-flight (TOF) mass spectrometry using a coincidence technique in which forward-scattered ions were detected with a Si semiconductor detector. Correlations between the TOF and the energy of forward-scattered ions were recorded for each event in list mode [2].

Figure 1 compares the TOF mass spectra of CH_3OH with CH_3OD droplets in the range of $m/z < 80$. We observed a variety of reaction product ions; i.e., $C_2H_i^-$ ($i = 0, 1$), $C_2H_iO^-$ ($i = 0, 1, 3, 5$), and $C_2H_iO_2^-$ ($i = 3, 5$). Comparing the peak shift due to deuterium substitution, we propose that the primary formation mechanism is association reactions of anion and neutral fragments, such as $CH_3O^- + CO \rightarrow C_2H_3O_2^-$. Quantum chemical calculations confirm that these reactions can proceed without energy barriers. This study proposes the importance of rapid anion–molecule reactions among fragments in fast heavy-ion-induced reactions.

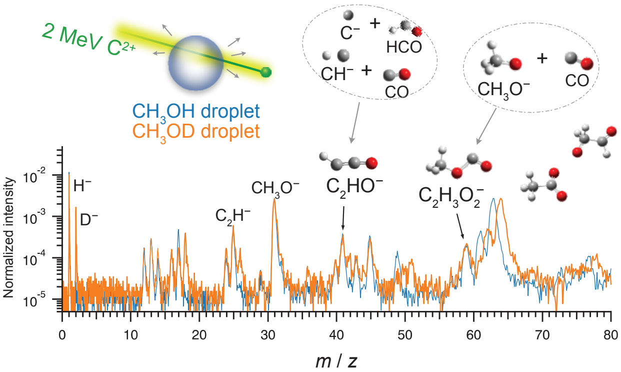

Figure 1. TOF mass spectra of the negative secondary ions from CH_3OH (blue line) and CH_3OD (orange line) droplets.

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SR MONDAY

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Nonradiative electron capture in collisions of fast Xe^{54+} with Kr and Xe

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Synopsis X rays emitted from the down-charged projectile ions produced by nonradiative electron capture in collisions of 95, 146, and 197 MeV/u Xe^{54+} projectiles with krypton or xenon gaseous targets were measured. The alignment of the projectile $2p_{3/2}$ state and the relative population of its magnetic substates were deduced from the observed angular distribution of the Lyman-α_1 transition of the Xe^{53+*} ions. Moreover, the population of excited projectile states involving single and double electron capture were investigated.

In collisions of fast highly charged ions with atoms, the nonradiative electron capture (NRC) is one of the fundamental processes [1]. In NRC, a bound electron of the target atom is captured into a bound state of the projectile with the energy and momentum being shared between the target and the projectile [1]. NRC often competes with the radiative electron capture (REC) mechanism, in which energy and momentum conservations are fulfilled by emission of a photon [2]. NRC becomes more important than REC with decreasing projectile energy and increasing target atomic number. Electron capture are important for predictions of state-charge distributions and the lifetime of stored ion beams when operation of heavy-ion accelerator and cooling storage rings, as well as research in plasma physics and astrophysics [1, 2].

In the present work, we measured x rays emitted from Xe^{53+*} and Xe^{52+*} produced by NRC in single collisions of 95-197 MeV/u Xe^{54+} ions with Kr or Xe atoms at observation angles of 35°, 60°, 90°, 120°, and 145°. Our experiments were carried out at the internal jet target of the HIRFL-CSR [3].

Figure 1 shows the energy-dependence of the alignment parameter of the $Xe^{53+}(2p_{3/2})$ state for Xe^{54+} + Kr collisions. A significant negative value of the alignment parameter at 95 MeV/u represents that NRC into the $m_j = \pm 1/2$ magnetic substates of the $2p_{3/2}$ state is about two times more probable than to the $m_j = \pm 3/2$ ones, and the Lyman-α_1 radiation is strongly linearly polarized. As the projectile energy increases, the corresponding population ratio steadily decreases and the population of the magnetic sublevels follows a statistical distribution at 197 MeV/u [4, 5]. The calculation of the alignment parameter of the REC process exhibits a rather weak dependence on the projectile energy for comparison. Moreover, the energy and target atomic number dependences of the population of excited projectile states involving single and double electron capture were investigated by means of the intensity ratios of the corresponding transitions [6].

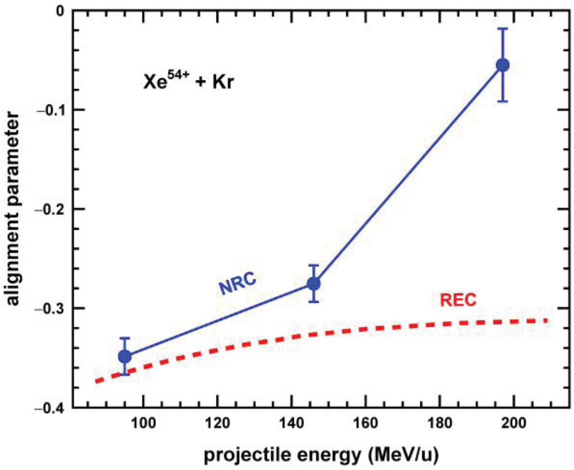

Figure 1. The experimentally determined alignment parameters of the $2p_{3/2}$ state of Xe^{53+*} ions following the NRC mechanism, as well as the theoretical results of the corresponding REC process for comparison.

We thank the crew of the accelerator department for their operation of HIRFL-CSR. This work is supported by the HIRFL research program No. HIR2021PY003 and "Young Scholars in Western China" of Chinese Academy of Sciences.

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Detailed Program

Tuesday, August 1

9:00 – 10:00	**Plenary Session V** • *Why are atomic and molecular dimers so exciting?* • *Room 214* Amine Cassimi (CIMAP laboratory, CEA/CNRS/ENSICAEN/UNICAEN, France) Chair: Stefan Schippers (Justus-Liebig-Universität Gießen, Germany)
10:00 – 10:30	**Coffee Break** • *Trillium Ballroom*
10:30 – 12:30	**Parallel Session IX A: Quantum Potpourri** • *Room 214* Chair: Marcelo Ciappina (Guangdong Technion-Israel Institute of Technology, China)
10:30	*PR: Electron emission from 2D materials induced by highly charged ions* Anna Niggas (TU Wien, Austria)
11:00	*PR: Ab-initio computation for attosecond electron dynamics in solids* Shunsuke Sato (University of Tsukuba, Japan)
11:30	*PR: Probing transient structures of nanoparticles by single-particle X-ray diffraction* Akinobu Niozu (Hiroshima University, Japan)
12:00	*PR: Modeling of EUV light source plasmas for nanolithography* John Sheil (ARCNL/Vrije Universiteit Amsterdam, The Netherlands)
10:30 – 12:30	**Parallel Session IX B: Cold Matter II** • *Room 213/215* Chair: Xavier Urbain (Université catholique de Louvain, Belgium)
10:30	*PR: Experiments with cold electrostatically trapped NO and N_2 molecules in high Rydberg states* Stephen D. Hogan (University College London, UK)
11:00	*PR: Design and underlying concepts of atomic community codes for high-precision atomic structure calculations* Bindiya Arora (Perimeter Institute for Theoretical Physics/Guru Nanak Dev University, Canada/India)
11:30	*PR: Spectroscopy of molecular ions at cryogenic temperatures - development of a novel method* Elisabeth Gruber (Universität Innsbruck, Austria)
12:00	*SR: Fragmentation upon collision-induced activation of cysteine–water cluster cations* Ewa Erdmann (Gdansk University of Technology, Poland)
12:15	*SR: Emergent s-wave dimers near a p-wave Feshbach resonance in a strongly confined Fermi gas* Kevin Xie (University of Toronto, Canada)

12:30 – 13:00	**Business Meeting** • *Room 214*
13:00 – 14:30	**Free Time**
14:30 – 16:00	**Parallel Session X A: Plasmonics/High Harmonic Generation on Surfaces** • *Room 214* Chair: Giulio Vampa (National Research Council, Canada)
14:30	*PR: Femtosecond control of plasmonic field enhancement by mode-mixing* Zsuzsanna Pápa (Wigner RCP/ELI-ALPS, Hungary)
15:00	*PR: High harmonic generation from metal surfaces* Shima Gholam-Mirzaei (University of Ottawa, Canada)
15:30	*SR: Controlling the polarization and phase of high-order harmonics with a plasmonic metasurface* Sohail Abdul Jalil (National Research Council of Canada and University of Ottawa, Canada)
15:45	*SR: Non-classical properties of light after strong-laser field processes in atomic and solid-state systems* Javier Rivera-Dean (IFCO, Spain)
14:30 – 16:00	**Parallel Session X B: Recombination** • *Room 213/215* Chair: Ann Orel (University of California Davis, USA)
14:30	*PR: Progress on dielectronic recombination spectroscopy at heavy-ion storage rings* Xinwen Ma (Institute of Modern Physics, Chinese Academy of Sciences, China)
15:00	*PR: Dissociative recombination of molecular ions in a cryogenic storage ring* Oldrich Novotny (Max-Planck-Institut für Kernphysik, Germany)
15:30	*SR: The effect of electron correlation on trielectronic recombination rate coefficients for Be-like argon* Chunyu Zhang (University of Strathclyde, UK)
15:45	*SR: Dissociative recombination of ArH^+ at the Cryogenic Storage Ring* Abel Kalosi (Columbia University/Max-Planck-Institut für Kernphysik, USA/Germany)

End of Conference

Why are atomic and molecular dimers so exciting?

A Cassimi

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Synopsis During the last 10-15 years, ion collisions have been used to unravel properties of van der Waals dimers from their fragmentation dynamics. This talk will review some recent highlights obtained in this field.

The large number of experimental and theoretical studies devoted to atomic and molecular van der Waals dimers for more than a decade is here to attest for their specific interest and the excitation they raised in the scientific community. One of their amazing feature is the monomers ability to interact at incredibly large distances through newly evidenced processes, due to the transition from closed to open shells upon ionization, such as Interatomic Coulombic Decay (ICD) [1]. However, this excitation is also due to the large amount of information obtained on the monomer themselves and in particular in the case of collisions with ions. Indeed, one of the first achievement has been to show that dimers behave as two quasi-independent monomers [2, 3].

Collision processes impact parameter dependent cross sections between an ion and an atom are not that easy to determine experimentally. The dimer geometry allows angular dependent measurements which give indirectly access to this impact parameter [3]. Dealing with molecules, the long standing question concerning the center to which the active electron belongs (could be reworded as “on which side of the molecule was the active electron during the interaction?”) has been answered thanks to the low electron mobility across an atomic dimer [3]. Furthermore molecular dimer fragmentation provides a smart way for metastable molecular state identification [4], one of the two monomers acting as a spectator probe to access the life time of the second monomer dissociating excited state.

Another strong motivation in studying ion-dimer collisions is to answer the question: to what extent gas phase results can be applied to the condensed phase. For example, can collision induced molecular fragmentation cross sections performed in the gas phase be used as the starting point (physical stage) for radiolysis chemical stage codes? Even if monomers tend to behave independently during a collision, interaction processes exist between them. Thus, while in low energy ion-atom collisions, electron emission vanishes, the ICD process appears as the projectile charge state decreases and becomes a new source of low-energy electrons. Such electrons are known to play a role in radiobiology and have to be taken into account at the end of the range, where the projectile ion stops in matter [5]. Van der Waals dimers mimic a simple environment while allowing keeping access to dynamics measurements using coincidence techniques such as COLTRIMS. However, it has also been shown experimentally that molecules may dissociate identically whether isolated or within a dimer [6]. This may validate the use of gas phase data in condense phase modelling.

Ion-dimer collision physics is rich and broad and has still plenty of topics to tackle. Theoretical calculations are just starting [7] and are highly needed to confirm the experimental data interpretations, as well as collision induced reactivity between the monomers within dimers [8].

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Electron emission from 2D materials induced by highly charged ions

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Synopsis We compare the electron emission from monolayers of semimetallic graphene and semiconducting MoS_2 triggered by the impact of highly charged ions. Although the potential energy deposition in both materials is similar, the electron yield varies strongly. A 6-fold higher electron yield of graphene is explained by the formation of a positive charge patch in MoS_2 upon ion impact, which prevents low-energy electrons from escaping the semiconducting material.

Ions in very high charge states, e.g., Xe^{40+}, possess large amounts of potential energy (several tens of keV) that equals the sum of binding energies of all missing electrons. Especially for slow highly charged ions with velocities v smaller than the Bohr velocity, the potential energy deposition upon material impact is confined to the very first surface layers and dominates the ion-solid interaction [1, 2]. Pumping large amounts of potential energy into the material leaves it in an excited state, which subsequently relaxes via various deexcitation channels including emission of secondary particles (electrons, x-rays, sputtered target atoms) and material modification [3]. However, depending on the (electronic) properties of the sample, the material response to the impact of highly charged ions can vary drastically. Here, we focus on one deexcitation regime, namely the emission of electrons and discuss the influence of material properties using semimetallic graphene and semiconducting MoS_2 as case study.

To exclude any secondary effects arising from ion interaction in deeper layers we rely on free-standing two-dimensional samples. We perform our measurements in a coincidence mode, i.e., we detect correlated pairs of transmitted ions and emitted electrons, where for the latter we can chose between either studying the energy distribution or the yield γ of emitted electrons. That way we can separate influences from support structures in order to study truly the primary electron emission from a solid surface.

Even though the potential energy deposition in monolayers of MoS_2 is similar compared to graphene [4], we find a smaller electron yield by a factor of 1/6 in MoS_2. This can be explained by a charging up of the material around the impact point which dissipates much faster in the semimetal than in the semiconductor. This charge patch prevents low-energy electrons from escaping the material and reduces the yield. Accordingly, it alters the electron energy distribution as well [5].

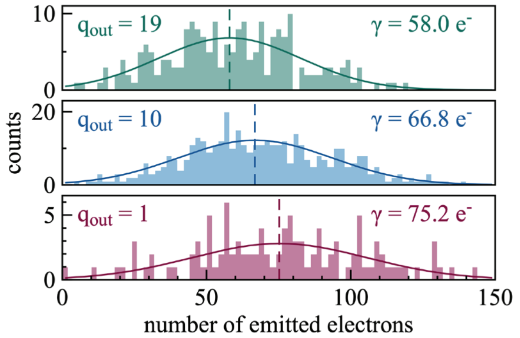

Figure 1. Electron emission spectra for 98 keV Xe^{30+} impinging on free-standing single-layer graphene with increasing electron yield γ for different ion exit charge states q_{out}.

For the high emission yields of graphene we can perform experiments in even more detail and compare the yield for different exit charge states q_{out}. Thereby we find that for decreasing q_{out}, i.e., more deposited potential energy, the electron yield γ increases as can be seen in Figure 1 for 98 keV Xe^{30+} incident projectiles. This underpins that the electron emission gives direct access to the neutralisation dynamics of highly charged ions at surfaces.

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Ab-initio computation for attosecond electron dynamics in solids

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Synopsis First-principles electron dynamics calculation based on the time-dependent density functional theory is a powerful tool for analyzing light-induced electron dynamics in solids. In this talk, we first introduce the numerical pump-probe experiment as a theoretical approach for studying ultrafast phenomena in solids. We then discuss the application of the pump-probe simulations to attosecond transient absorption spectroscopies in solids.

Thanks to the recent developments in laser technology, the experimental investigation on ultrafast electron dynamics in solids with attosecond time resolution has been realized. Such ultrafast spectroscopic experiments on solids provide valuable insights into nonlinear and nonequilibrium quantum dynamics of matter in the ultrafast regime. On the other hand, the experimental results are often difficult to interpret directly due to the complex electronic structure of solids.

First-principles calculations based on the time-dependent density functional (TDDFT) [1] is a powerful tool to investigate such complex electron dynamics in real materials and to provide microscopic insights into ultrafast phenomena. To demonstrate the capability of TDDFT calculations, we compute the electron dynamics in crystalline silicon induced by intense laser irradiation. Figure 1 shows the electron density distribution in Si before and after the intense laser irradiation. Clear covalent bonds (red region) can be found before the laser irradiation in Fig. 1 (a). In contrast, the covalent bonds are broken after the laser irradiation in Fig. 1(b) due to the strong electronic excitation. As demonstrated here, the TDDFT calculations allow us to microscopically analyze the nonlinear and nonequilibrium electron dynamics driven by the intense laser irradiation in solids.

In this talk, we will review the methodology for directly simulating attosecond transient absorption spectroscopy by mimicking pump-probe spectroscopy with TDDFT calculations [2]. We will also present the application of this first-principles pump-probe spectroscopy to transition metals such as Ti [3] and magnetic materials such as Co and Ni [4] to analyze the electron and spin dynamics driven by intense ultrashort pulsed light in these metals.

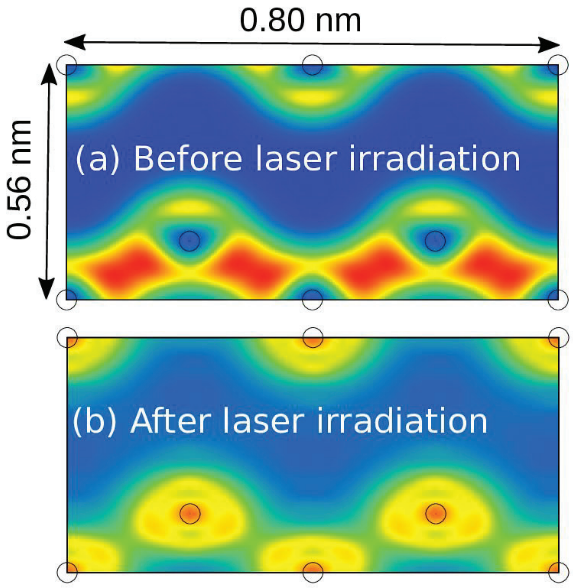

Figure 1. Electron density in crystalline Si (a) before and (b) after intense laser irradiation, as obtained by TDDFT calculations.

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Probing transient structures of nanoparticles by single-particle X-ray diffraction

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Synopsis We report the results of ultrafast single-particle X-ray diffraction of rare-gas nanoparticles at SACLA. We studied the crystallization dynamics of Xe nanoparticles by single-shot and single-particle X-ray diffraction. We also investigated the ultrafast structural dynamics of laser-induced plasmas by pump-probe X-ray diffraction.

The availability of ultrashort and intense pulses from X-ray free-electron lasers (XFELs) [1] has enabled novel experimental approaches in a wide range of research fields, including biology, chemistry, and materials science. Among the novel techniques using XFELs, ultrafast single-particle X-ray diffraction is a promising technique for elucidating the three-dimensional structures of nanoparticles and, moreover, structural dynamics on the nanoscale with unprecedented temporal resolution.

In this paper, we present the recent results of ultrafast X-ray diffraction of single rare-gas nanoparticles performed at SACLA [2]. The first topic is the crystallization dynamics of rare-gas nanoparticles nucleated in a supercooled gas jet [3, 4]. In the experiment, the crystal structures of Xe nanoparticles produced by adiabatic gas expansion were investigated by single-particle wide-angle X-ray diffraction. The diffraction data of the Xe nanoparticles suggested the formation of a stacking-disordered structure called the random hexagonal close-packed (rhcp) structure, as well as the face-centered cubic (fcc) structure, which is the expected bulk stable structure. Furthermore, we analyzed single-particle diffraction patterns and identified the coexistence of fcc and rhcp structures in individual nanoparticles. The observations provided meaningful insights into the crystallization kinetics of the Xe nanoparticles, supporting the initial crystal growth of the nanoparticles in the metastable rhcp phase and the subsequent transformation into the stable fcc phase.

Furthermore, the combination of XFEL and synchronized laser system allows the real-time observation of laser-induced structural dynamics on the femtosecond timescale [5]. In the second topic, we studied the ultrafast structural dynamics of nanometer-scale plasmas (nanoplasmas) induced by an intense near-infrared (NIR) laser pulse [6, 7]. We carried out pump-probe wide-angle X-ray diffraction experiments to investigate the crystalline order in the nanoplasmas. In the pump-probe diffraction data, Bragg diffraction intensities showed a decrease on a timescale of several hundred femtoseconds after the NIR excitation [6]. This means that the nanoparticles retain the crystalline order for several hundred femtoseconds after laser excitation, despite huge energy absorption in the nanoparticles. Furthermore, we observed an evident laser intensity dependence in the timescale of crystalline disordering [7], which was correlated to the speed of ions ejected from the nanoplasma.

The author is grateful to the co-authors of the papers [3, 4, 6, 7] with whom the experiments were conducted.

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Modeling of EUV light source plasmas for nanolithography

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Synopsis An overview is given on recent developments in modeling laser-driven EUV light source plasmas for nanolithography, from fundamental studies on atomic structures and opacities to radiation-hydrodynamic simulations of solid-state, laser-driven EUV source plasmas for future nanolithography.

EUV lithography is the process by which nanometre-scale patterns are inscribed on silicon wafers using extreme ultraviolet radiation to produce computer chips[1]. This radiation is generated in a hot and dense laser-driven plasma formed by irradiating tin targets with high-intensity laser radiation. In this progress report, I will give an overview of recent efforts in modeling these complex, mid-Z laser-driven plasmas.

First, I will discuss the atomic origins of this EUV radiation. Recently, we have shown that this radiation originates in large part from transitions between multiply excited states in $\mathrm{Sn}^{11+} - \mathrm{Sn}^{14+}$ ions[2]. This finding contradicts a well-known paradigm that transitions from singly excited states are the dominant source of EUV radiation in these plasmas. Recent work on understanding the role of such transitions in CO_2 laser-driven plasmas[3], as well as the role of radiation fields in determining the underlying atomic kinetics will be discussed.

Second, I will discuss the physics of ion expansion in laser-driven EUV source plasmas. Laser-produced plasmas generate copious amounts of high-energy ionic debris which could potentially damage sensitive optical components in EUV sources. Understanding and predicting the behaviour of such ions is essential for designing debris mitigation strategies. I will present recent work on this topic, where we have shown that single-fluid radiation hydrodynamics is capable of reproducing the shape of an absolutely calibrated ion kinetic energy distribution as well as the absolute number of ions detected in laser-plasma experiments[4]. I will also show how our simulations are capable of reproducing the anisotropy observed in experimental measurements of the ion kinetic energy distributions[5].

Finally, I will give an overview of our recent work in characterizing the properties of laser-plasmas driven by laser wavelengths in the $\lambda_{\mathrm{laser}} = 1.064-10.6$ μm range[6]. We have identified the establishment of steady-state plasma flows in the irradiation of tin droplets with said laser wavelengths, and moreover identified a temporal constancy in the energy components of the plasma (energy in radiation, kinetics, etc.). We identify and explain the origin of a peak in the conversion efficiency for $\lambda_{\mathrm{laser}} = 4$-$\mu$m-driven tin plasmas.

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Experiments with cold electrostatically trapped NO and N_2 molecules in high Rydberg states

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Synopsis Experiments performed with NO molecules that were decelerated and electrostatically trapped using the methods of Rydberg-Stark deceleration will be described. These molecules, in Rydberg states with principal quantum numbers between 32 and 48 were trapped > 1 ms. Effects of vibrational and rotational excitation of the NO^+ ion core on the trap decay rates were studied. The recent extension of this work to the first demonstration of electrostatic trapping cold N_2 molecules in Rydberg states will also be presented.

Atoms and molecules in Rydberg states with high principal quantum number n can posses large static electric dipole moments. These scale with n^2, exceed 3000 debye for values of $n \geq 30$, and allow forces to be exerted on samples in these states using inhomogeneous electric fields [1]. This approach, known as Rydberg-Stark deceleration, has been implemented to prepare cold, trapped gases of H, D, He, H_2, NO and now N_2. The most recent work with NO [2, 3, 4] and N_2 has allowed measurements of excited-state decay processes in these molecules over previously inaccessible timescales. The results obtained are of interest in understanding of the role high Rydberg states play in atmospheric physics and chemistry, including plasma recombination. The velocity-controlled beams generated in this work are well suited to studies of low-temperature ion-molecule reactions [5], and intermolecular resonant energy transfer [6].

In the experiments NO molecules, initially travelling at 800 m/s in pulsed supersonic beams, were photoexcited to high Rydberg states using the $n\ell\,\mathrm{X}^{+\,1}\Sigma^+ \leftarrow \mathrm{A}\,^2\Sigma^+ \leftarrow \mathrm{X}\,^2\Pi_{1/2}$ resonance-enhanced two-colour two-photon excitation scheme. They were then loaded into the travelling electric traps of a chip-based Rydberg-Stark decelerator and decelerated to rest in the laboratory-fixed frame of reference in a time of 250 μs ($\sim$ 100 mm). The apparatus was cooled to 30 K to minimise effects of blackbody radiation. The trapped molecules were detected by pulsed electric field ionisation. Studies were performed with Rydberg states in series converging to the lowest, $v^+ = 0$, and first excited, $v^+ = 1$, vibrational states of NO^+. These allowed effects of vibrational channel interactions on the excited-state decay rates to be identified, and bounds to be placed on rates of vibrational autoionisation. Experiments were also performed with molecules excited to Rydberg states in series converging to a range of rotational states of the NO^+ ion core to study effects of rotational excitation on the excited-state decay rates.

The same apparatus has also now been used to prepare cold trapped N_2 molecules in high Rydberg states for the first time. In this work Rydberg state photoexcitation was implemented using a three-photon excitation scheme [7]. This involved driving the two-photon transition from the $\mathrm{X}\,^1\Sigma_g^+$ state to the $\mathrm{a''}\,^1\Sigma_g^+$ intermediate state [8], followed by single-photon transitions to access long-lived $v^+ = 0$ Rydberg states converging to the $\mathrm{X}\,^2\Sigma_g^+$ state of N_2^+. In these experiments, molecules in states with values of n close to 40 were decelerated and trapped for times in excess of 1 ms.

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Design and underlying concepts of atomic community codes for high-precision atomic structure calculations

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Synopsis The talk will present a report on the development of code and web portal that are capable of calculating an extensive range of atomic properties to answer the significant needs of atomic, plasma, and astrophysics communities.

In a number of present applications, ranging from studies of fundamental interactions to the development of future technologies, accurate atomic theory is indispensable to the design and interpretation of experiments, with direct experimental measurement of relevant parameters at times being impossible or infeasible. Further rapid advances in applications involving atoms in the fields of quantum information, degenerate quantum gases, atomic clocks, precision measurements, studies of fundamental physics, and others will require accurate knowledge of basic atomic properties, most of which remain highly uncertain and difficult to measure experimentally. In this talk, I will discuss our research group's involvement in two projects which aim to solve this problem by developing general easily accessible community codes which provide high-precision atomic properties required for technological developments in the fields of cold atom physics, atomic clocks and quantum computing. In the first part of the talk, development of a general community code, easily accessible through a community web portal which provides accessible high-quality atomic data and user-friendly, broadly-applicable modern relativistic computational applications to treat electronic correlations will be discussed. In the second part, an easy-to-use Python package for the calculation of properties of atomic systems with the required precision will be discussed. The proposed package will be based both on relativistic and non-relativistic methods and will be able to calculate the properties of low-lying and high-lying Rydberg states. An option to use various basis sets within the package for calculating atomic properties will be provided. The role of basis set for calculating various atomic properties such as electric dipole moments, dipole and quadrupole polarizabilities, lifetimes, hyperfine constants, black body friction forces and parity non-conserving amplitudes will be discussed to get a fundamental insight of atomic systems.

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Spectroscopy of molecular ions at cryogenic temperatures – Development of a novel method

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Synopsis We present a novel experimental setup to perform messenger spectroscopy of mass-per-charge selected molecular (cluster) ions. The He-tagged ions are formed in the unique environment of highly charged helium nanodroplets. Moreover, the setup allows us to study the stabilization and solvation of multiply-charged dopant ions in the ultracold environment of HNDs.

Action spectroscopy is a very powerful method to explore the spectroscopy and dynamics of gas-phase molecules, and to provide benchmark data for quantum-chemical calculations. In the last decades, several devices have been developed which allow spectroscopic investigations of molecular ions at cryogenic temperatures. The cooling confines the ions in their vibrational ground state and simplifies the observed spectra due to the reduction of conformational heterogeneity and spectral congestion.

One of these methods uses superfluid helium nanodroplets (HNDs) as a cold, inert and optically transparent environment for doping atomic and molecular species [1]. The weak interaction between helium and the dopants is minimally perturbing and facilitates the collection of high-resolution absorption spectra.

In this contribution, we present a novel instrumental setup which allows us to efficiently produce He-tagged ions in order to study them by messenger spectroscopy [2]. Here, the dissociation of the weakly bound He tag is used as a messenger for photoabsorption. In the first step, HNDs are highly ionized by electron impact [3] and doped with the sample of interest. The charge centers are distributed across the droplet and attract the dopants, which are ionized by charge transfer processes. Cluster ions of a specific size and composition can be formed by using this technique [4]. Afterwards, the dopant ions are gently extracted by collision induced evaporation of the host droplet, delivering high yields of He-tagged ions of both polarities at cryogenic temperatures. In the next step, the ions are mass-per-charge selected in a quadrupole mass filter and merged with the laser beam. The emerging photofragments are detected in a time-of-flight mass-spectrometer. The high signal-to-noise ratio enables high quality spectra even for weak absorption lines at reduced data acquisition times.

Recently, we further enhanced the setup by the implementation of a second electron impact source after the pick-up region to enable the formation and study of cold multiply-charged dopant (cluster) ions [5]. The location of multiple charge centers in a single He droplet close to the surface makes them accessible for subsequent interactions with metastable He atoms, which leads to Penning ionization and the formation of cold multiply-charged dopant ions. We used this method to form doubly and triply charged rare gas cluster ions, and we obtained critical cluster sizes well below the values acquired by conventional measurements.

Acknowledgement

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Fragmentation upon collision-induced activation of cysteine–water cluster cations

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Synopsis Cysteine-water cluster cations have been prepared by assembly inside He droplets and subsequently analyzed by means of tandem mass spectrometry using collision-induced dissociation (CID). Quantum chemical calculations based on the Density Functional Theory as well as Monte Carlo approach provided theoretical support of the experimental findings. The energy redistribution within the clusters upon collision activation is investigated. A comparison between ergodic and non-ergodic processes is discussed.

Cysteine ($C_3H_7NO_2S$), one of the nonessential amino acids, plays a key role in many important biological processes. Benchmark experimental data for the clusters of cysteine and water are relevant from the point of view of radiation biology of peptides. In this work, cysteine-water cluster cations in the canonical form $Cys(H_2O)_{3;6}{}^+$ and protonated $Cys(H_2O)_{3;6}H^+$ have been prepared by assembly inside He droplets and subsequently analyzed by means of tandem mass spectrometry using CID. Complementary theoretical simulations allowed us to study energy redistribution in the cysteine-water system.

The theoretical approach applied in this work [1] follows our previous strategy [2, 3], which relies on the analysis of energetic structure and time propagation as well as entropy maximization for elucidation of the initial energy redistribution process. Firstly, the geometries of cysteine-water clusters were optimized at the M06-2X/6-31++G(d,p) level of theory. Secondly, for systems with three water molecules ab initio molecular dynamics simulations were carried out. To treat fragmentation dynamics of large clusters, such as $Cys(H_2O)_6^+$, a less computationally expensive method than ADMP is required. Therefore, the Microcanonical Metropolis Monte Carlo method, in its recent implementation in the M_3C code [4], was applied for the first time to obtain the fragmentation branching ratios for such complex molecular clusters.

The comparison of the experimentally measured appearance energies with dissociation energies for water loss channels obtained with the DFT calculations indicate that clusters do not fragment exclusively by sequential emission of single water molecules, but rather by the release of small water clusters. Through the fitting procedure of the M_3C-obtained data with experimental relative ion yields we can comment on the energy partitioning after collisional activation. We find that only some of the collision energy redistributes via the ergodic process, while the rest is transferred into a non-ergodic channel leading to the loss of a single water molecule from the cluster. We conclude that modelling of collision-induced activation of weakly bound clusters requires the consideration of the possible non-ergodic processes.

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Emergent s-wave dimers near a p-wave Feshbach resonance in a strongly confined Fermi gas

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Synopsis We present emergent s-wave interactions in a quasi-two-dimensional (quasi-2D) system of ^{40}K near a p-wave Feshbach resonance with orbital degrees of freedom. The emergent exchange symmetry is enabled by excited-band population in the strongly confined direction. We characterize the scattering channels by measuring dimer binding energies and "contact" parameters with radio-frequency (rf) methods.

Ultracold atomic gases are highly tunable platforms for exploring low-dimensional physics, but are often prepared in motional ground states, neglecting orbital dynamics. We demonstrate that scattering channels activated with orbital degrees of freedom provide new routes for exploring few- and many-body phenomena.

Here, we prepare orbitally excited systems of spin-polarized fermionic potassium (^{40}K) near a p-wave Feshbach resonance. An optical lattice generates a strongly confined quasi-2D regime. Orbital degrees of freedom are activated by manipulating atomic populations of the excited band of the confinement lattice. While ground-band interactions possess p-wave character, collisions between ground- and excited-band atoms allow emergent s-wave behavior to appear [1].

Interactions are enhanced near the confinement-induced resonance associated with each scattering channel. We characterize the resonances by measuring quasi-2D dimer binding energies with rf association. Emergent s-wave dimers appear when orbital bands hybridize with the p-wave dimer in the corresponding confinement direction, and we demonstrate this by performing measurements in two confinement geometries. The results are compared to a quasi-2D scattering model that include band excitations.

In a second set of measurements, we study the strengths of resonantly enhanced interactions for each quasi-2D dimer by measuring spin-flip rates from rf spectroscopy as a function of magnetic field and confinement strength with and without activated orbital degrees of freedom. The resulting atom-atom correlations are interpreted through a set of universal relations, revealing the contact parameters [2, 3]. These studies extend the paradigm previously established in quasi-one-dimensional confinement [1] and provide a comprehensive framework for engineering exotic interactions with orbital dynamics in low-dimensional systems.

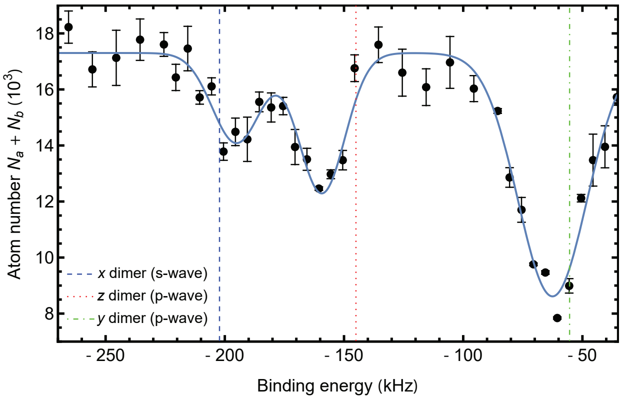

Figure 1. Typical dimer association loss measurement for an optical lattice along the x direction with activated orbital degrees of freedom. Blue dashed, red dotted, and green dot-dashed lines indicate predicted dimer energies and are labelled by the short-range 3D p-wave dimer direction and scattering channel.

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Femtosecond control of plasmonic field enhancement by mode-mixing

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Synopsis. Plasmonic field enhancement of tailored nanostructures is exploited in many applications. We demonstrate the nanoscale control of field enhancement factor on nanorods illuminated by femtosecond laser pulses having different polarization. We show that the observed differences in field enhancement factors originate from the simultaneous excitation of multiple plasmon modes of the nanorods, where the phase relations between these modes associated to the different polarization states play a fundamental role.

Plasmonic field enhancement and its measurement has received much attention in recent years. We developed an experimental method to determine the exact field enhancement factor of plasmonic nanostructures based on the measurement of the kinetic energy spectra of photoelectrons accelerated in the plasmonic near-fields [1]. Here, we use this method to quantify the field enhancement factor of nanorods illuminated by femtosecond laser pulses with different polarization states.

In our first experiment, arrays of plasmonic nanorods with lengths of 210, 240, 270, 300 nm, and constant width of 130 nm were illuminated from the backside by the 30-fs pulses of a fiber laser system having a central wavelength of 1030 nm in either linearly or circularly polarized states (Fig. 1 a)). Comparison of the measured data on these nanorods showed that in most cases circularly polarized illumination resulted in a larger field enhancement factors, than the ones observed with linear polarization, with the largest difference belonging to the 270 nm rod.

Analysis of the plasmonic response of the nanorods revealed that the role of circular polarization is twofold. 1) With circular polarization both the parallel and perpendicular plasmonic modes of the nanorods can be excited (Fig. 1 b)), and 2) the phase difference between the excitation of these modes is $\pi/2$. We found that the phase difference between the plasmonic modes of the nanorods clearly depends on the length-to-width ratio of the rods, and nearly $\pi/2$ phase difference belongs to the case where the length is twice the width for 270 nm long nanorod. This means that with circularly polarized light, these modes can be excited in a favorable phase. This in-phase addition of the plasmonic modes is the origin of the more efficient plasmon excitation observed with circularly polarized illumination [2].

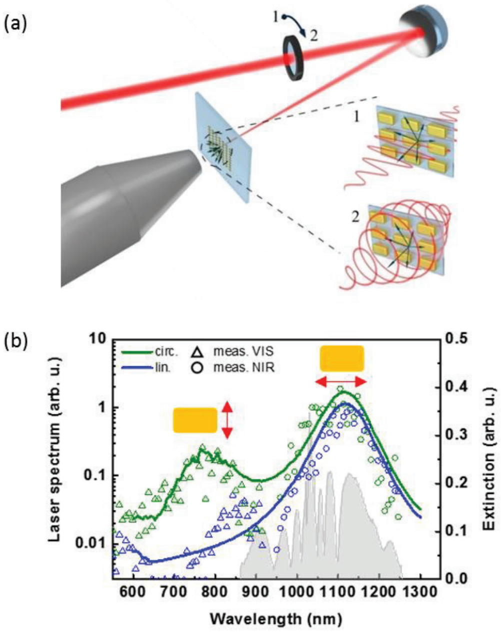

Figure 1. a) Scheme of the experimental setup. b) Extinction spectra of nanorod with 270 nm × 130 nm size.

This simple mode-mixing property of circularly polarized illumination provides an extra knob to control the near-field of plasmonic nanorods, which can be easily established in experiments. In my talk, I will show further applications of this phenomenon with different polarization states and specially designed nanostructures.

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High harmonic generation from metal surfaces

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Synopsis We observe extreme-ultraviolet (XUV) high harmonics from both epitaxial thin film and bulk crystalline silver (Ag) when exposed to the intense few-cycle near-infrared light pulses. Ag has a higher damage threshold than metallic titanium nitride, enabling high-harmonics generation up to photon energies of about 19 eV. As well, circularly polarized harmonics are efficiently generated by using circularly polarized incident light. High harmonic emission from metals can be a route to compact XUV frequency combs.

Since the observation of high harmonics in bulk ZnO [1], solid-state harmonics have been utilized as the spectroscopy technique to study the strong-field excitation, and the electronic and symmetry properties of various solids. Recently, the emission of high harmonics from metallic phase of titanium nitride (TiN) [2] suggests metals as novel media for high harmonic generation. Here, we report the emission of XUV high harmonics from both epitaxial thin film and bulk single crystal silver (Ag), thereby suggesting that high harmonics emission can be a universal feature in classical metals.

In the experiment, near-infrared (NIR) pulses (τ=30 fs, $\lambda_{\mathrm{center}}$=780 nm) from a commercial Ti:Sapph laser are spectrally broadened in a neon filled hollow-core fiber, and are compressed to two-cyle (τ=5.4 fs) pulses. The pulses are focused onto the 200 nm thick epitaxial Ag on a silicon substrate which is normal to the beam propagation. The reflected beam is sent to a grating spectrometer and the emitted harmonics are detected in the far-field. In this geometry, we observe high harmonics up to the 11th order (19 eV) when we reach the threshold intensity of several tens of TW/cm^2 (Fig 1. A), exceeding the experimentally measured damage threshold in TiN [2]. Additionally, when using the same pulse energy to generate harmonics from both TiN and Ag, the latter exhibits higher yield for the same harmonic order. We link these effects to the higher reflectivity and possibly lower electron scattering in Ag.

Next, we study the yield of emitted harmonics when altering the polarization state of incidentNIR beam. We find that the yield of 5th and 7th harmonics remains above 70% when the driving pluses is circularly polarized, and the space-time symmetry requires the harmonics to be circularly polarized. We further study the orientation dependence of the harmonics by rotating the polarization of the incident pulses relative to the crystal axis. The measured six-fold symmetry in the spectral yield of 5th and 7th is associated with the crystalline structure of (111) plane of the thin film target (Fig. 1. b).

In summery, we report the first observation of high harmonic emission from a standard metal. The results suggest that high harmonic emission is universal characteristic of metals when exposed to the intense light fields close to their damage threshold. The radiated XUV harmonics can utilized to probe and further control the electronic states of metal surfaces.

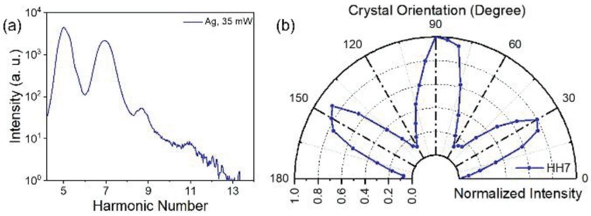

Figure 1. a) High harmonics spectrum from Ag reaching 19 eV. **b)** Orientation dependence of 7th harmonic.

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Controlling the polarization and phase of high-order harmonics with a plasmonic metasurface

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Synopsis Recently, metasurfaces have broken new ground in high-field attosecond science. We demonstrate the ability to control recolliding electrons and holes using a plasmonic metasurface, which results in the emission of high harmonics with controlled polarization and phase. Our metasurface enhances circularly polarized harmonics by approximately 43 times compared to unpatterned surfaces.

Nanostructured surfaces, or metasurfaces, offer precise manipulation of optical processes through the modification of electric and magnetic fields near wavelength-scale heterogeneities. In recent years, metasurfaces have made significant strides in high-field attosecond science by amplifying the typically inefficient process of high-order harmonics from femtosecond infrared laser pulses [1-4]. However, control of polarization and phase of the generated harmonics remained elusive.

Here we demonstrate the ability to control the polarization and phase of high harmonics using a plasmonic metasurface [5]. By creating perpendicularly aligned rectangular gold antennas on a silicon crystal, we generate circularly polarized deep-ultraviolet high harmonics from a circularly polarized infrared driver, providing a straightforward means of achieving circular emission from patterned crystals. Typically, circularly polarized drivers do not emit harmonics because electrons and holes are accelerated on trajectories that do not recollide. Our metasurface enhances the circularly polarized harmonics by approximately 43 times compared to the unpatterned surface, where the harmonics are suppressed.

Going forward, circularly polarized high harmonics will prove useful in sensing chiral laser-matter interactions and magnetic materials. This work opens the door to polarization control at even shorter, extreme ultraviolet wavelengths.

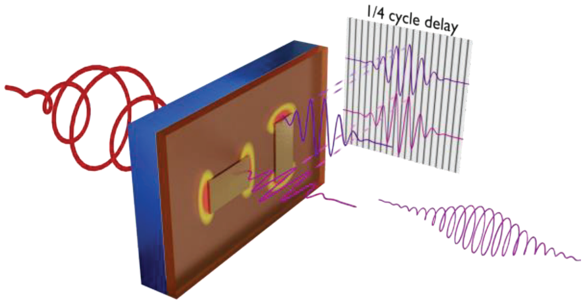

Figure 1. Each antenna resonates for the linear component of the incident circularly polarized driving field that aligns parallel to the antenna's major axis, thereby emitting linearly polarized odd-order high-harmonic radiation with half-cycle multiples of one quarter-cycle delay. Interference of pairs of antennas' emission results in circularly polarized high harmonics upon diffraction. The experiments are performed in reflection; however, transmission geometry is shown for clarity.

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Non-classical properties of light after strong-laser field processes in atomic and solid-state systems

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Synopsis The quantum optical characterization of strongly driven laser-matter interactions may allow extending current quantum technology platforms to unprecedented time and energy scales. Here, we present some of the recent progress that has been done in this direction, when considering atoms and solids as the matter system. We study the presence of two non-exclusive indications of non-classical behaviors in above-threshold ionization processes in atoms and in high-harmonic generation processes in solid-state systems, namely the presence of Wigner function negativities in the quantum optical state, and light-matter entanglement features.

The presence of non-classical states of light is usually witnessed by means of negative regions on its Wigner function representation, or by the presence of entanglement when more than one optical mode is considered. Exploiting the non-classical properties of light is crucial for the development of quantum technologies based in quantum optics [1]. However, as well as important is to find experimental setups that allow generating the desired quantum optical states. In this direction, it was proven theoretically and experimentally that laser-atom interactions driven by highly intense laser fields, can lead to the generation of non-classical states of light [2–5].

Here, we extend the theoretical approach used in Refs. [2–5] to study above-threshold ionization (ATI) processes in atoms, where photoelectrons with large values of kinetic energy are extracted from the atomic system; and high-order harmonic generation (HHG) processes in solid-state systems, where radiation in form of attosecond bursts with frequencies that range from the mid-infrared to the extreme ultraviolet are generated. In the first study [6], related to ATI in atoms, we observe that the final state of the light-field is entangled with that of the ionized electron, which allows for the generation of *hybrid-entangled* states, i.e., entangled states between light and matter. Moreover, if we only consider the field modes, we find a coherent state superposition where the amplitude of each coherent state within the superposition depends on the electronic properties: its final kinetic momentum and at what instant of time it has ionized. In the second study [7], related to HHG in solid-state media, we study how the interactions of the electrons in the solid get imprinted in the quantum optical state. By following the same experimental operations as the ones performed in Refs. [2–5], one can find two non-exclusive indications of non-classical behaviors, namely the presence of Wigner function negativities and entanglement features.

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Progress on dielectronic recombination spectroscopy at heavy-ion storage rings

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Synopsis The report will focus on the recent progresses of dielectronic recombination spectroscopy for Be-like argon/calcium, Na-like krypton and F-like nickel ions performed at the cooler storage rings CSRm and CSRe. The contributions of higher order effects of, such as quantum electrodynamics and electron-electron correlation in heavy ions by comparisons between experimental results with the state-of-the-art theoretical calculations will be discussed.

Dielectronic recombination (DR) is a resonant electron-ion scattering process when a free electron is captured into an ion while a core bound electron is excited to higher level if the excess energy released from capture matches the excitation energy. Therefore, DR is sensitive to the atomic structure of the ion. In the past three decades, DR measurements at electron beam cooling storage rings have been developed into a high resolution spectroscopic tool for investigation of the properties of highly charged ions (HCIs) [1, 2].

A series of DR experiments has been performed at the Cooler Storage Rings (CSR) at the Institute of Modern Physics, Chiese Academy of Sciences, Lanzhou, China. With improved DR energy resolution, various resonances are identified for HCIs such as $Ar^{12+, 13+, 14+, 15+}$, $Ca^{14+, 16+, 17+}$, Ni^{19+}, and $Kr^{25+, 30+}$ ions, by comparing with the theoretical calculations from FAC and AUTOSTRUCTURE codes. We observed significant contributions of trielectronic recombination (TR) process in Be-like ions at low collision energies. Some details of the measured DR spectroscopy and the investigation of electron-electron correlation effects, configuration mixing effects, quantum electrodynamics (QED) effects in these HCIs will be presented. Furthermore, DR resonances from metastable states of HCIs measured at storage rings suggests that, by appropriate preparations of the initial ion beam at storage ring, DR spectroscopy of metastable ions may be accessed. The spectroscopic data as well as the DR rate coefficients benchmark different atomic theoretical models used for modelling and understanding the astrophysical and other natural as well as man-made plasmas.

Last but not least, I will shortly introduce the status of the ongoing project – High Intensity Heavy Ion Accelerator Facility (HIAF) in China and the atomic physics program.

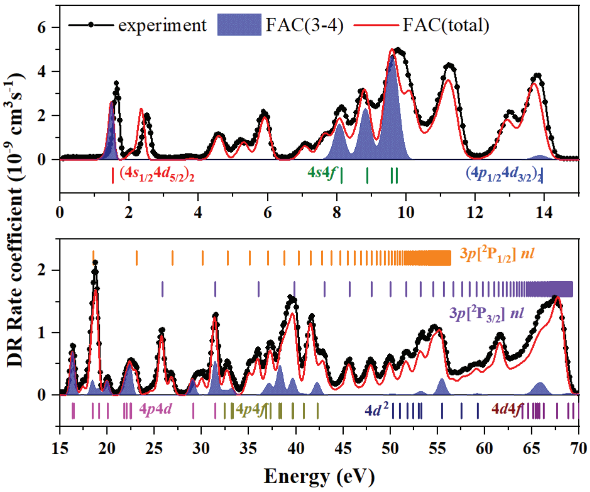

Figure 1. The DR rate coefficients of Na-like Kr^{25+} measured at the CSRe compared with the calculations by FAC in the energy range of 0-70 eV.

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Dissociative recombination of molecular ions in a cryogenic storage ring

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Synopsis Dissociative recombination on molecular ions in their lowest rotational states and other electron-ion interaction measurements performed at the Cryogenic Storage Ring are presented.

Dissociative recombination (DR) of molecular ions plays a key role in controlling the charge density and composition of cold plasmas, such as the cold interstellar medium (ISM). Experimental data on DR rate coefficients are required in order to understand the abundance of molecules in such astrophysical media. Experimentally, the main challenge is to acquire DR data at conditions relevant for the cold ISM, i.e., at collision temperatures of 10–100 K and at correspondingly low internal excitation. While past storage ring studies did reach collisional temperatures in the desired range, they did not have well-controlled access to internal excitation temperatures of the molecules below 300 K. This limitation was removed with the advent of electrostatic cryogenic storage rings.

The Cryogenic Storage Ring (CSR) [1] at the Max Planck Institute for Nuclear Physics, Heidelberg, is a multi-purpose electrostatic facility for studies with stored atomic, molecular and cluster ion beams. The cryogenic chamber temperatures of < 6 K, and the corresponding low residual gas densities, provide for beam lifetimes of hundreds to thousands of seconds. For many molecular ions this time is sufficient to relax down to their lowest ro-vibrational states by spontaneous photon emission [2,3]. Various experimental setups providing laser-, electron-, or even neutral atomic beams can be used for collision studies or as diagnostics for internal state populations. Furthermore, techniques for ion beam phase space cooling and isobaric purification [4] are available. The cryogenic environment and the excellent vacuum mimic the conditions in the cold ISM, making CSR an outstanding experimental setup for laboratory astrochemistry and for quantum dynamics studies with individual molecular state definition.

In the talk, recent CSR measurements on DR of molecular ions in their lowest rotational states will be discussed, including CH^+ [5], TiO^+ [6], OH^+, H_2D^+, D_2H^+, and ArH^+. Additionally, various other CSR studies on electron-ion interaction processes will be presented, such as rotational state-changing inelastic electron collisions of CH^+ [7], dielectronic recombination of low-charged atomic ions, and ion beam electron cooling at ultralow energies.

References

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The effect of electron correlation on trielectronic recombination rate coefficients for Be-like argon

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Synopsis The electron correlation between dielectronic and trielectronic recombinations (DR and TR) resonance states with different captured electron principal quantum numbers n can lead to an obvious enhancement in TR resonance strengths, which is cross-validated via the relativistic distorted-wave (RDW) approximation implemented in the Flexible Atomic Code (FAC) and the semi-relativistic distorted-wave (SRDW) approximation implemented in the AS code. However, previous theoretical calculations for this system did not include this form of electron correlation.

The merged-beam rate coefficients of dielectronic and trielectronic recombinations (DR and TR) within $\Delta N = 0$ channels for Be-like Ar^{14+} were measured by Huang *et al.* [Astrophy. J. Supp. Ser. 235, 2 (2018)] with the cooler storage ring at Lanzhou, China. Meanwhile, theoretical data were also calculated with AUTOSTRUCTURE (AS) code for comparison with the measured resonance spectrum. However, the AS calculations in most cases significantly underestimated TR resonance strengths. In the present work, we find that the electron correlation between DR and TR resonance states with different captured electron principal quantum numbers n can lead to an obvious enhancement in TR resonance strengths, which is cross-validated via the relativistic distorted-wave (RDW) approximation implemented in the Flexible Atomic Code (FAC) and the semi-relativistic distorted-wave (SRDW) approximation implemented in the AS code. Previous theoretical calculations for this system, however, did not include this form of electron correlation.

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Dissociative recombination of ArH^+ at the Cryogenic Storage Ring

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Synopsis
We have carried out experimental studies for dissociative recombination (DR) of rotationally cold ArH^+ molecules with free electrons at the Cryogenic Storage Ring (CSR) in Heidelberg, Germany. The low temperature DR rate coefficient for the electronic, vibrational, and rotational ground state of ArH^+ is important for astrochemical models of diffuse clouds, where observed abundances of ArH^+ are used to infer the cosmic ray ionization rate.

The cosmic ray ionization rate is an influential parameter of diffuse interstellar cloud models. ArH^+ formation is closely linked to the cosmic ray ionization rate via ionization of atomic Ar. The resulting Ar^+ can undergo hydrogen abstraction with H_2 to form ArH^+, which, in turn, can be destroyed by reactions with electrons through dissociative recombination (DR), with neutrals through proton transfer, or by ultraviolet photodissociation. A steady-state chemical model of this network enables one to estimate the cosmic ray ionization rate from the observed ArH^+ abundances. But such models require reliable rate coefficients that account for internal excitations of the reactants. A previous room-temperature storage ring experiment placed an upper limit on the DR rate coefficient for diffuse-cloud conditions [1]. Theoretical calculations have so far predicted a negligible rate coefficient at those conditions [2].

This contribution presents merged-beams experiments for ArH^+ interacting with free electrons produced in a low-energy electron cooler, which enables electron-ion collision studies at translational temperatures as low as ~ 10 K. For this, we have stored fast ArH^+ ion beams in the cryogenic environment of CSR. Previous studies showed that infra-red active diatomic hydrides relax to their lowest rotational states within minutes of storage inside CSR [3]. The DR rate coefficient for ArH^+ at low energies is expected to be several orders of magnitude smaller than the typical rate coefficient of other molecules. In the present experiment, we took special care with purifying the stored ion beam from potential isobaric contaminants before recording DR spectra as a function of center-of-mass collision energy.

In Figure 1, we compare our preliminary results with a theoretical calculation [2] in the collision energy range from 1 to 7 eV. In the poster, we will present our preliminary results for the full DR spectrum, particularly at the low energies relevant for diffuse clouds.

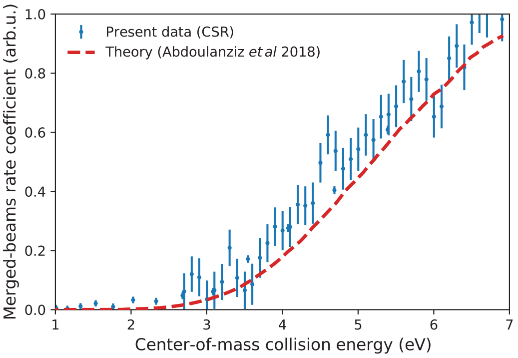

Figure 1. Merged-beams rate coefficients plotted as a function of center-of-mass collision energy. The preliminary dataset (CSR) is compared to a previous theoretical calculation [2]. The absolute scale of the experimental data is not yet fully determined.

This project is supported, in part, by the NASA Astrophysics Research and Analysis program under grant 80NSSC19K0969 and by the Max Planck Society.

References

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Posters

XXXIII International Conference on Photonic, Electronic and Atomic Collisions

July 25 - August 1, 2023, Ottawa, Canada

Poster abstracts can be found in the Book of Abstracts available online. Those contributions whose titles are marked by a star will also be presented as oral Special Reports.

Posters

Schedule

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Photon Molecule/Cluster	We028 – We055	Th026 – Th053	Fr026 – Fr054	Mo026 – Mo053
Photon Surface/Solid	We056 – We065			Mo054 – Mo064
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Absent Friends

a. Posters from Ukraine

AF001 **Electron-impact ionization of the $5p^6$ subshell in barium** • Oleksandr Borovik

AF002 **Photoluminescence of L-valine irradiated with 12.5 MeV electrons** • Yu. Bandurin, A. Zavilopulo, V. Maslyuk, N. Svatiuk

AF003 **Investigation of photoluminescence of glucose and fructose in the powder form** • Yu. Bandurin, A. Zavilopulo, V Maslyuk, N. Svatiuk

AF004 **Studies of the VUV luminescence excited by electron impact on the gas-phase glycine and alanine** • H. Bohachov, R. Tymchyk

AF005 **The near-threshold electron-impact resonance excitation of the In^+ ion** • A. N. Gomonai, V. Jonauskas, S. Kučas, V. Roman, A. I. Gomonai, Yu. Hutych, V. Zvenihorodsky

AF006 **Ramsauer-Townsend minima in the low-energy integral cross sections of elastic electron scattering by Sb, Xe and Bi, Rn atoms** • V. I. Kelemen, E. Yu. Remeta

AF007 **High-energy critical minima in differential cross sections of elastic electron scattering by Sb, Xe and Bi, Rn atoms** • V. I. Kelemen, E. Yu. Remeta

AF008 **Elastic and charge transfer cross sections for low energy H^+ + H collisions: Quantal and semiclassical calculations** • Mykhaylo V. Khoma

AF009 **Ionization of outer shells in the K atom by electron impact** • V. Roman

b. In Memoriam

AF010 **Electron Atom/Molecule Scattering and its Applications: A Tribute to Michael Brunger** • Stephen Buckman, Oddur Ingólfsson, Dragana Maric, Ronald White

AF011 **Electron Swarms as a Bridge Between Atom/Molecule Collisions and Gas Discharges: A Tribute to Robert W. Crompton** • Zoran Petrović, Stephen Buckman

AF012 **Multiphoton ionization and detachment of atoms and negative ions: A tribute to Anthony F. Starace** • Jean Marcel Ngoko Djiokap, Ilya I. Fabrikant

AF013 **In memoriam of past ICPEAC chairs and stalwarts** • Emma Sokell

Posters

Wednesday, July 26

Photon – Atom/Ion

We001 **Inner-shell ionization of low-charged silicon and iron ions** • Stefan Schippers, Alfred Müller, Simon Reinwardt, Michael Martins, Stephan Fritzsche for the PIPE collaboration

We002 **Relativistic and correlation effects in np photoionization Cooper minima of high-Z atoms** • S. Baral, J. Jose, P. C. Deshmukh, S. T. Manson

We003 **Angular distribution, spin polarisation and time delay studies of the potassium 4s orbital in the vicinity of Cooper minimum** • Nishita M. Hosea, Pranawa C. Deshmukh, Jobin Jose, Hari Varma Ravi, Steven T. Manson

We004 **New source for tuning the effective Rabi frequency in multiphoton ionization** • Dongdong Zhang, Wankai Li, Yue Lei, Xing Li, Tao Yang, Mei Du, Ying Jiang, Jialong Li, Aihua Liu, Lanhai He, Pan Ma, Sizuo Luo, Dajun Ding

We005 **Non-classical properties of light after strong-laser field processes in atomic and solid-state systems*** • Javier Rivera Dean, Philipp Stammer, Andrew S. Maxwell, Theocharis Lamprou, Andrés F. Ordóñez, Emilio Pisanty, Paraskevas Tzallas, Maciej Lewenstein and Marcelo F. Ciappina

We006 **Theoretical studies on high-order harmonic generation: from microscopic to macroscopic** • X. M. Tong, N. Toshima

We007 **Lorentz-force shifts in strong-field ionization with mid-IR laser fields** • Stephan Fritzsche, Birger Böning, Danish F. Dar

We008 **An atomic magnetometer to detect the oscillating magnetic field based on twisted light atom interaction** • S. Ramakrishna, R.P. Schmidt, A.A. Peshkov, A. Surzhykov, S. Fritzsche

We009 **Time-resolved Kapitza-Dirac effect** • Kang Lin, Maksim Kunitski, Sebastian Eckart, Alexander Hartung, Qinying Ji, Lothar Ph. H. Schmidt, Markus S. Schöffler, Till Jahnke, Reinhard Dörner

We010 **Pulse length effects in long wavelength driven non-sequential double ionization** • H. Jiang, M. Mandrysz, A. Sanchez, J. Dura, T. Steinle, J. S. Prauzner-Bechcicki, J. Zakrzewski, M. Lewenstein, F. He, J. Biegert, M. F. Ciappina

We011 **Ultrafast excitation dynamics for noble gas atoms subject to intense femtosecond laser fields** • S. P. Xu, M. Q. Liu, W. Quan, W. Becker, J. Chen, X. J. Liu

We012 **Visualization of a complex electron wavefunction in momentum space using an attosecond pulse** • Hiromichi Niikura, Takashi Nakajima, Tasuku Shinoda, D. M. Villeneuve

We013 **First commissioning results of the AMO endstation at the Shanghai soft X-ray free-electron laser facility** • Ruichao Dong, Xincheng Wang, Yuliang Guo, Jinze Feng, Mingjie Zhang, Hailong Guo, Yuhai Jiang

We014 **PCI effects following 2p double ionization of argon atoms** • Laura Sommerlad, Sven Grundmann, Florian Trinter, Max Kircher, Andreas Pier, Dennis McGinnis, Leon Kaiser, Jan Kruse, Angelina Geyer, Nils Anders, Niklas Melzer, Till Jahnke, Reinhard Dörner

We015 **Gauge-invariant absorption of light by coherent superposition states** • Axel Stenquist, Felipe Zapata, Marcus Dahlström

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We017 **Carrier-Envelope-Phase Effects for Multiphoton and Tunnel Excitation of Argon** • D. Chetty, R.D. Glover, X.M. Tong, B.A. deHarak, H. Xu, N. Haram. K. Bartschat, A.J. Palmer, A.N. Luiten, P.S. Light, I.V. Litvinyuk, R. T. Sang

We018 **Attosecond time delay during resonance-enhanced multiphoton ionization of noble gases in strong laser fields** • Lanhai He, Xing Li, Xuanhong Gao, Sizuo Luo, Song-Feng Zhao, Dajun Ding

We019 **Nonlinear scaling law in photon momentum transfer caused by two-electron effects** • Yong-Kang Fang, Hao Liang, Wei-Chao Jiang, Liang-You Peng

We020 **Rescattering sequential multiple ionization of cold Rb** • Z. H. Zou, J. Y. Yuan, X. C. Wang, H. Y. Ma, M. Weidemüller, Y. H. Jiang

We021 **Autoionization of two-electron-excited ^{88}Sr $5p_{1/2}$ nl_j states** • S. Yoshida, J. Burgdörfer, R. Brienza, G. Fields, F. B. Dunning

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We024 **Unexpected pathway to double-core-hole states in atoms and molecules** • Iyas Ismail

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We064 **Laser-based processing of dielectric chips for the generation of nano focused XUV radiation** • Parnia Bastani, Aleksey Korobenko, Giulio Vampa

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We069 **Theoretical investigation of electron-impact ionization of W^{8+} ion** • Shiping Zhang, D. H. Zhang, L. Y. Xie, X. B. Ding

We070 **Theoretical investigation of electron-impact ionization of W^{6+} ion** • Lili Ma, D. H. Zhang, L. Y. Xie, X. B. Ding

We071 **Theoretical study on the electron collision ionization of Sn^{11+} ions** • Fangjun Zhang, X. B. Ding, D. H. Zhang, C. Z. Dong

We072 **The state-resolved integral cross sections for atomic krypton studied by fast electron scattering** • Wanlu Ma, Zhiwei Nie, Linfan Zhu

We073 **Development of particle detectors for electron-ion collision spectroscopy with highly charged ions at the storage ring CSRe** • Zhongkui Huang, S. X. Wang, W. Q. Wen, H. B. Wang, W. L. Ma, S. Shao, H. K. Huang, D. Y. Chen, S. F. Zhang, L. F. Zhu, X. W. Ma for the DR collaboration@HIRFL

We074 **First Dielectronic Recombination Measurements at the Cryogenic Storage Ring** • Leonard Isberner, Manfred Grieser, Robert von Hahn, Zoltán Harman, Ábel Kálosi, Christoph H. Keitel, Claude Krantz, Daniel Paul, Daniel W. Savin, Suvam Singh, Andreas Wolf, Stefan Schippers, Oldřich Novotný

We075 **Electron recombination of deuterated triatomic hydrogen ions at the Cryogenic Storage Ring** • Aigars Znotins, Alexandre Faure, Joshua Forer, Chris Greene, Florian Grussie, Leonard Isberner, Abel Kalosi, Viatcheslav Kokoouline, Marco Pezzella, Damian Mull, Oldrich Novotný, Daniel Paul, Daniel Savin, Stefan Schippers, Jonathan Tennyson, Xavier Urbain, Andreas Wolf, Holger Kreckel

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We080 **Convergent close-coupling calculations of positron scattering from atomic oxygen** • Nicolas Mori, Liam Scarlett, Igor Bray, Dmitry Fursa

We081 **Differential positronium-formation cross-sections around zero degrees from atoms and molecules** • Donovan Newson, Michael Shipman, Sam Fayer, Simon Brawley, Rina Kadokura, Andrea Loreti, Gaetana Laricchia

We082 **Electron elastic scattering by Bk and Cf atoms: polarization effects** • Alfred Z. Msezane Zineb Felfli

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We083 **Theoretical investigation of bound and resonant states of imidogen radical NH** • Raju Ghosh, Kalyan Chakrabarti, Binayak S. Choudhury

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We087 **Isomerization dynamics of triatomic molecules driven by the electron-impact** • Lei Chen, Enliang Wang, Zhenjie Shen, Maomao Gong, Xu Shan, Xiangjun Chen

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We092 **Isotopic selectivity in the metastable dication production of benzene** • Lucas Sigaud, W. Wolff, E. C. Montenegro

We093 **Absolute cross sections for ionization and fragmentation of CO_2 by electron impact** • Ana Beatriz Monteiro-Carvalho, L. Sigaud, E. C. Montenegro

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We100 **Interaction of Singly Charged Sodium Ion with Nitrogen Atom: Total and Differential Ionisation Cross Sections** • M. Al-Ajaleen, Karoly Tőkési

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We119 **Efficient molecular oxidation in collisions with superoxide anions** • Sergio Diaz-Tendero, Carlos Guerra, Sarvesh Kumar, Fernando Aguilar-Galindo, Ana I. Lozano, Mónica Mendes, Paulo Limão-Vieira, Juan C. Oller, Gustavo García

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We125 **Precision Measurements of the $^2P_{1/2}$-$^2P_{3/2}$ fine-structure splitting in B-like S^{11+} and Cl^{12+} at SH-HtscEBIT** • X. Liu, X. P. Zhou, W. Q. Wen, Q. F. Lu, C. L. Yan, J. Xiao, A. V. Volotka, Y. S. Kozhedub, M. Y. Kaygorodov, X. Ma

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We128 **Development of microwave system for a high-precision Lamb shift spectroscopy of antihydrogen atoms** • Takumi Tanaka on behalf of the GBAR collaboration

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We130 **Determination of $2s^2\ 2p^5 \rightarrow 2s\ 2p^6$ transition energy in fluorine-like nickel utilizing a low-lying dielectronic resonance** • Shuxing Wang, Z. K. Huang, W. Q. Wen, H. B. Wang, S. Schippers, Z. W. Wu, Y. S. Kozhedub, M. Y. Kaygorodov, A. V. Volotka, K. Wang, X. Ma, L. F. Zhu for the DR collaboration@HIRFL

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We132 **The QED correction of the transition energy of Ne^{7+} and Ca^{17+} ions** • Bingbing Li, Jun Jiang, Lei Wu, D. H. Zhang, L. Y. Xie, D. X. Sun, C. Z. Dong

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We135 **Laser-assisted reduction of graphene oxide coated on melamine sponge for advanced application in electromagnetic interference shielding** • Yitbarek Fitwi Kidane, Lee Hun

We136 **Quantification of Pressure-Enhanced Electron-Phonon Coupling in Bi_2S_3 via Femtosecond Pump-Probe Spectroscopy** • Bowen Guan, Y. Chen, Ruiqi Wu, H. Liu, Y. Jiang, J. Dong, Qingyi Li, M. Jin

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We141 **Fine-structure energy levels, oscillator strengths and lifetimes in chromium** • Vikas Tayal

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Th005	**Spatially dependent laser assisted photoionization of He** • R. Della Picca, J. M. Randazzo, S. D. López, M. F. Ciappina, D. G. Arbó
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Th009	**Carrier-envelope-phase and helicity control of electron vortices and spirals in photodetachment** • Mateusz Majczak, F. Cajiao Vélez, J. Z. Kamiński, K. Krajewska
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Th012	**Relativistic calculations of electron-parent ion entanglement using the KRAKEN protocol** • C. Leon M. Petersson, Eva Lindroth

Th013 **Estimating Rare Gas Spectra with a New Theoretical Model for Pump-Probe Spectroscopy** • Miguel Alarcon, Chris Greene, Arvinder Sandhu, Alex Plunkett, James Wood, Dipayan Biswas

Th014 **Tracking Few-Femtosecond Auger Decay by Synchrotron Radiation** • Tatsuo Kaneyasu, Yasumasa Hikosaka, Masaki Fujimoto, Hiroshi Iwayama, Masahiro Katoh

Th015 **Phase-resolved photoelectron-imaging of potassium atoms in two-color laser fields** • Wankai Li, Yixuan Wang, Dongdong Zhang, Dajun Ding

Th016 **Strong-field Effects on Time Delays in Correlated Ionization** • Wei-Chao Jiang, M. -C. Zhong, Y. -K. Fang, S. Donsa, I. Brezinova, L. -Y. Peng, J. Burgdörfer

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Th021 **Coulomb focusing in attosecond angular streaking measurement of strong field tunneling ionization** • Xiaokai Li

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Th027 **Investigation of Interatomic Coulombic Decay after inner-shell ionization in heterogeneous rare gas clusters by multi-coincidence spectroscopy** • Catmarna Küstner-Wetekam, Lutz Marder, Dana Bloß, Nils Kiefer, Uwe Hergenhahn, Arno Ehresmann, Premysl Kolorenc, Andreas Hans

Th028 **DFT study of d-electron photoionization of $x@C_{60}$ with $x = Cu^+, Cu, Cu^-, Zn$** • Dalton Forbes, Sanjay Prabhakar, Ruma De, Himadri Chakraborty

Th029 **Photofragmentation of cyclo-dipeptides in the gas-phase and routes to the formation of peptide chains** • Paola Bolognesi, Darío Barreiro Lage, Jacopo Chiarinelli, Robert Richter, Henning Zettergren, Mark Stockett, Laura Carlini, Sergio Diaz-Tendero, Lorenzo Avaldi

Th030 **Strong evidence for neighbor-induced recapture obtained by electron-photon-coincidence spectroscopy** • Nils Kiefer, Carolin Honisch, Catmarna Küstner-Wetekam, Lutz Marder, Niklas Golchert, Arno Ehresmann, Andreas Hans

Th031 **Probing conical intersection dynamics in the dissociative photoionization of formaldehyde at FLASH** • David Chicharro Vacas, Weiyu Zhang, Hannes Lindenblatt, Florian Trost, Pedro Recio, Alexandre Zanchet, Roger Y. Bello, Jesús González-Vázquez, Ulrike Fruehling, Markus Braune, Sonia Marggi Poullain, Luis Bañares, Thomas Pfeifer, Robert Moshammer

Th032 **Investigating the UV-Induced Dynamics of Methylated Cyclopentadiene with XUV Photoelectron Spectroscopy at FLASH** • Zane Phelps, Lisa Huang, Tristan Fehl, Dennis Meyer, Fabiano Lever, Stefan Duesterer, Artem Rudenko, Martin Centurion, Adam Kirrander, Peter M. Weber, Markus Guehr, Daniel Rolles

Th033 **Electron-rotation coupling in diatomics by intense UV pulses** • Y. R. Liu, V. Kimberg, Y. Wu, J. G. Wang, O. Vendrell, S. B. Zhang

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Th036 **Isotope labelling as a tool for atto-chemistry** • Morgane Vacher, Alexie Boyer, Vincent Loriot, Franck Lépine, Saikat Nandi

Th037 **Time-resolved imaging of an elusive molecular reaction: hydrogen roaming in acetonitrile** • Aaron Laforge, Debadarshini Mishra, Lauren Gorman, Sergio Díaz-Tendero, Fernando Martín, Nora Berrah

Th038 **Valence photo double ionization of CH3OD: Insights into Molecular Dynamics and Electron Correlation** • S. Kumar, M. Shaikh, W. Iskandar, R. Thurston, M. A. Fareed, D. Call, R. Enoki, C. Bagdia, N. Iwamoto, T. Severt, J. B. Williams, I. Ben-Itzhak, D. S. Slaughter, Th. Weber

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Th045 **Imaging the nuclear wavepacket dynamics of multiply charged Ar_2 using a two-color laser field** • Arnab Sen, M. J. J. Vrakking, A. Rouzée

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Th047 **Capturing electron-driven molecular chirality** • Vincent Wanie, Etienne Bloch, Erik P. Månsson, Lorenzo Colaizzi, Krishna Saraswathula, Sergey Ryabchuk, Andrea Trabattoni, Valérie Blanchet, Nadia Ben Amor, Marie-Catherine Heitz, Yann Mairesse, Bernard Pons, Francesca Calegari

Th049 **Time-resolved Imaging of CH_4 Fragmentation in Strong Laser Fields** • Weiyu Zhang, David Chicharro Vacas, Thomas Pfeifer, Robert Moshammer

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Th053 **Accurate molecular ab initio calculations in support of strong-field attosecond physics experiments** • Giorgio Visentin, Bo Ying, Gerhard G. Paulus, Stephan Fritzsche

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Th054 **Effect of the Breit interaction on the angular distribution of Auger electrons following electron-impact excitation of Be-like ions** • Zhongwen Wu, Yong Li, Zhouwang Tian, Chenzhong Dong, Stephan Fritzsche

Th055 **Linear polarization and angular distribution of the Lyman-α_1 line following electron-impact excitation of H-like ions** • Zhongwen Wu, Zhongmang He, Zhouquang Tian, Zhongwen Dong, Stephan Fritzsche

Th056 **Classical description of the ionization of carbon by electron impact** • N. Bachi, S. Otranto, Karoly Tőkési

Th057 **Impact Parameter and Kinematic Information for Differential Ionization of Argon by 1 keV Positrons and Electrons** • Karoly Tőkési, R. D. DuBois

Th058 **Convergent close-coupling calculations of positron scattering from carbon** • Nicolas Mori, Liam Scarlett, Igor Bray, Dmitry Fursa

Th059 **Low-energy elastic scattering of positrons by helium** • Xian-Jun Li, M. -S. Wu, J. Jiang, J. -Y. Zhang, Z. -C. Yan, K. Varga

Th060 **Laser-assisted positron-H scattering in reduced quantum mode** • Xiao Hu Ji, Li Guang Jiao, Aihua Liu

Th061 **Low-energy total cross-sections of positronium scattering from the inert atoms** • Donovan Newson, Simon Brawley, Rina Kadokura, Andrea Loreti, Michael Shipman, Gaetana Laricchia

Th062 **Collective effects in positronium formation from rare gas atoms** • Paul-Antoine Hervieux, Adrien Andoche, Kévin Lévêque, Himadri Chakraborty

Th063 **Calculation and Wigner law analysis of scattering cross sections for collisions of antihydrogen atom with excited positronium** • Takuma Yamashita, Yasushi Kino, Emiko Hiyama, Svante Jonsell, Piotr Froelich

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Th065 **Electron impact excitation of Ar-like Kr XIX** • Aloka Kumar Sahoo, Nitish Ghosh, Lalita Sharma

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Th069 **Theoretical investigation of KLL dielectronic-recombination processes of highly charged Cu ions** • Jianhu Deng, Shengbo Niu, Wenliang He, Yulong Ma, Luyou Xie, Chenzhong Dong

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Th072 **Measurements of positron and electron scattering from biomolecules** • David Stevens, Zoe Cheong, Tamara Babij, Josh Machacek, James Sullivan

Th073 **Quantum Monte Carlo study on positron binding to atomic anion dimers** • S. Ito, D. Yoshida, Y. Kita, T Shimazaki, M. Tachikawa

Th074 **Low-energy positronium scattering from O_2** • Donovan Newson, Rina Kadokura, Harriet Allen, Samuel Fayer, Simon Brawley, Michael Shipman, Gaetana Laricchia, Robyn Wilde, Ilya Fabrikant, László Sarkadi

Th075 **Production of O_2^+ following the double ionization of CO_2*** • Ana Beatriz Monteiro-Carvalho, L. Sigaud, E. C. Montenegro

Th076 **Observation of ultrafast proton and energy transfer in hydrated pyrrole dimers induced by electron impact*** • J. Zhou, S. Jia, X. Xue, X. Hao, Q. Zeng, X. Ren

Th077 **Development of atomic momentum spectroscopy of polyatomic molecules** • Satoru Kanaya, Yuuki Onitsuka, Noboru Watanabe, Hirohiko Kono, Masahiko Takahashi

Th078 **Development of a new molecular spectroscopy technique: mapping atomic motions and elemental composition analysis of a molecule** • Yuuki Onitsuka, Yuichi Tachibana, Satoru Kanaya, Hirohiko Kono, Masahiko Takahashi

Th079 **Velocity slice imaging probed for kinematically complete measurements of dissociative electron attachment to OCS molecule** • Narayan Kundu, Vikrant Kumar, Dhananjay Nandi

Th080 **Fragmentation dynamics of $BrCN^{q+}$ (q = 2-6) induced by 1-keV electron impact** • Wenchao Zhao

Th081 **Elastic scattering and rotational excitation of H_2 by electron impact: Convergent close-coupling calculations** • Liam Scarlett, Una Rehill, Mark Zammit, Nicolas Mori, Igor Bray, Dmitry Fursa

Th082 **Resonances in electron scattering from SO_2** • Peter Bingham, Jimena Gorfinkiel

Th083 **Comparison of electron induced reactions of $(CH_3)AuP(CH_3)_3$ under single collision conditions and its deposition composition in UHV FEBID** • Ali Kamali, Elif Bilgilisoy, Alexander Wolfram, Thomas Xaver Gentner, Gerd Ballmann, Sjoerd Harder, Hubertus Marbach, Oddur Ingólfsson

Th085 **Dynamics of Dissociative Electron Attachment to Acetylacetone*** • Surbhi Sinha, Vaibhav Prabhudesai

Th086 **Effect of Background on Momentum Images on a Crossed-Beam Experiment** • Sukanta Das, Vaibhav S Prabhudesai

Heavy Particle – Atom/Ion

Th087 **AEgIS: Synthesis of mid-heavy antiprotonic atoms at CERN** • Adam Linek on behalf of the AEgIS collaboration

Th088 **Nonradiative electron capture in collisions of fast Xe^{54+} with Kr and Xe*** • Bian Yang

Th089 **An improved short-range description for CDW-EIS model with dressed projectiles** • Nicolás Esponda, Michele Quinto, Roberto Rivarola, Juan Monti

Th090 **Target atomic number dependence of the electron capture and excitation process for the relativistic hydrogen-like Cs ions** • Caojie Shao, H. Q. Zhang, B. Yang, D. Y. Yu, Z. Y. Song, P. F. Li, H. Yuan, Z. D. Cheng, S. Ha, H. W. Zhang, Y. S. Kozhedub, W. Wang, M. W. Zhang, J. L. Liu, Y. L. Xue, C. L. Wan, Y. Cui, K. Yao, Z. H. Yang, X. H. Cai, R. Schuch, X. M. Chen

Th091 **State-selective single-electron capture in 1 keV/u Ar^{2+} -Ar collisions** • Shucheng Cui

Th092 **State-selective single electron capture in 9 keV N^+-He collisions** • Da Xing

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Heavy Particle – Atom/Ion

Th093 **Fully Differential Study of Non-PCI Higher-Order Contributions to Ionization of Helium by Proton Impact** • Shruti Majumdar, Sujan Bastola, Ramaz Lomsadze, Ahmad Hasan, Michael Schulz

Th094 **Energy and angular distributions of electrons produced in intermediate-energy proton-helium collisions** • Kade Spicer, Corey Plowman, Shukhrat Alladustov, Ilkhom Abdurakhmanov, Igor Bray, Alisher Kadyrov

Th095 **Single ionization of helium by protons in the parabolic quasi-Sturmians approach** • Sergey A. Zaytsev, Darya S. Zaytseva, Alexander S. Zaytsev, Lorenzo Ugo Ancarani, Konstantin A. Kouzakov, Yuri V. Popov

Th096 **A 22-pole RF ion trap experimental setup to study the ion-neutral and ion-photon interactions relevant to astrophysical environments** • Roby Chacko, Nihar Ranjan Behera, Saurav Dutta, Saroj Barik, Aravind Gopalan

Th097 **Upcoming atomic physics studies of ion-ion collisions** • Mariette Jolly, Emily Lamour, Alain Méry, Angela Bräuning-Demian, Alain Dubois, Jean-Yves Chesnel, Alexandre Gumberidze, Christoph Hahn, Michael Lestinsky, Stéphane Macé, Christophe Prigent, Jean Marc Ramillon, Jimmy Rangama, Patrick Rousseau, Uwe Spillmann, Sébastien Steydli, Thomas Stöhlker, Martino Trassinelli, Dominique Vernhet

Th098 **Three-particle one-dimensional model for ionization collisions: A simple laboratory to test perturbative approximations** • T. Guarda, V. D. Rodríguez, Raul Barrachina

Heavy Particle – Molecule/Cluster

Th099 **Dissociation pathways of methane dication** • Jyoti Rajput, Diksha Garg, A. Cassimi, A. Mery, X. Flechard, J. Rangama, C. P. Safvan

Th100 **Fragmentation upon collision-induced activation of cysteine–water cluster cations*** • Lukas Tiefenthaler, Paul Scheier, Ewa Erdmann, Néstor F. Aguirre, Sergio Díaz-Tendero, Thomas F. M. Luxford, Jaroslav Kočišek

Th101 **Swift heavy ion irradiation of water, carbon monoxide, and methanol mixture in the solid phase** • Ana De Barros, C. Mejía, A. Domaracka, P. Boduch, C. P. da Costa, H. Rothard, E. F. da Silveira

Th102 **Probing the fragmentation pathways of an Argon dimer in slow ion-dimer collisions** • Md Abul Kalam Azad Siddiki, Lokesh C. Tribedi, Deepankar Misra

Th103 **Single-electron capture and ionisation in He^{2+} - H_2 collisions** • Akshit Kotian, Corey Plowman, Igor Bray, Alisher Kadyrov

Th104 **Differential ionisation in proton collisions with molecular hydrogen** • Corey Plowman, Ilkhom Abdurakhmanov, Igor Bray, Alisher Kadyrov

Th105 **Role of different electron capture mechanisms in fragmentation of CO_2^{3+} into $O^+ + C^+ + O^+$** • Kamal Kumar, Md Abul Kalam Azad Siddiki, Jibak Mukherjee, Deepankar Misra

Th106 **Giant quadrupole plasmon resonance in C_{60} in high perturbation collisions** • Lokesh Tribedi. S. Kasthurirangan, E. Suraud

Th107 **Lifetime measurement of collision-induced delayed fragmentation from singly charged intermediate ions** • Tomohiko Nakao, Riyon Takasu, Siyao Li, Hidetsugu Tsuchida, Manabu Saito, Takuya Majima

Th108 **Ion molecule reaction dynamics of the radical anion O- with deuterated methane CD_4 and methyl iodide CH_3I** • Atilay Ayasli, Tim Michaelsen, Arnab Khan, Thomas Gstir, Fabio Zappa, Roland Wester

Th109 **Survival of Interstellar Carbon Knockout Fragments** • Naemi Florin, Michael Gatchell, João Ameixa, MingChao Ji, Mark Stockett, Ansgar Simonsson, Suvasthika Indrajith, Peter Reinhed, Stefan Rosén, Henrik Cederquist, Henning Schmidt, Henning Zettergren

Low Energy to Ultracold

Th110 **Cold molecular dynamics and chemical reactions of H_2 (D_2) in strong laser fields*** • Lianrong Zhou, J. Qiang, H. Ni, Z. Jiang, W. Jiang, W. Zhang, P. Lu, K. Lin, H. Stapelfeldt, J. Wu

Th111 **Collective electron dynamics in large ultracold atomic ensembles** • Mario Großmann, Julian Fiedler, Jette Heyer, Amir Khan, Markus Drescher, Klaus Sengstock, Philipp Wessels-Staarmann, Juliette Simonet

Th112 **Magneto-optical trap reaction microscope for strontium atoms** • Shushu Ruan

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Low Energy to Ultracold

Th113 **Microwave Spectroscopy of high-*n* low-*l* ^{84}Sr Rydberg states in a cold gas** • Robert Brienza, Yi Lu, Chuanyu Wang, Soumya Kanungo, Thomas Killian, Barry Dunning, Shuhei Yoshida, Joachim Burgdörfer

Th114 **Cold collisions of atomic and molecular hydrogen with astrochemically relevant anions** • Christine Lochmann, Sruthi Purushu-Melath, Markus Nötzold, Robert Wild, Francesco A. Gianturco, Roland Wester

Th115 **Theoretical Studies of Mutual Neutralization** • Ann Orel, Åsa Larson

Th116 **Theoretical studies of reactive scattering processes involving the H_2 reaction complex** • Johan Hörnquist, Patrik Hedvall, Åsa Larson, Ann E. Orel

Th117 **Mutual neutralization of $^{1,2}H^-$ with Li^+, O^+, N^+ and C^+ at DESIREE*** • Alice Frederike Schmidt-May, G. Eklund, S. Rosén, M. C. Ji, J. Grumer, P. S. Barklem, H. Cederquist, H. Zettergren, H. T. Schmidt

Th118 **Mutual neutralization in collision of Na^+ with O^- and S^-** • Antoine Aerts, Arnaud Dochain, Jacky Liévin, Xavier Urbain, Nathalie Vaeck

Th119 **Charge transfer in Sodium Iodide collisions** • Patrik Hedvall, Michael Odelius, Åsa Larson

Th120 **Molecular-rotation-induced splitting of the binary ridge in the velocity map of sub-eV H^+ (D^+) ions ejected from H_2 (D_2) molecules by ion impact** • Zoltán Juhász, Sándor T. S. Kovács, Violaine Vizcaïno, Péter Herczku, Sándor Demes, Richárd Rácz, Béla Sulik, Sándor Biri, Nicolas Sens, Duncan V. Mifsud, Gergő Lakatos, Rahul K. Kushwaha Jean-Yves Chesnel

Th122 **Two-photon optical shielding of collisions between ultracold polar molecules*** • Charbel Karam, Mara Meyer zum Alten Borgloh, Romain Vexiau, Maxence Lepers, Silke Ospelkaus, Nadia Bouloufa-Maafa, Leon Karpa, Olivier Dulieu

Th123 **Emergent s-wave dimers near a p-wave Feshbach resonance in a strongly confined Fermi gas*** • Kevin Xie

Th124 **Resonant processes and their impact in many-body dynamics*** • Robin Côté

Th125 **Dynamical instabilities and macroscopic quantum self-trapping in a rotating Bose-Einstein condensate** • Denise Kamp, Duncan, O'Dell

Th126 **Observation of Sequential Tunneling in Driven Optical Lattices** • X. X. Ma, X. Y. Tong, N. C. Zhang, X. Zhang, K. K. Huang, Xuanhui Lu

Th127 **Two-Dimensional Turbulence in dipolar Bose-Einstein condensate** • Sabari Subramaniyan, Ramavarmaraja Kishor Kumar, Lauro Tomio

Structure and Spectroscopy

Th128 **Electronic *K* x rays emitted from muonic atoms: an application of density functional theory** • X. M. Tong, D. Kato, T. Okumura, S. Okada, T. Azuma

Th129 **High precision theory for the Rydberg states of helium up to n = 24: test of a 7σ discrepancy with experiment** • Gordon Drake, Aaron Bondy, Eric Ene, Evan Petrimoulx, Lamies Sati

Th130 **Theoretical study on radii of neutral atoms and singly charged negative ions** • Mingmin Luo, Guangxin Min, Guannan Guo, Xuemei Zhang

Th132 **The planetary states of the Sr atom** • Matthieu Génévriez, Ulli Eichmann

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Th133 **Table-top setup for independent phase and timing control of XUV pulse pairs** • Sarang D. Ganeshamandiram, Ronak N. Shah, Fabian Richter, Ianina Kosse, Jahanzeb Muhammad, Lukas Bruder, Frank Stienkemeier, Giuseppe Sansone

Th134 **Intensity variation of N_2 and CO in the presence of two-color ultrafast pulses** • Madhusudhan P, Rajesh Kumar Kushawaha

Th135 **Ultrafast Imaging of Molecular Chirality with Photoelectron Vortices** • Xavi Planas, Andres Ordóñez, Maciej Lewenstein, Andrew Maxwell

Th136 **Ionization dynamics of CO_2 in intense XUV and strong IR pump/probe at REMI end station FLASH2** • Atia Atia Tul Noor

Th137 **Geometry dependence of photoionization asymmetry parameter of CH_3I** • Paresh Modak, Loren Greenman

Th138 **Molecular ion time-dependent rotational relaxation dynamics probed by photo-electron in an ion trap** • Abhishek Shahi, Deepak Sharma, Sunil Kumar, Saurabh Mishra, Igor Rahinov, Oded Heber, Daniel Zajfman

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Post Deadline

Th139 **Cusp-electron production in collisions of open-shell O^{6+}(1s2s) ions with He** • Stefanos Nanos, N. J. Esponda, P. -M. Hillenbrand, A. Biniskos, A. Laoutaris, M. A. Quinto, N. Petridis, E. Menz, T. J. M. Zouros, Th. Stöhlker, R. D. Rivarola, J. M. Monti, E. P. Benis

Th140 **Suppression of three-body loss near a p-wave Feshbach resonance in a quasi-1D ultracold fermionic system** • Kenta Nagase, Z. Xu, N. Takahashi, T. Mukaiyama

Th141 **Precise measurement of the electron affinity of C_{60}** • José Eduardo Navarro Navarrete, P. Martini, M. Kristiansson, S. Indrajith, M. Björkhage, S. Rosén, A. Simonsson, P. Reinhed, J. D. Alexander, M. Gatchell, H. Cederquist, H. T. Schmidt, H. Zettergren

Th142 **X-ray spectra of highly charged Nd in an EBIT plasma: line identifications and effect of metastable states on ionization balance** • Adam Hosier, Joseph Tan, Timothy Burke, Dipti, Galen O’Neil, Endre Takacs, Yuri Ralchenko

Th143 **CollisionDB: An online repository of plasma collisional data sets** • Christian Hill, Dipti, Martin Haničinec

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Photon – Atom/Ion

Fr001 **Characterization of the longitudinal gas density profile in the microfluidic gas cell** • Janez Turnšek, Klemen Bučar, Matjaž Žitnik, Marcello Coreno, Anna Gabriella Ciriolo, Rebeca Martinez Vazquez

Fr002 **Laser cooling experiments at the CSRe: explanation for the observed wide deceleration range on a coasting ion beam by a cw laser** • Dongyang Chen, H. B. Wang, W. Q. Wen, Y. J. Yuan, D. Winters, S. Klammes, Th. Walther, U. Schramm, M. Bussmann, X. Ma and Laser Cooling Collaboration

Fr003 **Quantum Holography in Above Threshold Ionization** • Sebastián López, Diego Arbó

Fr004 **First principles simulation of high harmonic generation using quantum computer** • Hiroki Gi, Yuki Orimo, Kenichi L. Ishikawa, Yukio Kawashima, Tanvi Gujarati, Takeshi Sato

Fr005 **Impact of nondipole corrections on photoelectron rescattering off atomic targets in intense midinfrared laser pulses** • Resad Kahvedzic, Stefanie Gräfe

Fr006 **Attosecond-resolved Non-dipole Electron Dynamics** • Jintai Liang, Meng Han, Yijie Liao, Jia-bao Ji, Leung Chung Sum, Wei-Chao Jiang, Kiyoshi Ueda, Yueming Zhou, Peixiang Lu, Hans Jakob Wörner

Fr007 **Multi-photon double ionization of helium by ultrashort XUV pulses: probing the role of electron correlations** • Wei-Chao Jiang, M. Ederer, S. Donsa, J. Feist, I. Brezinova, J. Burgdörfer

Fr008 **Precise control of intracycle interference with a phase-stabilized polarization-gated laser pulse** • Yanlan Wang

Fr010 **Twisted attosecond pulse trains driven by amplitude-polarization pulses** • E. G. Neyra, D. Biasetti, F. Videla, L. Rebón, M. Ciappina

Fr011 **Tailoring the spectral phase of attosecond pulse trains generated by intense, femtosecond, two-color fields** • Trevor Olsson, Spenser Burrows, Swapneal Jain, Jody Davis, Scott Chumley, William Medlin, Guillaume Laurent

Fr012 **Study of the effect of higher-order dispersions on photoionisation induced by ultrafast laser pulses** • István Márton, László Sarkadi

Fr014 **Carrier-phase envelope control of nondipole effects in ionization** • Julia Derlikiewicz, Mihai C. Suster, Jerzy Z. Kaminski, Katarzyna Krajewska

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Fr016 **Spin-polarized electron vortices generated in single-photon ionization of atoms** • Yibo Hu, Qiangfei Ma, Kunlong Liu

Fr017 **Measuring the photoelectron angular distribution after nonlinear interaction of two photons with two active electrons in helium** • Michael Straub, Thomas Ding, Marc Rebholz, Gergana D. Borisova, Alexander Magunia, Hannes Lindenblatt, Severin Meister, Florian Trost, Yimeng Wang, Steffen Palutke, Markus Braune, Stefan Düsterer, Rolf Treusch, Chris H. Greene, Robert Moshammer, Thomas Pfeifer, Christian Ott

Fr018 **Multi-sideband interference structures observed via high-order photon-induced continuum-continuum transitions in helium** • Divya Bharti, Hemkumar Srinivas, Farshad Shobeiry, Robert Moshammer, Thomas Pfeifer, Kathryn R. Hamilton, Aaron T. Bondy, Soumyajit Saha, Klaus Bartschat, Anne Harth

Fr019 **Extended RPAE method for cross sections and delays** • A. Ljungdahl, J. Vinbladh, C. L. M. Petersson, S. Saha, J. Sörngård, Eva Lindroth

Fr020 **Disentangling interferences in the photoelectron momentum distribution from strong-field ionization** • Tian Wang, Zack Dube, Yonghao Mi, Giulio Vampa, David M. Villeneuve, Paul B. Corkum, Xiaojun Liu, Andre Staudte

Fr021 **Energy variation of double K-shell photoionization of Ne** • T. W. Gorczyca, S. T. Manson, S. H. Southworth, S. Li, D. Koulentianos, G. Doumy, L. Young, D. A. Walko, R. Püttner, D. Céolin, R. Guillemin, I. Ismail, O. Travnikova, M. N. Piancastelli, M. Simon

Fr022 **R-matrix with time dependence theory for double photoionization of general atoms** • Gregory Armstrong, Martin Plummer, Andrew Brown, Hugo van der Hart

Fr023 **Angular Distributions of Attosecond Time Delay in the Photoionization of ns Subshells of Atomic Systems: Relativistic and Nondipole Effects** • R. Hosseini, P. C. Deshmukh, Steven Manson

Fr024 **Singlet/triplet branching ratios in core-valence double photoionization of neon** • Takeshi Odagiri, Yuma Sugawara, Tatsuo Kaneyasu, Jun-ichi Adachi, Hirokazu Tanaka, Isao H. Suzuki, Sakura Suzuki, Yasumasa Hikosaka

Fr025 **Photoionization of a quantum grating formed by a single atom** • Shaofeng Zhang, B. Najjari, X. Ma

Photon – Molecule/Cluster

Fr026 **Recurrent fluorescence rates of tetracene cations $C_{18}H_{12}^{+}$ measured at two electrostatic Storage Rings: DESIREE and Mini-Ring** • Jérôme Bernard, MingChao Ji, Suvasthika Indrajith, Mark H Stockett, José E. Navarro Navarrete, Naoko Kono, Henrik Cederquist, Serge Martin, Henning T Schmidt, Henning Zettergren

Fr027 **Resonant intercluster Coulombic decay in the photoionization of Na_{20} confined inside C_{240}** • Rasheed Shaik, Kuldeep Prajapat, Hari Varma Ravi, Himadri S. Chakraborty

Fr028 **Efficient indirect interatomic Coulombic decay induced by photoelectron impact excitation in large pure He nanodroplets** • Ltaief Ben Ltaief, Keshav Sishodia, Suddhasattwa Mandal, Subhendu De, Sivarama Krishnan, Cristian Medina, Nitish Pal, Robert Richter, Thomas Fennel, Marcel Mudrich

Fr029 **The primary steps of ion solvation in helium nanodroplets** • Simon Høgh Albrechtsen, Jeppe Christensen, Constant Schouder, Albert Muñoz, Manuel Barranco, Marti Pi, Henrik Stapelfeldt

Fr030 **Carrier-envelope-phase measurement of sub-cycle UV pulses using angular photofragment distributions** • X. X. Dong, Y. R. Liu, V. Kimberg, O. Vendrell, Y. Wu, J. G. Wang, J. Chen, S. B. Zhang

Fr031 **Chiral Molecular Frame Photoelectron Angular Distributions in achiral formic acid** • Dimitrios Tsitsonis, Florian Trinter, Till Jahnke, Reinhard Dörner, Markus Schöffler

Fr032 **Ultrafast imaging of molecular chirality via low-order nonlinear interactions** • Josh Vogwell, Laura Rego, Olga Smirnova, David Ayuso

Fr033 **Revealing the wave-function-dependent zeptosecond birth time delay in molecular photoionization** • Xuanyang Lai, S. P. Xu, S. G. Yu, M. W. Shi, Y. L. Wang, W. Quan, X. J. Liu

Fr034 **Time-Resolved Images of Intramolecular Charge Transfer in Organic Molecules** • Francisco Fernández-Villoria, Jesús González-Vázquez, Alicia Palacios, Fernando Martín

Fr035 **Theory of molecular photoionization time delays** • Adrian J. Suñer-Rubio, Roger Y. Bello, Christoph Lemell, Joachim Burgdörfer, Alicia Palacios, Fernando Martín

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Fr036 **Ultrafast competition between H_2^+ and H_3^+ formation via roaming H_2 mechanism** • Krishnendu Gope, Itamar Luzon, Dror Bittner, Ester Livshits, Roi Baer, Daniel Strasser

Fr037 **Ionization Dynamics in H_2 by Interference of One- and Two-Photon Pathways employing VUV FEL Pulses** • Fabian Holzmeier, Alberto Gonzalez-Castillo, Thomas Baumann, Carlo Callegari, Michele Di Fraia, Matteo Lucchini, Michael Meyer, Danielle Dowek, Oksana Plekan, Kevin Prince, Eleonore Roussel, Rene Wagner, Alicia Palacios, Fernando Martin, Danielle Dowek

Fr038 **Chiral photoelectron angular distributions from ionization of achiral atomic and molecular species** • Andreas Pier, Kilian Fehre, Sven Grundmann, Isabel Vela-Perez, Nico Strenger, Max Kircher, Dimitrios Tsitsonis, Joshua B. Williams, Arne Senftleben, Thomas Baumert, Markus S. Schöffler, Philipp V. Demekhin, Florian Trinter, Till Jahnke, Reinhard Dörner

Fr039 **The Big, the Small & the Shoulder: Controlling OCS post-Ionization Dynamics*** • Tomoyuki Endo, Karl Michael Ziems, Martin Richter, Akiyoshi Hishikawa, Stefanie Gräfe, François Légaré, Heide Ibrahim

Fr040 **Exploration of VUV photodissocaition of aniline as a soruce of astronomically important HC2N** • S. Muthuamirthambal, S. Arun, K. Ramanathan, R. Richter, N. Pal, P. Bolognesi, L. Avaldi, M. V. Vinitha, C. S. Jureddy and U. Kadhane

Fr041 **Differentiating Molecular Structures using Laser-induced Coulomb Explosion Imaging*** • Huynh Van Sa Lam, Anbu Selvam Venkatachalam, Surjendu Bhattacharyya, Keyu Chen, Vinod Kumarappan, Artem Rudenko, Daniel Rolles

Fr042 **Fully differential double photoionization of linear molecules beyond H_2** • Frank Yip, R. R. Lucchese, T. N. Rescigno, C. W. McCurdy

Fr043 **First principle approach to the simulation of attosecond XUV pump XUV probe spectra for small organic molecules** • Gilbert Grell, Jesús González-Vázquez, Piero Decleva, Alicia Palacios, Fernando Martín

Fr044 **Sub-cycle resolved tunnel ionization of chiral molecules** • Max Hofmann, Angelina Geyer, Daniel Trabert, Nils Anders, Jan Kruse, Jonas Rist, Lothar Schmidt, Till Jahnke, Maksim Kunitski, Markus Schöffler, Sebastian Eckart, Reinhard Dörner

Fr045 **UV-induced ring-opening dynamics investigated by time-resolved Coulomb explosion imaging** • Keyu Chen, Surjendu Bhattacharyya, Anbu Venkatachalam, Huynh Lam, Kurtis Borne, Sergey Usenko, Björn Senfftleben, Daniel Rivas, Terence Mullins, Thomas Baumann, Benjamin Erk, Aljoscha Rörig, Philipp Schmidt, Sharath Sasikumar, Simon Dold, Tommaso Mazza, Michael Meyer, Basile Curchod, Mike Ashfold, Felix Allum, Alice Green, Emily Warne, Joseph McManus, Michael Burt, Mark Brouard, Ruaridh Forbes, Pedro Nunes, Martin Centurion, Peter Weber, Arnaud Rouzee, Rico Tanyag, Henrik Stapelfeldt, Kang Lin, Rebecca Ingle, Enliang Wang, Florian Trinter, Till Jahnke, Rebecca Boll, Daniel Rolles, Artem Rudenko

Fr046 **Resonant Double-Core Excitation of N_2** • Eetu Pelimanni, Adam Fouda, Phay Ho, Thomas Baumann, Alberto De Fanis, Simon Dold, Iyas Ismail, Dimitris Koulentianos, Tommaso Mazza, Michael Meyer, Maria Novella Piancastelli, Ralph Püttner, Daniel Rivas, Björn Senfftleben, Marc Simon, Linda Young, Gilles Doumy

Fr047 **Metrology of Attosecond Soft X-ray Pulses at European XFEL** • Markus Ilchen, Sadia Bari, Thomas M. Baumann, Rebecca Boll, Markus Braune, Günter Brenner, Francesca Calegari, Alberto De Fanis, Kristina Dingel, Stefan Düsterer, Felix Egun, Arno Ehresmann, Benjamin Erk, Lars Funke, Andreas Galler, Gianluca Geloni, Gesa Goetzke, Tais Gorkhover, Jan Grünert, Patrik Grychtol, Marc Guetg, Andreas Hans, Arne Held, Ruda Hindrikson, Moritz Hoesch, Till Jahnke, Fini Jastrow, Reinhard Kienberger, Stephan Kuschel, Joakim Laksman, Mats Larsson, Jia Liu, Jon Marangos, Lutz Marder, David Meier, Michael Meyer, Najmeh Mirian, Jacobo Montano, Terence Mullins, Valerija Music, Christian Ott, Thorsten Otto, Yevheniy Ovcharenko, Christopher Passow, Thomas Pfeifer, Nils Rennhack, Daniel Rivas, Daniel Rolles, Artem Rudenko, Patrick Rupprecht, Sara Savio, Albert Schletter, Frank Scholz, Jörn Seltmann, Svitozar Serkez, Philipp Schmidt, Evgeny Schneidmiller, Bernhard Sick, Richard D. Thomas, Kai Tiedtke, Sergey Usenko, Jens Viefhaus, Peter Walter, Vincent Wanie, Niclas Wieland, Lasse Wülfing, Mikhail Yurkov, Vitali Zhaunerchyk, Wolfram Helml

Fr048 **XUV-induced dynamics in complex molecular ions in the gas phase** • Richard Brédy, Alexie Boyer, Marius Hervé, Isabelle Compagnon, Franck Lépine

Fr049 **Mass spectrometry at the limits of biological objects: viruses, bacteria and amyloid fibers** • Sylvain Maclot, Rodolphe Antoine, Philippe Dugourd

Fr050 **Observation of H_3^+ formation from molecular hydrogen dimers** • Yonghao Mi, Enliang Wang, Zack Dube, Tian Wang, Andrei Naumov, David Villeneuve, Paul Corkum, Andre Staudte

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Photon – Molecule/Cluster

Fr051 **Coincidence Measurements of Photodouble Ionization of Thiophene** • Nicholas Wong, Jason Howard, Emma Sokell, Paola Bolognesi, Lorenzo Avaldi

Fr052 **On the role of isomerisation in the photo dissociation of PANHs : A casestudy with methyl amidogen abstraction** • Subramani Arun, Karthick Ramanathan, S. Muthuamirthambal, Robert Richter, Nitish Pal, J. Chiarinelli, Paola Bolognesi, Lorenzo Avaldi, M. V. Vinitha, Chinmai Sai Jureddy, Umesh R. Kadhane

Fr053 **Diatomic molecular vibrations in a strong infrared laser field: an analytic treatment of the laser-dressed Morse potential** • Szabolcs Hack, Sándor Varró, Gábor Paragi, Péter Földi, Imre Ferenc Barna, Attila Czirják

Fr054 **Fragmentation of methanol molecules after valence photoexcitation studied by negative-ion positive-ion coincidence spectroscopy** • Hanan Sa'Adeh, Antti Kivimäki, Christian Stråhlman, Kevin C. Prince, Richard D. Thomas

Photon – Other

Fr055 **Unexpected enhanced terahertz radiation in two-foci cascading plasmas** • Jingjing Zhao

Fr056 **Realtime tracking of ultrafast dynamics in liquid water*** • Gaia Giovannetti, Sergey Ryabchuk, Ammar bin Wahid, Hui-Yuan Chen, Erik Petter Maansson, Andrea Trabattoni, Vincent Wanie, Hugo Marroux, Majed Chergui, Francesca Calegari

Fr057 **Enhanced cutoff energies in strong-field photoelectron emission of plasmonic nanoparticles** • Erfan Saydanzad, J. A. Powell, A. Rudenko, Uwe Thumm

Fr058 **Nonadiabatic Tunneling of Photoelectrons Induced by Few-Cycle Near-Fields** • B. Lovász, Václav Hanus, P. Sándor, G. Z. Kiss, B. Bánhegyi, Z. Pápa, J. Budai, C. Prietl, J. R. Krenn, P. Dombi

Fr059 **Photoionization of H Debye plasmas in strong field approximation** • Yugang Yang, Li Guang Jiao, Aihua Liu

Fr060 **Shake-up and shake-off satellites as probe of ultrafast charge delocalization in liquid water*** • Florian Trinter, B. Winter, S. Thürmer

Fr061 **High-order harmonic generation and confinement in artificial atoms** • Harshitha Nandiga Gopalakrishna, Raktim Baruah, Christian Hünecke, Viacheslav Korolev, Martin Thümmler, Alexander Croy, Ulf Peschel, Stefanie Gräfe, Maria Wächtler, Daniil Kartashov

Fr062 **Studying the Optical Properties of 1-decanol for Ultrashort Pulse Generation** • Nathan Drouillard, TJ Hammond

Fr063 **Supercontinuum amplification for nonlinear optics** • Nathan Drouillard, Sagnik Ghosh, TJ Hammond

Fr064 **Application of LIBS spectral data fusion in quantitative analysis of Astragalus** • P. Zhao, W. W. Han, D. X. Sun, G. D. Zhang, Maogen Su

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Mo059 **Electron excitation dynamics in silicon irradiated by femtosecond double pulses of different wavelength combination** • Eiyu Gushiken, Mizuki Tani, Kenichi Ishikawa

Mo060 **Visualization of ultrafast plasmon by nonlinear multi-photon photoemission electron microscopy** • Boyu Ji, Peng Lang, Yang Xu, Xiaowei Song, Jingquan Lin

Mo061 **Orbital perspective of high-harmonic generation in ReS_2** • Álvaro Galán, Chandler Bossaer, Guilmot Ernotte, Andrew Parks, Rui Silva, David Villeneuve, André Staudte, Thomas Brabec, Adina Luican-Mayer, Giulio Vampa

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Mo063 **Tunable spectral shift of high-order harmonic generation in atoms by a plasmon-assisted shaping pulse** • Yuan Wang, Qingyi Li, Zhou Chen, Jun Wang, Fuming Guo, Yujun Yang

Mo064 **Far-ultraviolet (FUV) emission from laser-produced plasma of Al, Fe, Cu and Inconel** • Shuichiro Tamaki, Hiroki Ohnishi, Yoko Shiina, Yuji Nakano

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Mo066 **Recent progress of muon catalyzed fusion study: III. Alternative measurement of nuclear fusion reaction in muonic molecule** • K. Okutsu, T. Yamashita, Yasushi Kino, R. Nakashima, R. Konishi, K. Sasaki, K. Miyashita, Y. Toyama, S. Okada, M. Sato, T. Oka, N. Kawamura, S. Kanda, K. Shimomura, P. Strasser, S. Takeshita, M. Tampo, S. Doiuchi, Y. Nagatani, H. Natori, S. Nishimura, A. D. Pant, Y. Miyake, K. Ishid

Mo067 **Triple-differential cross sections in three-dimensional kinematics for electron-impact-ionization dynamics of tetrahydrofuran at 250-eV** • X. Xue, D. M. Mootheril, E. Ali, M. Gong, S. Jia, J. Zhou, E. Wang, J. Li, X. Chen, D. H. Madison, A. Dorn, and X. Ren

Mo068 **Molecular ionization cross-sections using complex Gaussian representations of the continuum** • Abdallah Ammar, Arnaud Leclerc, Lorenzo Ugo Ancarani

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Mo070 **Many-body theory calculations of positron binding to halogenated hydrocarbons** • Jack Cassidy, Jaroslav Hofierka, Brian Cunningham, Charlie Rawlins, Charles Patterson, Dermot Green

Mo071 **Low-energy positron collisions with tetrachloroethylene (C_2Cl_4) molecule** • Rafael O. Lima, Alessandra S. Barbosa, Márcio H. F. Bettega, Sergio d`A. Sanchez, Giseli Moreira

Mo072 **Electron and Positron impact ionisation of few biologically relevant molecules for coplanar and perpendicular plane emission of electrons** • Alpana Pandey, Ghanshyam Purohit

Mo073 **Electronic excitation of benzene by electron impact: a theoretical and experimental investigation** • Alan Guilherme Falkowski, Romarly Fernandes da Costa, Marco Aurélio Pinheiro Lima, Alexi De Avila Cadena, Ronald Pocoroba, Murtadha A. Khakoo, Fábris Kossoski

Mo074 **Scaled Born approximation for electron impact excitations of N_2 molecule** • Jorge Lino

Mo075 **Electron Impact Induced Fragmentation of ND_3^+** • M. O. A. El Ghazaly, J. J. Jureta, Ola Al-Hagan, P. Defrance

Mo076 **Elucidating geometrical features of e-C_{60} interaction from their elastic scattering spectra** • R. Aiswarya, Jobin Jose, Rasheed Shaik, Hari Varma Ravi, Himadri S. Chakraborty

Mo078 **Tracing the expansion of molecular plasma with electron collision** • Guangqing Chen, Zonglin Yao, Xu Shan, Xiangjun Chen

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Mo080 **Effects and data of electron collisions on various molecules for medical applications** • Yeunsoo Park, Mi-Young Song, Mareike Dinger, Woon Yong Baek

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Mo082 **Secondary electron emission & detection of low-energy charged particles impacting channel electron multipliers** • Donovan Newson, Simon Brawley, Michael Shipman, Rina Kadokura, Tamara Babij, David Cooke, Dawn Leslie, Gaetana Laricchia

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Mo088 **Quantum vortices in the fully differential cross section for the ionization of atoms by the impact of protons and positrons** • Tamara Guarda, Francisco Navarrete, Raul Barrachina

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Mo094 **Probing the formation of quasi-molecules in collisions of Kr^{q+}-ion with Pb and Bi** • C. V. Ahmad, K. Chakraborty, R. Gupta, D. Swami and P. Verma

Mo095 **Efficiency enhancement of the dynamical capture of ion bunches by instantanous ion-mode coupling** • Stefan Ringleb, Markus Kiffer, Sugam Kumar, Manuel Vogel, Wolfgang Quint, Thomas Stöhlker, Gerhard G. Paulus

Mo096 **Resonance-Enhanced Electron Capture in the Laser-Assisted Proton-Hydrogen Collision** • S. Gao, F. Zhu, L. G. Jiao, Aihua Liu, U. Thumm

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Mo097 **Development of electrospray ion source and setup for collision induced dissociation experiments of large molecules** • Kamal Kumar, Md Atiqur Rehman, Deepankar Misra

Mo098 **Dissociation dynamics in Chloroform molecule induced by ion impact** • Nirmallya Das, Sankar De, Pragya Bhatt, C. P. Safvan, Abhijit Majumdar

Mo099 **Excitation processes in collisions of He$^+$ ions with N$_2$, O$_2$ molecules** • Malkhaz Gochitashvili, Ramaz A. Lomsadze, Roman Ya Kezerashvili, Michael Schulz

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Mo101 **A travelling-wave ion-mobility system for preparation of conformationally pure molecular targets for collision experiments** • Marcelo Goulard, Klaas Bijlsma, Martje Nieuwenhuis, Jente Damm, Thomas Schlathölter

Mo102 **Ultrafast rotational energy transfer initiating by Coulomb explosion in two-body dissociation of CO_2^{3+}** • Weiqing Xu, Ruichao Dong, Xincheng Wang, Yuhai Jiang

Mo103 **Statistical Analysis of X-ray Spectra of Aqueous Tripeptides** • Eemeli Eronen, Anton Vladyka, Florent Gerbon, Christoph Sahle, Johannes Niskanen

Mo104 **The role of molecular collisions in the conversions of nuclear spin isomers of methanol gas** • Zhen-Dong Sun

Mo105 **Combining momentum-space wavefunctions and frontier orbital theory for providing predictive insights into pharmacological activity** • Long Sihan, Y. Onitsuka, S. Nagao, M. Takahashi

Mo106 **Probing the internal dynamics of homonuclear dimer anions via time-dependent electron detachment inside an electrostatic ion trap*** • Roby Chacko, Stav Knaffo, Nikolaj Klinkby, Oded Heber, Daniel Zajfman

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Mo107 **Ultralong-range Rydberg Molecules: Electronic Structure and Rydberg blockade** • D. Mellado-Alcedo, J. Gacia-Garrido, A. Guttridge, D. K. Ruttley, C. S. Adams, S. L. Cornish, H. R. Sadeghpour, R. Gonzalez-Ferez

Mo108 **Inner-shells effect for positrons and electrons traversing cold matter and plasmas** • Claudio Archubi, Claudia Montanari, Néstor Arista, Diego Arbó

Mo109 **Stereodynamical control of cold collisions between two aligned D_2 molecules** • Pablo Jambrina, James F. E. Croft, J. Zuo, Hua Guo, F. J. Aoiz, N. Balakrishnan

Mo110 **Improved method to treat asymptotic non-adiabatic couplings in scattering processes** • Patrik Hedvall, Åsa Larson

Mo111 **Low-energy collisions between two indistinguishable tritium-bearing hydrogen molecules: HT+HT and DT+DT** • Renat Sultanov

Mo112 **Mutual neutralization between diatomic cation and atomic anion** • Arnaud Dochain, M. Poline, Ansgar Simonsson, Stefan Rosén, MingChao Ji, Henning Schmidt, R. D. Thomas

Mo113 **A new approach for measuring the reaction rates of low-energy ion—polar-molecule reactions for astrochemistry** • Kunihiro Okada, Kazuki Sugata, Naoki Kimura, Kazuhiro Sakimoto, Hans A. Schuessler

Mo114 **Observation of radiative vibrational cooling of N_2O^+ ions using a cryogenic electrostatic ion storage ring: contribution of Fermi resonance** • Sakumi Harayama, S. Kuma, N. Kimura, K. C. Chartkunchand, Y. Nakano, T. Yamaguchi, T. Azuma

Mo115 **Mutual Neutralization in sub-eV $C_{60}^+ + C_{60}^-$ collisions** • Raka Paul

Mo116 **Slow decay processes of molecular anions during long-time storage in a cryogenic storage ring** • Viviane Charlotte Schmidt, Klaus Blaum, Roman Čurík, Paul Fischer, Lisa Gamer, Sebastian George, Jürgen Göck, Manfred Grieser, Florian Grussie, Robert von Hahn, Oded Heber, Mark A. Iron, Ábel Kálosi, Claude Krantz, Holger Kreckel, Evangelos Miliordos, Preeti M. Mishra, Damian Müll, Oldřich Novotný, Felix Nuesslein, Milan Ončák, Daniel Paul, Hendrik B. Pedersen, Lutz Schweikhard, Kaija Spruck, Yoni Toker, Andreas Wolf, Aigars Znotiņš

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Mo118 **CO_2 activation by Cu clusters in superfluid helium nano-droplets** • Olga Lushchikova, M. Gatchell, J. Reichegger, S. Kollotzek, F. Zappa, P. Scheier

Mo119 **A versatile ion source for cold ions using superfluid helium nanodroplets** • Paul Martini, Henning Zettergren, Henning Schmidt, Michael Gatchell

Mo120 **Mid-infrared spectroscopy of aromatic molecular cations in helium nanodroplets** • Arisa Iguchi, Susumu Kuma, Hajime Tanuma, Toshiyuki Azuma

Mo121 **Supersolidity in a quasi-2D spinor Bose-Einstein condensate with SO-coupling** • Pardeep Kaur, Sandeep Gautam, S.K. Adhikari

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Experimental Developments

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Mo125 **Present and future opportunities at the CAMP instrument at the Free-Electron Laser FLASH** • Benjamin Erk

Mo127 **Direct measurement of few-cycle electric fields using a lock-in detection** • Ronak Narendra Shah, Jahanzeb Muhammad, Ianina Kosse, Samuel Bengtsson, Riccardo Mori, Mario Niebuhr, Fabio Frassetto, Luca Poletto, Giuseppe Sansone

Mo128 **A hybrid mode-locking Yb:fiber laser for generations of vector dissipative solitons** • Kun Chen, Tao Cao, Shaozhen Liu, Qi Xu, Zhou Li, Jiahui Peng

Mo130 **The CSR-ReMi – A cryogenic in-ring reaction microscope** • Felix Herrmann, David V. Chicharro, Robert Moshammer, Claus Dieter Schröter, Thomas Pfeifer

Mo131 **The (only) way towards low-energy, heavy, highly charged ions: the HITRAP deceleration facility** • Nils Stallkamp, Zoran Andelkovic, Svetlana Fedotova, Wolfgang Geithner, Frank Herfurth, Max Horst, Dennis Neidherr, Simon Rausch, Sergiy Trotsenko, Gleb Vorobjev

Mo132 **ErUM-FSP APPA: BMBF Collaborative Research Center at FAIR** • Stefan Schippers, Thomas Stöhlker for the APPA collaboration

Post Deadline

Mo133 **A real-time gas monitoring system based on ion mobility spectrometry for high concentration** • Kazunari Takaya, Masayoshi Hagiwara, Shiro Matoba, Mitsutoshi Takaya, Nobuyuki Shibata

Mo134 **Development of a universal in-ring COLTRIMS Reaction Microscope for CRYRING@ESR** • G. Kastirke, L. Ph. H. Schmidt, T. Jahnke, R. Dörner, M. S. Schöffler

Mo135 **Novel High Harmonic Beamline Design for Ultrafast X-ray Spectroscopy** • Philippe Burden, Patrick Elten, Andrey E. Boguslavskiy, Claude Marceau, Iain Wilkinson, Arnaud Rouzée, Paul Corkum, Albert Stolow

Mo136 **The development of marking system of secondary battery anode and cathode using nanosecond laser with in situ tracking module** • Seungsik Ham, Jaesung Park, Taeho Jun, Ho Lee

Mo137 **Development of Polymer Dispersed Liquid Crystal (PDLC)-based switchable spatial filter using femtosecond laser micro-patterning** • Jaesung Park, Jong-Wook Park, Ho Lee

Mo138 **Ultrafast electron-stimulated desorption to form ion pulses for time-resolved ion surface collision experiments** • Marius C. Chirita Mihaila, Gabriel L. Szabo, Alexander Redl, Markus Goldberger, Richard Wilhelm

Mo139 **Development of portable Electron Beam Ion Traps at NIST** • Joseph Tan, David La Mantia, Aung Naing, Albert Henins, Alessandro Banducci, Samuel Brewer

Mo140 **Toward a new type of gas phase spectroscopy for complex organic ions** • Stav Knaffo, M. L. Rappaport, H. Kreckel, K. Blaum, A. Wolf, Th. Henning, Y. Toker, S. Sunil Kumar, O. Heber, D. Zajfman

Mo142 **Recent progress of muon catalyzed fusion study: IV. Nuclear reaction processes in the dtμ molecule** • Masayasu Kamimura, Yasushi Kino, Takuma Yamashita

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XXXIII International Conference on Photonic, Electronic and Atomic Collisions

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8:30		**ICPEAC Opening (8:45)** • *Room 214*	
9:00		**Plenary** • Kenji Ohmori • Chair: Friedrich Aumayr • *Room 214*	**Plenary** • Ursula Keller • Chair: Dominique Vernhet • *Room 214*
9:30	**Tutorial I** • Paul Corkum • Chair: A. Staudte • *Room 4007, Faculty of Social Sciences Building, 120 University Private, Ottawa, ON K1N 6N*		
10:00		**Coffee Break** • *Trillium Ballroom*	**Coffee Break** • *Trillium Ballroom*
10:30	**Coffee Break**	**Atto I** • Averbukh (PR), Cryan (PR), Douguet (PR), Geyer (SR), Hutcheson (SR) • *Room 214* **Antimatter** • Bray (PR), Nagata (PR), Green (PR), Graves (SR), Nauta (SR) • *Room 213/215*	**FEL** • Hishikawa (PR), Callegari (PR), Rohringer (PR), Nandi (PR) • *Room 214* **Bio** • Andersen (PR), Rousseau (PR), Kočišek (PR), Lozano (PR) • *Room 213/215*
11:00	**Tutorial II** • Eva Lindroth • Chair: T. Kirchner • *Room 4007, Faculty of Social Sciences Building, 120 University Private, Ottawa, ON K1N 6N*		
11:30			
12:00	**Free Time**		
12:30		**Free Time**	**Free Time**
13:00			
13:30	**Tutorial III** • Emily Lamour • Chair: M. Horbatsch • *Room 4007, Faculty of Social Sciences Building, 120 University Private, Ottawa, ON K1N 6N*		
14:00		**Ultrafast** • Centurion (PR), X.Liu (PR), Palacios (PR), Pan (SR), Pajek (SR) • *Room 214* **Astro** • Petrignani (PR), de Barros (PR), Hama (PR), Schneider (PR) • *Room 213/215*	**Cold I** • Wester (PR), Steinberg (PR), Ishida (PR), Coté (SR), Boulou-fa-Maafa (SR) • *Room 214* **Exotic Methods** • Y.Liu (PR), Choubisa (PR), Ngoko Dijokap (PR), Osaku (SR), Giovanetti (SR) • *Room 213/215*
14:30	**Coffee Break**		
15:00	**Tutorial IV** • Jonathan Tennyson • Chair: J. Gorfinkiel • *Room 4007, Faculty of Social Sciences Building, 120 University Private, Ottawa, ON K1N 6N*		
15:30			
16:00	**Registration and Welcome Reception** • *Rideau Canal Atrium*	**Poster Session I** • *Trillium Ballroom*	**Poster Session II** • *Trillium Ballroom*
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18:00	**Executive Committee Meeting and Dinner** • *Room 210*		
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19:00			
19:30			
20:00		**Public Lecture I** • Donna Strickland • Chair: P. Corkum • *Room 214*	**Public Lecture II** • Teresa Scassa • *Room 214*
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21:00			
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Time	Friday, July 28		…	Monday, July 31		Tuesday, August 1	
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9:00				**Poster Session IV** • *Trillium Ballroom*		**Plenary** • Amine Cassimi • Chair: Stefan Schippers • *Room 214*	
9:30	**IUPAP Prize Talk** • Hong-Guang Duan • Chair: Rosario González-Férez • *Room 214*						
10:00	**Coffee Break** • *Trillium Ballroom*					**Coffee Break** • *Rideau Canal Atrium Centre*	
10:30	**Atto II** • D.Boll (PR), Ruchon (PR), Kheifets (PR), Weber (SR), Magunia (SR) • *Room 214*	**El-Molecule** • Houfek (PR), Sinha (SR), Watanabe (SR), Kopyra (PR), Monteiro-Carvalho (SR), Bondy (SR) • *Room 213/215*				**Quantum Potpourri** • Niggas (PR), Sato (PR), Niozu (PR), Sheil (PR) • *Room 214*	**Cold II** • Hogan (PR), Arora (PR), Gruber (PR), Erdmann (SR), Xie (SR)
11:00							
11:30				**Plenary** • Alexander Dorn • Chair: Emma Sokell • *Room 214*			
12:00							
12:30	**Free Time**			**Free Time**		**Business Meeting** • *Room 214*	
13:00						**Free Time**	
13:30							
14:00	**Imaging** • Blume (PR), Wang (PR), R. Boll (PR), Ibrahim (SR), H.V.Sa Lam (SR) • *Room 214*	**Spectroscopy** • Okumura (PR), Hori (PR), Loetzsch (PR), Pfäfflein (SR), Zhou (SR) • *Room 213/215*		**Synchrotron** • Ganguly (PR), Milosavljevic (PR), Sisourat (SR), Dutta (SR), Trinter (SR) • *Room 214*	**Storage Rings** • Hanstorp (PR), Zettergren (PR), Lestinsky (PR), Chacko (SR), Schmidt-May (SR) • *Room 213/215*		
14:30						**Plasmonics** • Pápa (PR), Gholam-Mirzaei (PR), Jalil (SR), Rivera-Dean (SR) • *Room 214*	**Recombination** • Ma (PR), Novotny (PR), Zhang (SR), Kalosi (SR) • *Room 213/215*
15:00							
15:30							
16:00	**Poster Session III** • *Trillium Ballroom*			**Coffee Break** • *Rideau Canal Atrium Centre*		End of Conference	
16:30				**Complex** • Schöffler (PR), Varella (PR), Ren (SR), Segui (SR) • *Room 214*	**Ion Collisions** • Wei (PR), Wolff (PR), Majima (SR), Yang (SR) • *Room 213/215*		
17:00							
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19:00				**Conference Dinner** • *Trillium Ballroom*			
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