



D Y N
RESEARCH
TRAINING
GROUP

C A M
DYNAMICS OF CONTROLLED
ATOMIC AND MOLECULAR
SYSTEMS



BOOK OF ABSTRACTS



Annual Convention 2026 ***RTG DynCAM***

Dynamics of Controlled Atomic and Molecular Systems

Juli 27 to August 1, 2026

Institute of Physics

Hermann-Herder-Straße 3

D - 79104 Freiburg

universität freiburg



Imprint

RTG 2717 / Dynamics of Controlled Atomic and Molecular Systems

Spokesperson: Giuseppe Sansone

Coordination: Simone Ortolf

Institute of Physics

University of Freiburg

Hermann-Herder-Straße 3

D - 79104 Freiburg

E-Mail: info-dyncam@physik.uni-freiburg.

General Information

Duration

Monday, Juli 27, 2026, 9:00 a.m.

Saturday, August 1, 5:00 p.m.

Location

University of Freiburg Institute of Physics

Hermann-Herder-Straße 3

D - 79104 Freiburg

<https://uni-freiburg.de/phys/>

Accommodation

Our guests from Vancouver will be accommodated in the rooms of the Caritas Academy. You will have a single room with bathroom; breakfast is included. Outside reception hours, you can arrive via the late check-in box.

There is a library, a fireside lounge and a chapel in the main building, which are accessible and may be used at any time. There is also a small bistro with coffee, drinks and snacks for self-service. Furthermore, you can rent e-bikes on site for excursions, or nordic walking sticks for a hike.

Meals & Drinks

Two coffee breaks (morning and afternoon) are included for conference participants, as well as lunch each day. On Monday we will have an evening to welcome the participants in the Common Room of the Physics-building. The Conference Dinner on Thursday will be at the Caritas Academy.

Group Activities

(1) Afternoon Trip on Wednesday, July 29th, there will be a short hike to a nearby lake. We will start at a tram station and walk from there past several small highlights towards a lake to spent the evening here. **(CANCELLED)**

(2) On Saturday, August 1st we will drive by bus to Orbey in Alsace and walk the **“Three Lakes” Hike in the Vosges**. It will take around four hours and we will return around 5 p.m. A packed lunch will be provided. We'll be leaving from the Physics Institute at 8:00.

Travel information

BY PUBLIC TRANSPORT

If you arrive at Frankfurt Main Airport (FRA) you can get to Freiburg by train either through a direct connection or with a transfer in Mainz or Mannheim in roughly 2-3 hours. If you arrive at Zurich Airport (ZRH) you can take a train to Basel SBB and then to Freiburg Hauptbahnhof in roughly 2-2.5 hours.

Arrival at Central Station, Freiburg

To the Institute of Physics:

- take the tram line 3 in the direction “Zähringen” to the stop “Tennebacher Straße”.
- Cross the Street towards the large red building, then walk left. At the next opportunity, take a right and follow that street to the next intersection. Cross it and you have reached your destination. The Institute of Physics is on the left.

To the Accomodations at the Caritas Academy:

- take tram line 3 in the direction “Zähringen” to the stop “Europaplatz” (formally “Siegesdenkmal”). From there, you walk for about 5 minutes (ca. 0,5 km) on the right side of the street “Auf den Zinnen”. After that you should reach a bridge leading over the crossroads into the park, “Stadtgarten”. Then keep to the right and follow the street f17/19.

Please keep in mind that this street is very steep, so getting there by foot and with luggage might be a bit of a chore.

- the academy is about 25 minutes by foot from the central station of Freiburg.
- you can also take a taxi from the central station. It will approximately cost 15-20 €.
- traveling by bus will most likely mean that you arrive the ZOB (Central Bus Station), which is at the south side of the central station.

Distances:

Central train station:

To the Institute: 1,1 km

To Caritas Academy: 2,1 km

Nearest tram/bus station:

To the Institute: 290 m

To the Caritas Academy: 1,1 km

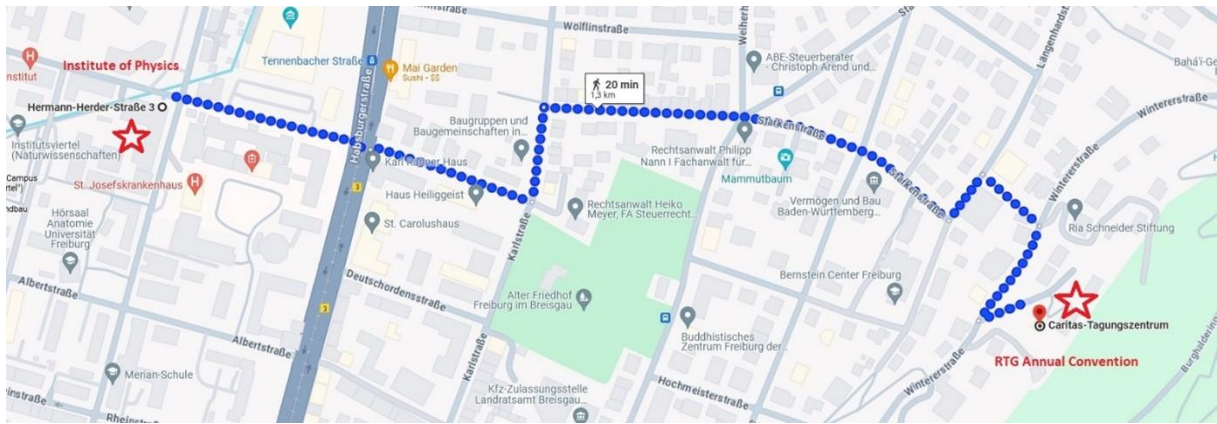
City-Center: (Freiburger Münster, Old Town):

To the Institute: 950 m-1 km

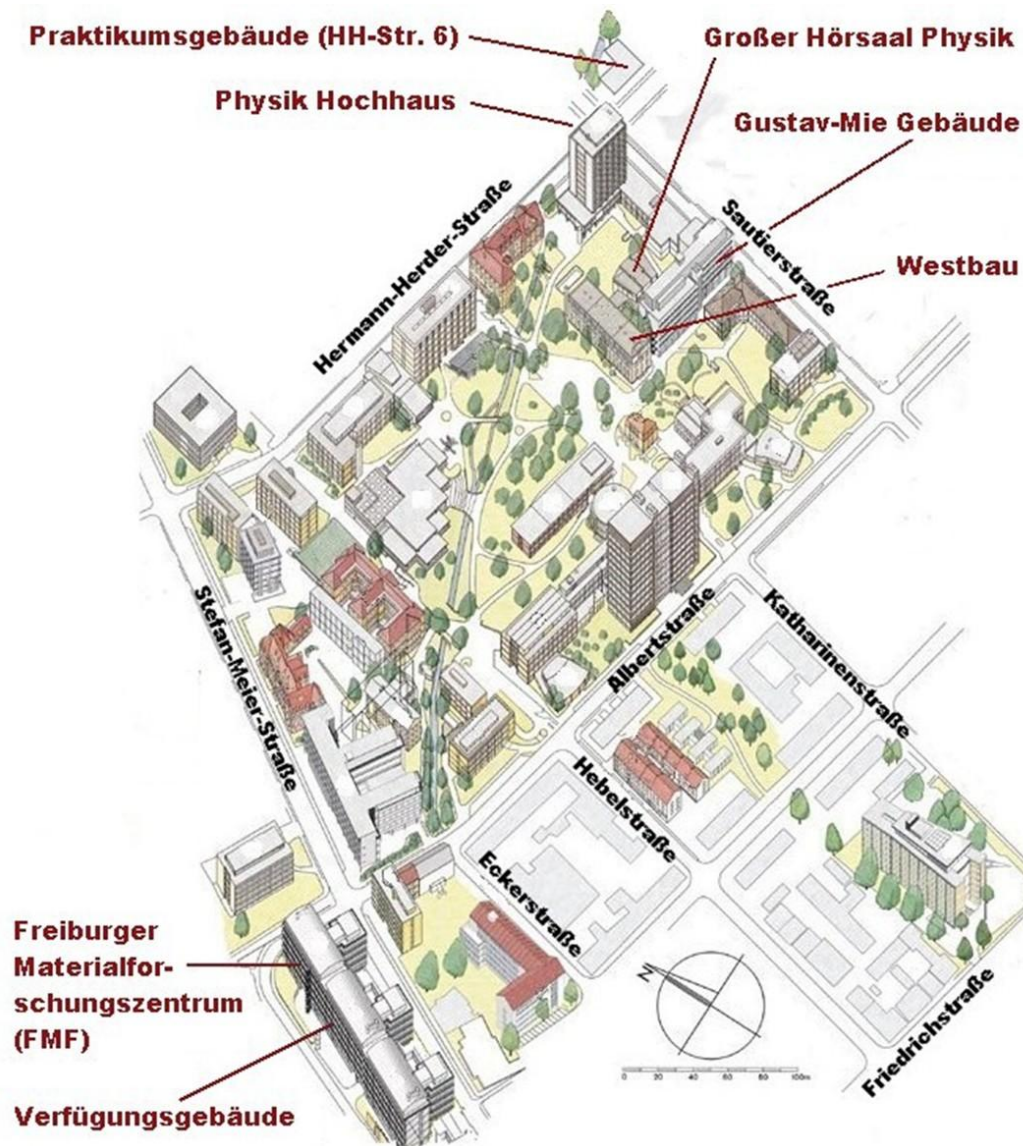
To the Caritas Academy: 1,4 km

Maps

Caritas Academy – Institute of Physics:



Site plan Institute of Physics:



Program

Monday, July 27, 2026

Lecture Hall I, Physics Highrise

9:00	Arrival & Welcome – Giuseppe Sansone
	Chair: Lukas Bruder
9:30	PI Lecture – Alessandra Colla <i>Thermodynamics of arbitrary open quantum systems: from average quantities to fluctuation relations</i>
10:30	Coffee Break
11:00	PHD presentation – Leonie Werner <i>Energy transfer processes in molecules and molecular complexes using ultracold rare-gas clusters</i>
11:20	PHD presentation – Tim Ehret <i>A Lindblad master equation for twisted photons in a turbulent atmosphere</i>
11:40	PHD presentation – Marvin Schmoll <i>Two-sideband RABBIT</i>
12:00	Lunch Break
	Chair: Bernd von Issendorff
2:00	PHD presentation – Alexander Döring <i>Interaction-Induced Dynamics in Ultracold Atom-Ion Mixtures</i>
2:20	PHD presentation – Abhir Mehrotra <i>How wrong is too wrong: A numerical study on the relevance of positional memory in the generalized Langevin equation</i>
2:40	PHD presentation – Nishtha Lakkhanpal <i>A new setup for Free Electron Laser based photoelectron spectroscopy</i>
3:00	Coffee Break
3:30	Lab Tours
4:00	PI Meeting <i>MMR 1, Westbuilding</i>
6:00	Welcome Evening <i>Common Room, Physics Highrise</i>

Tuesday, July 28, 2026

Lecture Hall I, Physics Highrise

	Chair: Tanja Schilling
9:00	PI Lecture – Edward Grant <i>Emergent Constraints and Collective Dynamics in a Molecular Ultracold Plasma</i>
10:00	PostDoc presentation – Ioannis Makos <i>Entanglement in Photoionization Reveals the Effect of Ionic Coupling in Attosecond Time Delays</i>
10:30	Coffee Break
11:00	PHD presentation – Farouk Albalacy <i>Many-body state tomography in a three-mode mach-zehnder interferometer</i>
11:20	PHD presentation – Aleksandr Demianenko <i>Helium cluster-isolation spectroscopy of quinacridone</i>
11:40	PHD presentation – Kaleb Julius Strahringer <i>Helium Nanodroplet Isolation Spectroscopy of Quinacridone and its Microsolvation Complexes</i>
12:00	Lunch Break
	Chair: Alessandra Colla
2:00	PHD presentation – Joachim Siemund <i>Quantum statistics on atom-ion Feshbach resonances</i>
2:20	PHD presentation – Qianqian Zhang <i>Generation of Slow Hydrogen Atomic Beam</i>
2:40	PHD presentation – Steve Takouan Tchounga <i>Angle-resolved photoelectron spectroscopy of Gold clusters</i>
3:00	Coffee Break
3:30	PAC Meetings
3:30	Lab Tours
5:00	Poster Session Foyer Lecture Hall I
7:00	Free Evening

Wednesday, July 29, 2026

Lecture Hall I, Physics Highrise

	Chair: Frank Stienkemeier
9:00	PI Lecture – Jale Schneider <i>The journey of silicon from ingot to photovoltaic module</i>
10:00	PostDoc presentation – Pascal Pessier <i>Photo-Induced Dynamics of Bridged Azobenzenes in a Molecular Beam</i>
10:30	Coffee Break
11:00	PHD presentation – Nils-Oliver Schütz <i>Generation of broad-bandwidth deep ultraviolet pulses with achromatic second harmonic generation</i>
11:20	PHD presentation – Felix Selz <i>Simple and efficient temporal compression scheme of a high-power frequency-doubled Yb laser</i>
11:40	PHD presentation – Maziyar Kazemi <i>In search of superconductivity in Niobium clusters</i>
12:00	Lunch Break
2:00	PAC Meetings
6:00	Free evening
7:00	PI Dinner at Oma's Küche, Hildastraße 66, 79102 Freiburg

Thursday, July 30, 2026

Lecture Hall I, Physics Highrise

	Chair: Tobias Schätz
9:00	PI Lecture – Takamasa Momose <i>Hydrogen/Antihydrogen Spectroscopy and Laser Cooling</i>
10:00	PHD presentation – Benjamin Steiner <i>Attosecond time delays in the Ar dimer</i>
10:30	Coffee Break
11:00	PHD presentation – Grigorios Bolougiannis – cancelled - <i>From Nonlinear Absorption to Ablation: Towards Predictive Ultrashort Pulse Laser Processing of Transparent Materials for Photovoltaics</i>
11:20	PHD presentation – Anutthama Alape <i>Development and Optimization of a Home-Built Multipass Cell, High-Harmonic Generation Setup, and Ultrafast Pulse Autocorrelator</i>
11:40	PHD presentation – Brendan Wouterlood <i>Local and Non-Local Double Ionisation of Micro-Solvated Nucleobases</i>
12:00	Lunch Break
	Chair: Sebastian Hartweg
2:00	PHD presentation – Linda Zeng <i>Asymmetric Photolysis of Valine in Parahydrogen Crystals</i>
2:20	PHD presentation – Sitanath Mondal <i>Study of dissociative single and double ionization of pyridine and thymine using coincidence spectroscopy</i>
2:40	PHD presentation – Merline Cherukarathadathil Ulahannan <i>Design for a Monochromatic, High-Repetition-Rate XUV Beamline for Time-Resolved Photoelectron–Photoion Coincidence Spectroscopy</i>
3:00	Coffee Break
3:30	Lab Tours & PAC Meetings
6:00	Conference Dinner at Caritas Tagungszentrum, Wintererstr. 17-19, 79104 Freiburg
7:00	After Dinner Talk – Marc Vrakking <i>Attosecond Science in the Age of Entanglement</i> at Caritas Tagungszentrum, Wintererstr. 17-19, 79104 Freiburg

Friday, July 31, 2026

Lecture Hall I, Physics Highrise

	Chair: Giuseppe Sansone
9:00	PI Lecture – Tanja Schilling <i>Why Life Is Hot</i>
10:00	PHD presentation – Karin Thalmann <i>Triplet-triplet annihilation upconversion in covalently coupled acene dimers</i>
10:30	Coffee Break
11:00	PHD presentation – Lotar Kurti <i>Novel Apparatus for Synchrotron X-ray Photoelectron Spectroscopy of Size-Selected Gas-Phase Clusters</i>
11:20	PHD presentation – Frederike Dörr <i>Stroboscopic Ramsey Spectroscopy for Phase-Space Characterisation of Trapped-Ion Motion</i>
11:40	Final Remarks – Giuseppe Sansone
12:00	Lunch Break
2:00	PAC Meetings
3:00	Coffee Break
3:30	Lab Tours & PAC Meetings
6:00	Free evening

Saturday, August 1, 2026

Excursion: **“The Three Lakes” Hike, Orbey**, Alsace (France)

Start at 8:00 a.m., Institute of Physics, Hermann-Herder-Str. 3

Return around 5:00 p.m.

PAC Meetings

Seminar Rooms II & III, located right next to Lecture Hall II, have been reserved for the PAC meetings—you're also welcome to use the PI offices or the Physics Garden instead.

Tuesday, July 28

- 3:30 – 4:15 p.m. **Alexander Döring** – Tobias Schätz – Kirk Madison
- 3:30 – 4:15 p.m. **Qianqian Zhang** – Takamasa Momose – Frank Stienkemeier
- 3:30 – 4:15 p.m. **Marvin Schmoll** – Giuseppe Sansone – Bernd v. Issendorff
- 4:15 – 5:00 p.m. **Joachim Siemund** – Tobias Schätz – Kirk Madison
- 4:15 – 5:00 p.m. **Linda Zeng** – Takamasa Momose – Frank Stienkemeier
- 4:15 – 5:00 p.m. **Nishtha Lakhanpal** – Bernd v. Issendorff – Giuseppe Sansone

Wednesday, July 29

- 2:00 – 2:45 p.m. **Aleksandr Demianenko** – Frank Stienkemeier – Bernd v. Issendorff
- 2:00 – 2:45 p.m. **Frederike Dörr** – Tobias Schätz – Kirk Madison
- 2:45 – 3:15 p.m. **Maziyar Kazemi** – Bernd v. Issendorff – Frank Stienkemeier
- 2:45 – 3:15 p.m. **Felix Selz** – Lukas Bruder – Giuseppe Sansone
- 3:30 – 4:15 p.m. **Nils-Oliver Schütz** – Lukas Bruder – Frank Stienkemeier
- 3:30 – 4:15 p.m. **Merline Cherukarathadathil Ulahannan** – Sebastian Hartweg – Giuseppe Sansone
- 4:15 – 5:00 p.m. **Brendan Wouterlood** – Frank Stienkemeier – Takamasa Momose

Thursday, July 30

- 3:30 – 4:15 p.m. **Grigorios Boulogiannis** – Jale Schneider – Giuseppe Sansone
- 3:30 – 4:15 p.m. **Benjamin Steiner** – Giuseppe Sansone – Lukas Bruder

PI-TALKS

ABSTRACTS

(in alphabetical order)

Thermodynamics of arbitrary open quantum systems: from average quantities to fluctuation relations

Allesandra Colla

Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

We present a framework for defining thermodynamic quantities in open quantum systems strongly coupled to non-Markovian environments. It relies on an exact time-local master equation for the system's evolution, circumventing the need to explicitly characterize the environment. Extending this beyond average quantities, we investigate thermodynamic fluctuations by proposing a two-point measurement scheme based on dynamics-dependent observables. The approach allows for the derivation of exact equalities for fluctuations of path-dependent quantities like work and heat, and enables the isolation of correction factors to Jarzynski's equality, all while requiring access only to the system's degrees of freedom.

Emergent Constraints and Collective Dynamics in a Molecular Ultracold Plasma

Amin Allahverdian and Edward Grant

Department of Chemistry, University of British Columbia, Vancouver, BC V6T 1Z3, Canada

Avalanches occur in systems that appear to have little in common, microscopically: epidemics, forest fires, fractures, catalytic reactions, neuronal cascades, Rydberg facilitation, and the spontaneous ionization of dense molecular Rydberg gases. But all these systems share an underlying dynamics in which the stochastic amplification of a rare seed gives way to extinction, saturation, or arrest. Molecular ultracold plasmas provide an unusual setting in which microscopic collision dynamics inseparably link stochastic avalanche growth, long-range Coulomb interactions, molecular dissociation, and arrested many-body relaxation. Dense nitric oxide Rydberg gases undergo Penning ionization and electron-impact avalanche, then evolve to form a long-lived state that resists the relaxation expected of either a cold plasma or a dense molecular Rydberg ensemble. This persistent arrested state is not a simple absorbing configuration of neutral particles. Instead, it contains ions, weakly bound electrons, high- n , high- ℓ Rydberg molecules, exhibiting collective charge confinement. These observations invite questions of theoretical framework. Does plasma evolution best conform to a directed-percolation-like absorbing-state transition, a self-organized critical branching process, a dynamically depleted reaction-diffusion system, or collapse to a prethermalized state? This talk offers a unified conceptual framework for the evolution observed experimentally. We begin with experimentally motivated ionization and recombination kinetics, connect these dynamics to branching processes, reaction/diffusion models with an absorbing-state transition, and a contact process supporting directed percolation. We examine how long-range transport, dynamically generated correlations, angular-momentum mixing, and kinetic arrest demand reasoning beyond those basic constructs. We refer to time-resolved ensemble measurements of avalanche-size distributions and cellular-automaton modelling, which uncover a relation between microscopic reversibility and macroscopic irreversibility, leading to self-organization and a gapped state of arrested relaxation

Hydrogen/Antihydrogen Spectroscopy and Laser Cooling

Takamasa Momose

Department of Chemistry, The University of British Columbia

Spectroscopy of the hydrogen atom has played a central role in the development of modern physics, providing the foundation for quantum mechanics, quantum electrodynamics (QED), and the Standard Model. Today, comparisons between hydrogen and antihydrogen offer one of the most critical tests of CPT symmetry and may provide clues to the long-standing mystery of the apparent absence of antimatter in the universe.

Our group participates in the international ALPHA (Antihydrogen Laser Physics Apparatus) collaboration at CERN, where we develop precision spectroscopy and laser cooling techniques for trapped antihydrogen atoms. Recently, we demonstrated laser cooling of antihydrogen using 121.6 nm vacuum-ultraviolet laser pulses, cooling trapped antihydrogen atoms to temperatures below 10 mK. This achievement significantly enhances the precision of fundamental spectroscopic measurements, including the 1S-2S transition, as well as measurements of the gravitational behavior of antimatter.

The ultimate precision of antihydrogen spectroscopy is intrinsically linked to our ability to characterize hydrogen itself. To address this challenge, we have also initiated a complementary program on trapping laser-cooled hydrogen atoms and performing ultrahigh-precision spectroscopy on hydrogen using similar trapping and laser-cooling techniques. These parallel efforts will provide improved benchmarks for CPT tests while advancing precision atomic spectroscopy more broadly.

In this talk, I will review recent advances in antihydrogen laser cooling and spectroscopy, discuss our new program on ultracold hydrogen spectroscopy, and outline future prospects for ultracold hydrogen and antihydrogen as complementary platforms for precision tests of fundamental physics.

Why Life Is Hot

Tanja Schilling

Institute of Physics, University of Freiburg

Living organisms ubiquitously produce heat. According to biology textbooks, this is necessary to compensate for the loss of entropy caused by biological ordering processes. I.e. to satisfy the Second Law of Thermodynamics, enough heat must be exported from the cell to raise the entropy of the environment to give a net positive entropy change. However, estimates on the change in entropy associated with biological ordering processes such as polymerisation, compartmentalisation, etc. show that these processes make up less than one percent of the total dissipated heat.

We propose a different explanation. The process of evolution by natural selection leads to phenotypes of increasing fitness. For cellular chemical reaction networks, this means optimising a variety of fitness functions such as robustness, precision, or sensitivity to external stimuli. We argue that these diverse goals can be achieved by a versatile, generic mechanism: coupling chemical reaction networks to reservoirs that are strongly out of equilibrium. We show that this mechanism of optimisation comes at the price of significant heat dissipation. Then we demonstrate that the degree of optimality achievable saturates, and that Nature appears to operate near saturation despite high energetic costs. We conclude that 'life is hot' largely because of the need for a versatile mechanism to optimise a variety of fitness functions.

The journey of silicon from ingot to photovoltaic module

Jale Schneider

Fraunhofer Institute for Solar Energy Systems ISE, Heidenhofstr.2, D-79110 Freiburg, Germany

In this talk, I will introduce the long production chain of solar cells starting from wafering to module interconnections. From wafer to functional solar cell; several mechanical, chemical, optical, and heat-induced processes interlock with one another. The wafer is doped with phosphorus or boron to create the essential p-n junction. The surface gets texturized to reduce light reflection. Additional steps include antireflective coating deposition, passivation layers to minimize recombination losses, and screen-printed metallization for front and rear contacts. Each process demands tight environmental control, as even trace contaminants can significantly degrade performance.

A special emphasis will be put on perovskite tandem solar cells, which represent the next frontier in photovoltaic technology. By stacking a perovskite absorber (with tunable bandgaps of 1.5-2.3 eV) atop a silicon bottom cell, theoretical efficiencies exceeding 30% become achievable—beyond the limit of single-junction silicon devices. However, challenges remain, including perovskite stability, and scalable manufacturing. And the mystery remains: how can such a complex device, requiring dozens of high-precision steps and complex facilities, be produced so inexpensively?

After Dinner Talk

Attosecond Science in the Age of Entanglement

Marc J.J. Vrakking

Max-Born Institute (MBI), Berlin

The development of quantum mechanics during the first decades of the 20th century sparked intense discussions about its interpretation in terms of a realistic world-view. In [1], Albert Einstein and co-workers pointed out the consequences of situations where the wave function of a multi-component system cannot be written as a direct product of wave functions describing the individual parts, but rather, describes an entangled state. Quantum mechanics' prediction for entangled systems is that measurements on one part of the composite system determine the properties of other parts of the system that do not take part in the experiment. To Einstein, this prediction was unacceptable, and smelled of "spooky action at a distance" ("spukhafte Fernwirkung") [2]. He concluded that quantum mechanics must be incomplete, and that the results of measurements must be influenced by "hidden variables" not described by the theory. Nearly three decades later, John Bell proposed an experiment to rule out the possible existence of hidden variables [3]. Violations of Bell's inequality were subsequently demonstrated in several experiments (see e.g. [4, 5]), and were recognized by the Nobel Prize in physics in 2022, which was jointly awarded to Alain Aspect, John Clauser and Anton Zeilinger.

Subsequently, in 2023, Pierre Agostini, Anne L'Huillier and Ferenc Krausz received the Nobel Prize for the discovery of High-Harmonic Generation (HHG)[6] and subsequent demonstrations that this technique produces isolated attosecond laser pulses (IAPs) [7] or attosecond pulse trains (APT) [8]. While at first sight these two Nobel Prizes have little in common, they are in fact strongly connected. The attosecond pulses that are produced by HHG have photon energies in the extreme-ultraviolet (XUV) part of the spectrum. These photon energies exceed the binding energies of any compound (atom, molecule, liquid or solid) that may be exposed to the attosecond pulses, leading to ionization. In its simplest form, this leads to the formation of a bi-partite quantum system consisting of an ion and a photoelectron, which are entangled if their wavefunction cannot be written as a single direct product of ion and photoelectron wavefunctions. In my talk I will show how entanglement between the ions and the photoelectrons formed by attosecond ionization leads to measurable consequences, and how the properties of attosecond pulses can be tailored to control the degree of entanglement [9-11].

1. Einstein, A., B. Podolsky, and N. Rosen, *Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?* Physical Review, 1935. **47**(10): p. 777-780.
2. Einstein, A., H. Born, and M. Born, *The Born-Einstein letters: correspondence between Albert Einstein and Max and Hedwig Born from 1916-1955*. 1971, [London]: Macmillan. xi, 240 p., 5 plates.
3. Bell, J.S., *On the Einstein Podolsky Rosen paradox*. Physics Physique Fizika, 1964. **1**(3): p. 195-200.
4. Freedman, S.J. and J.F. Clauser, *Experimental Test of Local Hidden-Variable Theories*. Physical Review Letters, 1972. **28**(14): p. 938-941.
5. Aspect, A., J. Dalibard, and G. Roger, *Experimental Test of Bell's Inequalities Using Time-Varying Analyzers*. Physical Review Letters, 1982. **49**(25): p. 1804-1807.
6. Ferray, M., et al., *Multiple-harmonic conversion of 1064 nm radiation in rare gases*. Journal of Physics B: Atomic, Molecular and Optical Physics, 1988. **21**(3): p. L31.

7. Hentschel, M., et al., *Attosecond metrology*. Nature, 2001. **414**(6863): p. 509.
8. Paul, P.M., et al., *Observation of a train of attosecond pulses from high harmonic generation*. Science, 2001. **292**(5522): p. 1689-1692.
9. Vrakking, M.J.J., *Control of Attosecond Entanglement and Coherence*. Physical Review Letters, 2021. **126**(11): p. 113203.
10. Koll, L.-M., et al., *Experimental Control of Quantum-Mechanical Entanglement in an Attosecond Pump-Probe Experiment*. Physical Review Letters, 2022. **128**(4): p. 043201.
11. Koll, L.M., et al., *Entanglement and electronic coherence in attosecond molecular photoionization*. Nature, 2026. **652**(8108): p. 82-88.

ABSTRACTS

(in alphabetical order)

Development and Optimization of a Home-Built Multipass Cell, High-Harmonic Generation Setup, and Ultrafast Pulse Autocorrelator

Anutthama Alape

Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

This project focuses on the development and optimization of a home-built ultrafast laser platform comprising a gas-filled multipass cell for nonlinear pulse compression, a gas-cell-based high-harmonic generation (HHG) beamline, and an ultrafast pulse autocorrelator. The work involves the integration of ultrafast laser systems, vacuum and gas-delivery infrastructure, XUV detection, and pulse diagnostics to establish a reliable experimental platform for strong-field laser–matter interactions. Ongoing optimization of parameters such as pulse duration, gas target conditions, and beamline alignment is aimed at improving harmonic generation efficiency while enabling the generation and characterization of ultrashort laser pulses. This platform provides the foundation for future research in ultrafast optics, attosecond science, and XUV spectroscopy.

Many-body state tomography in a three-mode mach-zehnder interferometer

Farouk Albalacy

Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

We study the interplay of single- and many-body interference effects by injecting one quantum object per port in a generalized Mach-Zehnder (GMZ) interferometer with three ports. Single-body interference is controlled by the phase shifts between the paths of the interferometer. The effect of bosonic many-body interference is singled out by tuning the individual constituents' mutual distinguishabilities through their internal states. We then formulate a tomographic reconstruction protocol to infer the internal state parameters of the injected many-body state from the counting statistics on output of the GMZ. In addition, we determine which values of the phase shifts allow for a reliable estimation of the internal parameters in the presence of noise in the counting statistics.

From Nonlinear Absorption to Ablation: Towards Predictive Ultrashort Pulse Laser Processing of Transparent Materials for Photovoltaics

Grigorios Boulogiannis

Fraunhofer Institute for Solar Energy Systems ISE, Heidenhofstr.2, D-79110 Freiburg, Germany

Ultrashort pulse (USP) laser processing enables precise structuring, surface functionalization, and targeted modification of transparent and semi-transparent materials central to next-generation photovoltaics, including transparent conductive oxides, wide-bandgap semiconductors such as 4H-SiC and GaN, transparent dielectrics, and perovskites. Predictive control of these processes, however, remains challenging: analytical models established for metal processing do not readily transfer to materials in which energy deposition is governed by nonlinear absorption mechanisms such as multiphoton absorption and Kerr-type nonlinearities.

This work aims to investigate the complete interaction chain, from nonlinear optical absorption through electron-lattice energy transfer and phonon excitation to heat accumulation, ablation, and plasma formation. The aim is to establish analytical scaling relations that link laser parameters (wavelength, pulse duration, fluence, repetition rate) to temperature-dependent linear and nonlinear material properties.

First results from two complementary experimental approaches are presented. Using a fully automated, in-house-built Z-scan setup covering wavelengths from 310 to 2600 nm and substrate temperatures up to 1500 °C, the nonlinear refractive index n_2 and the 4-photon absorption coefficient of soda-lime glass were determined. In parallel, USP processing of 4H-SiC was studied: ablation thresholds were mapped as a function of laser parameters, and dicing experiments reveal how these parameters govern achievable dicing speed as well as kerf geometry and cut quality. An outlook on upcoming temperature-dependent

measurements on PV-relevant materials and the validation of scaling relations across material classes concludes the contribution.

Helium cluster-isolation spectroscopy of quinacridone

Aleksandr Demianenko, Kaleb Strahringer, Sebastian Hartweg, and Frank Stienkemeier

Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Organic chromophores are essential components of organic solar cells, field-effect transistors, light-emitting diodes, and supramolecular organic semiconductors. Their electronic and vibrational energy levels play a central role in determining collective molecular behaviors, including charge transport, exciton motion, and self-assembly.

In this talk, I will present helium cluster isolation spectroscopy to study the chromophore quinacridone. Although mostly known as an organic dye, quinacridone also shows highly interesting properties in its aggregation. Since it is a prochiral molecule it can be seen as a chiral object when attached to surfaces, where it can either aggregate in homochiral linear chains or more complex heterochiral structures.

The superfluid helium environment can be seen as isotropic thus allowing the aggregation of quinacridone molecules as non-chiral objects. Additionally, the ultracold temperature of the helium nanodroplets restrict population to vibrational ground states and produces well-resolved spectra for both monomers and oligomers in a minimally perturbing ultracold matrix. By combining a wavelength-tunable nanosecond laser, we obtain high-resolution laser-induced fluorescence spectra. These are presented in comparison with spectra on surfaces and in organic solvents.

The spectra in helium nanodroplets are interpreted by simulating them given the experimentally determined electronic origin and a number of vibrational modes. The analysis shows a main totally symmetrical vibrational mode, a number of higher-frequency modes, and their combination bands. Interestingly, a series of transitions is also observed to the red of the 0_0^0 line. I will discuss the assignment and the possible nature of the red-shifted peaks in detail. Doping-temperature dependent measurements are done to identify oligomer contributions in the spectrum. Finally, a quinacridone derivative – fluorinated quinacridone – has been also measured in helium nanodroplets, and compared to the non-modified molecule.

Overall, this work gives insight to electronic and vibrational transitions in one of the most popular organic dyes, with theoretical treatment of the experimental data well on its way.

Interaction-Induced Dynamics in Ultracold Atom-Ion Mixtures

Alexander Döring

Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

We investigate quantum atom-ion scattering in the s-wave regime using a hybrid apparatus comprising a single $^{138}\text{Ba}^+$ ion in a linear Paul trap and a ^6Li Fermi gas. The atomic sample is prepared via sequential cooling in a magneto-optical trap (MOT) and a compressed MOT (cMOT) before confinement in a crossed optical dipole trap (xODT). Inelastic collision rates are manipulated via magnetically tunable Feshbach resonances. To overcome micromotion-induced energy limits in RF traps, we use radial displacement fields E_{dc} to control the ion's excess kinetic energy ΔE_{ion} . This technique, calibrated via molecular dynamics (MD) simulations, allows for the systematic tuning of collision energies over four orders of magnitude, from the classical $E^{-3/4}$ scaling regime to below the s-wave limit $E_s = 8.8 \mu\text{K} \cdot k_B$.

We present a characterization of the Feshbach spectrum between 240 G and 340 G with an average resonance density of $0.58(1) \text{ G}^{-1}$, utilizing fluorescence-based detection of ion survival probability P_{surv} . Technical emphasis is placed on the manipulation of the substructure of individual three-body resonances. We demonstrate that the resonance position, width, and amplitude are modulated by the external fields and the ion's driven motion. These techniques enable high-speed interaction control, a prerequisite for future many-body quantum simulations.

Stroboscopic Ramsey Spectroscopy for Phase-Space Characterisation of Trapped-Ion Motion

Frederike Dörr

Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

We introduce a stroboscopic Ramsey spectroscopy technique that probes the phase-space dynamics of a single trapped ion via Doppler-sensitive interrogation. By synchronising short interrogation pulses with the ion's oscillation, the accumulated Ramsey phase becomes sensitive to the instantaneous Doppler shift — and hence the ion's velocity — at a chosen phase of its trajectory; the ion thereby acts as a sensitive probe of its own dynamics. The finite, sub-microsecond pulse duration sets the velocity resolution: shorter pulses resolve fine spectral structures that longer pulses average out, so the reconstruction sharpens directly as the pulses are shortened. Accumulating the signal coherently over $\gtrsim 100$ oscillation periods at MHz motional frequencies yields spectra from which we reconstruct the phase-space trajectory. For coherently displaced motional states we demonstrate reconstruction of the trajectory, position and momentum-dependent phase evolution, and a relation linking the measured spectrum to the ion's dynamics. The scheme extends naturally to a broad class of periodic motional dynamics.

A Lindblad master equation for twisted photons in a turbulent atmosphere

Tim Ehret

Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

The propagation of photonic spatial modes carrying orbital angular momentum (OAM) through a turbulent atmosphere is an active area of research, both from a fundamental perspective and for practical applications. A standard approach to account for atmospheric effects on spatial modes is based on the stochastic parabolic equation [1] and the numerical multiple phase screen method derived therefrom. Notwithstanding the success of these approaches, a fully quantum treatment of the propagation of twisted photons through turbulence, taking full advantage of the open quantum system toolbox, may pave the way for a much more efficient treatment of the problem. However, until recently, this had yet to be realized. In the present contribution, we derive a GKLS master equation for the disorder-averaged density operator of single photons populating Laguerre-Gauss (LG) modes that are phase-distorted by turbulence. This equation relies on a mapping between open and disordered quantum systems [2], which we here generalize to twisted photons in Kolmogorov turbulence to analyze crosstalk in the atmosphere. We present numerical results that reproduce established features of the crosstalk matrix of LG photons and derive an entanglement decay law for a maximally entangled photon pair that is consistent with known results [3].

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In search of superconductivity in Niobium clusters

Mazyar Kazemi

Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Among the superconducting materials, Nb stands out due to its high critical temperature and is often used as a model system, to investigate superconductivity-related physics. The question arises at what size Nb clusters will exhibit properties related to superconductivity, namely Cooper pair formation. Some hints for this to happen already at small sizes have been found by de Heer and coworkers [1]. We have measured photoelectron spectroscopy of size -selected Nb clusters in similar size ranges, with temperatures between 3.9-50 K in the gas phase, employing a recently developed photoelectron magnetic bottle spectrometer with a resolution of $\Delta E/E = 0.2\%$. Vibrationally resolved spectra have been obtained for several sizes, but no direct evidence for unusual temperature effects yet.

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Novel Apparatus for Synchrotron X-ray Photoelectron Spectroscopy of Size-Selected Gas-Phase Clusters

Lotar Kurti¹, Phillip Stöcks¹, Fabian Bär¹, Lukas Weise¹, Bernd von Issendorff¹

¹ *Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

A newly developed apparatus enables X-ray photoelectron spectroscopy on mass-selected cluster ions at synchrotrons. The heart of this system is a liquid nitrogen-cooled linear Paul trap, where stored cluster ions interact with synchrotron radiation. The emitted electrons are guided by a specially designed magnetic field into a Hemispherical Energy Analyzer, where the photoelectron spectra are recorded. Clusters are produced in a magnetron cluster source, mass-selected using a quadrupole mass spectrometer, and then introduced into the linear ion trap. This setup will allow for element-specific binding energy measurements of core levels and hence detailed insights into the chemical bonding of pure and mixed metal and semiconductor clusters. In this contribution, we present the current status of the new apparatus and some initial commissioning results. We show that the electron optical path has been successfully tested by imaging electrons created by the ionization of ambient air on the MCP phosphor screen, demonstrating the efficiency of the magnetic guiding system. [1]

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A new setup for Free Electron Laser based photoelectron spectroscopy

Nishtha Lakhanpal

Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Clusters serve as ideal model systems for examining fundamental phenomena such as multi-particle quantum dynamics, phase transitions, and strong field effects. A new setup for photoelectron spectroscopy is currently under construction to investigate size-selected, deeply cold clusters, with a focus on characterizing ultrafast electronic processes. The constructed parts of the machine include a deflector, a radiofrequency (RF) quadrupole mass selector, a cryogenic RF ion trap, and an optimized accelerator unit. Prior to the design phase, various simulations were performed using SIMION software to determine the optimal ion trajectory. The setup will enable the exploitation of the huge potential of FELs for photoelectron spectroscopy studies, utilizing their high intensity and the ability to perform high resolution, time-resolved, two-colour pump-probe experiments to characterize ultrafast dynamics in nanoscale matter.

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

Ioannis Makos¹, David Busto^{1,2}, Jakub Benda³, Dominik Ertel¹, Benjamin Steiner¹, Barbara Merzuk¹, Fabio Frassetto⁴, Luca Poletto⁴, Claus Dieter Schröter⁵, Thomas Pfeifer⁵, Robert Moshhammer⁵, Serguei Patchkovskii⁶, Van-Hung Hoang⁷, Uwe Thumm⁷, Zdeněk Mašín³, and Giuseppe Sansone^{1,8}

¹ *Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

² *Department of Physics, Lund University, SE-221 00 Lund, Sweden*

³ *Institute of Theoretical Physics, Charles University, Prague 8, Czech Republic*

⁴ *Istituto di Fotonica e Nanotecnologie, CNR, 35131 Padova, Italy*

⁵ *Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany*

⁶ *Max Born Institut, D-12489 Berlin, Germany*

⁷ *J. R. Macdonald Laboratory, Kansas State University, Manhattan, Kansas 66506, USA*

⁸ *Freiburg Institute for Advanced Studies (FRIAS),*

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

In molecules, however, the IR field can induce polarization of the ion. In CO₂, this corresponds to the dipole coupling between B ²Σ_u⁺ and C ²Σ_g⁺ cationic states. This extends the conventional two-path interference picture of the RABBIT technique, with an additional pathway arising [5, 6]. The interference between these three pathways introduces a measurable additional time delay in photoelectron emission associated with the B ²Σ_u⁺ cationic state. The observed effect, consistent with theoretical predictions using a stationary multiphoton molecular R-matrix approach [5], is not mediated by the Coulomb interaction between the ion and the photoelectron but depends on the degree of entanglement of the reduced density matrix of the ionic subsystem conditioned on the energy absorbed from the harmonic 2q+1 [7]. Furthermore, looking into the dissociative channels and measuring in coincidence with O⁺, the same ionic coupling leads to a pronounced phase jump, close to a π phase shift, in the photoelectron wavepacket [8].

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[8] I. Makos *et al.*, arXiv:2604.23441 (2026).

How wrong is too wrong: A numerical study on the relevance of positional memory in the generalized Langevin equation

Abhir Mehrotra

Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

If a generalized Langevin equation contains a potential of mean force, it cannot at the same time contain a linear memory kernel and a fluctuating force that obeys a second fluctuation dissipation theorem in the sense of Kubo, and be exact. As modelers often prefer to use generalized Langevin equations that have the first three properties, one needs to ask how close the model dynamics is to the dynamics of the underlying microscopic system.

Here, we test this by analyzing a simple model system in which the potential of mean force can be well approximated by a polynomial of low order. The exact generalized Langevin equation of this model contains memory terms in addition to the linear one. Further, we show that these additional terms, at least for the model system regarded in this article, are important for the dynamics and cannot be neglected if one intends to model core aspects of the underlying system correctly.

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

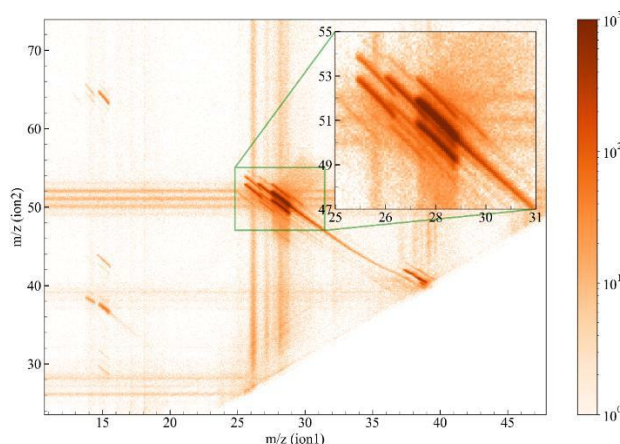
Sitanath Mondal¹, Brendan Wouterlood¹, Gustavo A. Garcia², Laurent Nahon², Frank Stienkemeier¹, Sebastian Hartweg¹

¹ *Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

² *Desirs Beamline, Synchrotron Soleil, St. Aubin, France*

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

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



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Photo-Induced Dynamics of Bridged Azobenzenes in a Molecular Beam

Pascal Pessier, Felix Selz, Nils-Oliver Schütz, Leonie-Katharina Werner, Jo Schropp and Lukas Bruder

Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Bridged azobenzenes have drawn considerable attention in the last decade due to their superior photochemical properties compared to conventional azobenzene (AB). The bridged derivatives exhibit higher isomerization yields and bi-directional switching abilities upon irradiation in the visible region of the electromagnetic spectrum [1]. Examples for prototypical molecules are the $-C_2H_4-$ bridged diazocine (Dz) [2] and the $-CH_2-$ bridged diazepine (Dzp). The higher ring strain in the Dzp molecule suggests a consecutive reaction mechanism involving a transient saddlepoint, consisting of first an ultrafast unfolding motion and second a torsional motion. However, this proposed isomerization mechanism lacks so far clear experimental evidence.

We conducted a beam time at ELI Beamlines Prague with the premise to elucidate this consecutive isomerization mechanism using the Legend-HHG-MAC beamline. A systematic study of three different Dzp molecules, plain Dzp and two halogenated derivatives, was proposed. First results and limitations of this beamtime will be presented. In the end, an outlook on the experimental setup of the MULTIPLEX project to finalize this study will conclude this talk.

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Trapping Ammonia Molecules Using a Fabry-Perot MW Cavity

Hugh Gao, Manish Vashishta, Pavle Djuricanin, and Takamasa Momose Amirhossein Rashidi

Department of Chemistry, The University of British Columbia, Canada

This project aims to trap pre-decelerated ammonia molecules in a Fabry-Perot cavity. This approach relies on the AC-Stark effect of the microwaves on the rotational energy levels of ammonia. Trapping can be achieved by using standing microwaves with a frequency close to the inversion splitting at the vibrational ground state of ammonia (0.79 cm^{-1})

This approach provides a larger trap volume and a higher trap depth with similar input power compared to DC traps which makes the use of an AC-Stark cavity desirable for trapping ammonia (and several other polar molecules).

To trap a sufficient number of molecules, first we need to lower down their temperature. The process begins with a supersonic expansion into a vacuum through a pulsed nozzle and an orifice acting as a collimator which produce a molecular beam as cold as a few kelvins. The resulting supersonic molecular beam is too fast for trapping. To fix that, we use a DC-Stark decelerator which consists of 180 electrode pairs alongside the beam propagation axis which under right operation can reduce the molecular beam velocity down to 20 m/s . Previously, we have made and tested a superconducting Fabry-Perot microwave cavity as the trap unit and our recent focus has been on deceleration patterns and minimizing the molecular beam velocity while keeping the number density high enough for detection and further experiments. Our latest work and progress on deceleration and superconducting microwave cavity trap will be discussed.

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Two-sideband RABBITT

M. Schmoll¹, M. Jahanzeb¹, S. Majoni¹, P. Weizel¹, R. N. Shah¹, K. Hall¹, C. Manzoni² and G. Sansone¹

¹ *Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

² *Institute for Photonics and Nanotechnology - CNR, Piazza Leonardo da Vinci 32, 20133 Milano, Italy*

Over recent years it has become possible to measure the phase shifts induced by photoionization of atoms and molecules with increasing precision. One of the most common methods to achieve this is RABBITT (reconstruction of attosecond beating by interference of two-photon transitions), which relies on ionization by an extreme ultraviolet (XUV) frequency comb and the interaction of the released electron with an infrared (IR) probe field. If the IR photon energy is half the comb spacing of the XUV frequencies, as is typically achieved by using HHG (high order harmonic generation) to generate the XUV comb, sidebands emerge in the photoelectron spectrum, which oscillate with the XUV-IR delay. The phase of these oscillations gives access to the Wigner phase experienced during photoionization.

However the IR interaction also has an influence on the resulting phase. In the asymptotic approximation one can view this as an additional continuum-continuum-Phase, which can mathematically be separated from the Wigner Phase [1].

In this contribution we will present a novel setup where the IR energy is shifted to a third of the XUV comb spacing using an Optical Parametric Amplifier (OPA) resulting in sideband pairs. Comparing the phases of two neighboring sidebands allows us to check for the limits of the asymptotic approximation.

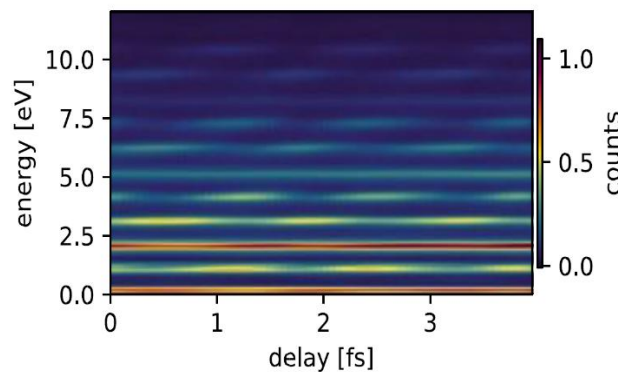


Figure 1: Two-sideband RABBITT spectrogram showing the photoelectron spectrum of Helium as a function of XUV-IR delay.

We will present the setup used to acquire these scans with a focus on the active delay stabilization between pump and probe reaching stability better than 50 as in two different modes of operation [2]. We will also show the measured sideband oscillation as a function of both carrier-envelope-phase (CEP) and delay and conclude with a first analysis hinting at the breakdown of the asymptotic approximation.

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Generation of broad-bandwidth deep ultraviolet pulses with achromatic second harmonic generation

Nils-Oliver Schütz, Lukas Bruder, Ferdinand Bergmeier, and Ulrich Bangert

Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

The generation of deep ultraviolet optical pulses featuring broad spectral bandwidth and short pulse durations is a challenging task, especially when using high repetition rate ($> 100\text{kHz}$) laser systems that provide low pulse energies to drive the nonlinear conversion processes. We present a scheme based on second harmonic generation of the output of a non-collinear optical parametric amplifier. To increase the bandwidth and efficiency of the second harmonic generation we employ achromatic phase matching [1]. Through ray-tracing simulations, the impact of different geometrical arrangements of the setup on the compression of the UV pulses was investigated. The results, together with the characterization of the UV pulses, are presented.

[1] P. Baum, S. Lochbrunner, and E. Riedle, Opt. Lett. 29, 1686 (2004)

Simple and efficient temporal compression scheme of a high-power frequency-doubled Yb laser.

Felix Selz¹, Ulrich Bangert¹, Pascal Pessier¹, Nils-Oliver Schütz¹, Gaspard Beaufort², Anne-Lise Viotti², Lukas Bruder¹

¹*Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

²*Department of Physics, Lund University, P.O. Box 118, SE-22100 Lund, Sweden*

Producing pulses that are only a few-tens of femtoseconds long is essential for many emerging ultrafast applications, such as high-harmonic generation, time-resolved spectroscopy or resonant-dispersive-wave emission. The rapid rise of ytterbium-based laser systems, driven by their high average power, high repetition rates and excellent low-noise characteristics, has created a growing need for post-compression techniques for the typically >200 fs-long fundamental laser pulses. Moreover, there is an increasing demand to produce short pulses at the second harmonic output of the Yb-lasers around 515 nm. The shorter wavelength is advantageous, *e.g.*, for high-flux extreme ultraviolet laser sources [1] or few-cycle deep ultraviolet pulse generation [2].

In our work, we demonstrate the highly efficient compression of a frequency-doubled Yb-laser at 518 nm. This compression is achieved by exploiting self-phase modulation of the frequency-doubled fundamental in a pressured argon gas tube and a single-pass transmission-grating compressor. With this setup, we preserve > 90 % of the initial 518 nm pulse energy and 50 % of the fundamental

1036 nm pulse energy, obtaining sub-35 fs pulses (eight-fold compression). The compression factor can be readily tuned by adjusting the gas pressure and the grating compressor, providing a flexible setup for various applications.

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Quantum statistics on atom-ion Feshbach resonances

Joachim Siemund¹, Fabian Thielemann¹, Jonathan Grieshaber¹, Wei Wu¹, Patrick Mullan¹, Panagiotis Giannakeas², Krzysztof Jachymski³, and Tobias Schätz¹

¹*Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

²*Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany*

³*Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland*

Hybrid atom–ion systems combine the precise control of a single radio-frequency-trapped atomic ion with the rich few- to many-body phenomena of ultracold degenerate quantum gases trapped in light fields. In these systems, long-range atom–ion interactions can be enhanced via Feshbach resonances, enabling access to regimes where three-body recombination dominates the dynamics. We combine a single $^{138}\text{Ba}^+$ ion with a two-component Fermi gas of ^6Li near an atom–ion Feshbach resonance, enabling a direct comparison of recombination involving identical and distinguishable fermions. By tuning the spin composition while keeping the total density and temperature fixed, we observe a suppression of recombination involving identical fermions. The observations are consistent with theoretical predictions, identifying fermionic exchange symmetry as the dominant origin of this suppression. Our work establishes atom–ion systems as a platform for controlling three-body collisions via quantum statistics and demonstrates that exchange-symmetry effects remain robust even under thermal averaging, highlighting the potential of a single trapped ion as a local probe of many-body quantum statistics.

Attosecond time delays in the Ar dimer

Benjamin Steiner¹, I. Makos¹, S. Discher¹, K. Kumar¹, S. Majoni¹, B. Merzuk¹, N. Diehl², N. M. Novikovskiy², Ph. V. Demekhin² and G. Sansone¹

¹*Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

²*Department of Physics, University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany*

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

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

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

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[9] J. Rist et al., Nat. Commun. 12, 6657 (2021)

Helium Nanodroplet Isolation Spectroscopy of Quinacridone and its Microsolvation Complexes

K. J. Strahringer¹, A. Demianenko¹, F. Stienkemeier¹, and Sebastian Hartweg¹

¹*Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

Organic chromophores with conjugated π -electron systems, efficiently absorb light in a spectral region between near IR and UV, largely determined by the spatial extent of the electronic system. Besides playing a key role in nature, they are utilized in modern technology, with organic solar cells being a notable example, and have recently emerged as candidates for photocatalytic water splitting [1]. One such candidate is quinacridone, a widely used printing pigment that absorbs in the visible region [2].

We use helium nanodroplet isolation spectroscopy to elucidate the vibronic structure of quinacridone molecules. The ultracold inert environment of the helium nanodroplets ensures cooling of the molecules to the vibrational ground state while not altering the vibronic structure significantly [3]. This technique furthermore enables us to form and investigate cold molecular clusters and complexes under controlled conditions. In our experiments we combine these techniques with pulsed dye lasers to obtain vibronic excitation spectra with a resolution below 1 cm^{-1} .

The recorded excitation spectra exhibit an intriguing structure, pointing toward contributions from different tautomers. By varying the experimental doping conditions, different molecular clusters and complexes can be formed and investigated. These include for example hydrogen-bonded molecular dimers and quinacridone–water complexes. The latter are of particular interest for potential photon driven water splitting reactions. Various excitation energy shifts are observed and attributed to complexes. Surprisingly, peaks assigned to tautomers exhibit significantly different behavior upon water co-doping.

The potential formation of dark states and non-radiative relaxation pathways in these complexes will be investigated in future experiments using alternative detection schemes based on the photoionization of excited molecular complexes. A final assignment of the observed spectral features is expected through quantum chemical calculations.

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Angle-resolved photoelectron spectroscopy of Gold clusters

Steve Takouan Tchounga

¹*Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

Angle-resolved spectroscopy provides an important test of the theoretical description of clusters since these spectra carry more information than the bare electron binding energies. Specifically, the anisotropy of photoelectron spectra depends on the angular momentum state [1].

In the experiment cluster anions are produced in a magnetron sputter source, cooled to 7K, and enter a time-of-flight spectrometer for mass selection. Electrons are then detached by linear polarised laser light and projected onto an MCP detector in a velocity map imaging setup.

The presented analysis utilizes the additional information from angle-resolved spectroscopy to gain a better understanding of the electronic structure of the cluster. For Au⁻ 33 an electronic shell closing is expected, leading to the opening of a new shell for Au⁻ 34. The angular momentum character of this new shell is not in accordance with a simple shell model. It also differs from the mixed character as observed for Sodium clusters of the same size [2]. Possible influences of the high-lying d-band are discussed.

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[2] C. Bartels, C. Hock, R. Kuhnen, M. Walter, and B. v. Issendorff, Physical Review A (2013), 88.

Triplet-triplet annihilation upconversion in covalently coupled acene dimers

K. S. Thalmann¹, S. R. Reddy², P. B. Coto³, and M. Thoss¹

¹ *Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

² *Department of Chemistry, School of Chemical Sciences and Pharmacy, Central University of Rajasthan, NH-8, Bandarsindri, Ajmer, 305817 Rajasthan, India*

³ *Nanomaterials and Nanotechnology Research Center (CINN), CSIC-University of Oviedo-Principality of Asturias and Donostia International Physics Center (DIPC), Avda. de la Vega 4-6, 33940 El Entrego, Spain*

Triplet–triplet annihilation upconversion (TTA) is a process transforming two low-energy triplet excitons to a higher-energy excited singlet exciton. Together with its reverse process, singlet fission (SF) [1], TTA belongs to the multiexciton processes which could be utilised in solar cells to increase their efficiency by mitigating thermalization losses [2]. While efficient SF was previously studied in covalently coupled pentacene dimers [3], the interplay between SF and TTA across shorter acene systems remains less understood. In this contribution, we investigate SF and TTA in covalently coupled anthracene and tetracene dimers with two different linkers using a combined technique of ab initio multireference perturbation theory and quantum dynamical simulations based on a linear vibronic coupling Hamiltonian. In detail, we analyse the population transfer between the locally excited states and the multiexcitonic triplet state mediated by charge transfer and doubly excited states. Our results, together with previous calculations on pentacene dimers [3], reveal a clear trend across the acene series. Whereas SF is the most efficient in pentacene dimers, reducing the acene length suppresses SF while it enhances TTA, with the strongest TTA for the anthracene dimers. In contrast, the change in linkers only has a minor effect on the dynamics. Our findings provide valuable insight into the mechanisms of SF and TTA in covalently coupled acenes, guiding the molecular design of materials for next-generation applications.

[1] M. B. Smith, J. Michl, *Chem. Rev.* 110, 6891–6936 (2010).

[2] A. J. Carrod, V. Gray, K. Börjesson, *Energy Environ. Sci.* 15, 4982 (2022).

[3] S. R. Reddy, P. B. Coto, M. Thoss, *J. Phys. Chem. Lett.* 9, 5979–5986 (2018).

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

Merline Cherukarathadathil Ulahannan¹, Ulrich Bangert¹ and Sebastian Hartweg¹

¹*Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

Many molecular level processes, relevant in fundamental science and modern technology occur naturally in a condensed environments. The details of the molecular environment, while crucial for an exact description of the process poses challenges in the experimental and theoretical study of such processes. Molecular clusters and complexes can in some cases be used to study the effect of complex environments, while circumventing some of the challenges posed by larger condensed samples.

Photoelectron photoion coincidence spectroscopy has been demonstrated to provide detailed cluster-size resolved information on various molecular processes and properties. However, such cluster-size resolved experiments, do not routinely extend to ultrafast time-resolved techniques like time-resolved photoelectron spectroscopy. One bottleneck for such measurements is the existence of femtosecond, monochromatized VUV and XUV light sources operating at the high repetition rates necessary for coincidence detections.

We present our plans for an XUV beamline based on high-harmonic generation driven by a high-repetition-rate Yb laser, operating at up to 120 kHz. The beamline will be based on a high harmonic generation (HHG) scheme driven by an Yb laser. The NIR pulses will first be spectrally broadened by self-phase modulation in a gas-filled multipass cell and compressed to pulse durations of ~40 fs. The XUV radiation, generated by HHG of the fundamental (1030 nm) or second harmonic (515 nm) of the driving Laser [1] in a rare gas jet, will be coupled to a single-grating time-preserving monochromator [2]. With a plane diffraction grating in off-plane geometry, the monochromator will enable spectral selection of individual harmonics while minimizing temporal broadening to maintain pulse durations of tens of femtoseconds. In contrast to many existing HHG-based beamlines, we focus on the relatively low photon energy range of 10–20 eV. Using not only the fundamental but also the second harmonic to drive the HHG process provides several advantages. At these photon energies, conversion efficiency can be increased by driving with the second harmonic of the Yb laser while the shorter driving wavelength also simplifies the spectral isolation of individual harmonic orders. The latter allows the use of low-groove-density gratings, further reducing the temporal broadening introduced by the monochromator.

A home-built nonlinear optical parametric amplifier pumped by the same Yb Laser will supply frequency-tunable ultrashort pump pulses in the visible and UV spectral range. This beamline will be used in performing time-resolved XUV photoelectron–photoion coincidence spectroscopy in molecular complexes.

[1] Comby et al., Opt. Express 27, 20383 (2019).

[2] Frassetto et al., Opt. Express 19, 19169 (2011)

Energy transfer processes in molecules and molecular complexes using ultracold rare-gas clusters

Leonie Werner¹, Ulrich Bangert¹, Sebastian Hartweg¹, Yilin Li¹, Arne Morlok¹, Felix Riedel¹, Frank Stienkemeier¹, and Lukas Bruder¹

¹ *Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

Polycyclic aromatic hydrocarbons (PAHs), such as tetracene, are promising materials for organic semiconductor technologies, especially since they support singlet fission processes.

Helium nanodroplet isolation spectroscopy offers a suitable technique to investigate charge transfer and singlet fission processes in well-defined ultracold gas-phase molecular systems. However, a detailed understanding of the interactions between the embedded molecules and the surrounding environment is essential. Combining this cluster isolation technique with time-resolved photoelectron spectroscopy, we establish a powerful approach to probe the influence of different environments on electronic properties and intramolecular dynamics.

At a first step in this direction, we investigated the dynamics of single tetracene molecules dissolved in helium nanodroplets and attached to solid-argon clusters. Our experiments reveal distinct influences of the two environments as well as interaction dynamics upon photoexcitation of the molecule. Understanding these dynamics constitutes an important step towards developing a spectroscopic method capable of identifying singlet fission pathways.

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

Brendan Wouterlood¹, Sitanath Mondal¹, Madhusree Roy-Chowdhury², Gustavo A. Garcia-Macias²,
Laurent Nahon², Frank Stienkemeier¹, Sebastian Hartweg¹

¹*Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

²*Synchrotron SOLEIL, L'Orme des Merisiers, St. Aubin BP 48, 91192 Gif sur Yvette Cedex, France*

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

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

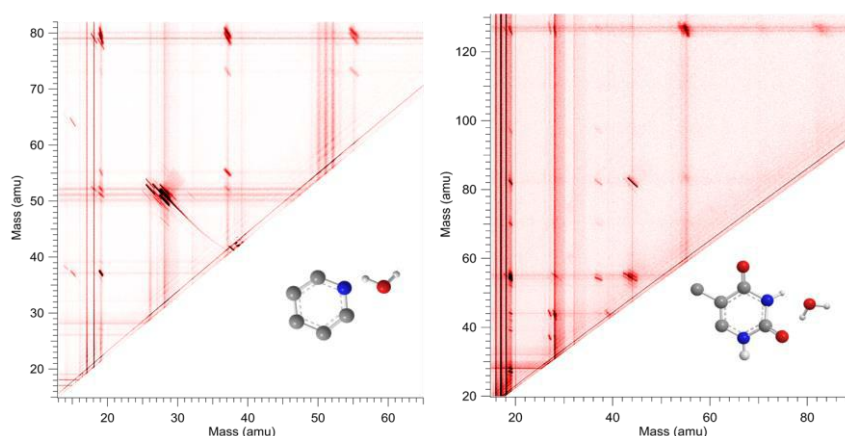


Figure 2: Left (right) ion-ion coincidence map of pyridine (thymine) - water complexes after ionisation by synchrotron radiation at 36 eV.

Asymmetric Photolysis of Valine in Parahydrogen Crystals

Linshan Zeng and Takamasa Momose

The University of British Columbia, CANADA

The origin of biological homochirality may be linked to extraterrestrial environments, where interactions between chiral molecules and polarized photons in interstellar space could have generated an initial enantiomeric imbalance that eventually evolved into the homochirality observed in living systems on Earth. To investigate this possibility, we have studied the asymmetric photolysis of amino acids using parahydrogen matrix-isolation spectroscopy. Parahydrogen matrices are particularly well suited for such studies because their soft quantum crystal nature allows in situ photochemical processes and reactive intermediates to be observed more effectively than in conventional rare gas matrices.

In this work, we investigated the photolysis of valine isolated in a parahydrogen matrix. Under these conditions, several of the most stable conformers of valine can be trapped in their neutral (non-zwitterionic) form, which is expected to be relevant for amino acids in the gas phase under interstellar conditions. UV photolysis of valine at 213 nm produced the HOCO radical, indicating decomposition of the original chiral structure of valine. We also carried out photolysis experiments using circularly polarized UV light. We will discuss the latest results on asymmetric photolysis of valine and their implications for the extraterrestrial origin of homochirality.

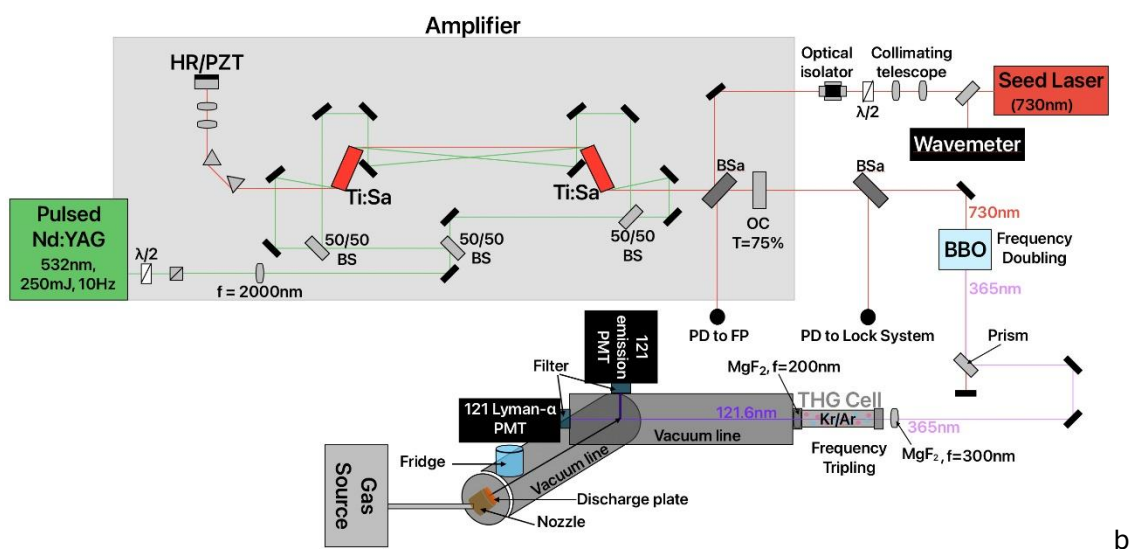
- [1] K. Öberg, *Chem. Rev.* 2016, **116**, **17**, 9631–9663
- [2] N. Kaifu, M. Morimoto, K. Nagane, K. Akabane, T. Iguchi, K. Takagi, *Astrophys. J. Lett.* 1974, **191**, 135-137
- [3] C. Meinert, D. Garcia, J. Topin, *Nat Commun.* 2022, **13**, 502
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Generation of Slow Hydrogen Atomic Beam

Qianqian Zhang and Takamasa Momose

The University of British Columbia, CANADA

We report on the development of a high-density hydrogen, slow atomic beam generated using a pulsed source combined with supersonic expansion, discharge configurations and Zeeman deceleration techniques. A pulsed CRUCS valve was used to produce short and intense gas pulses, while an electric discharge dissociated molecular hydrogen into atomic hydrogen. Different nozzle geometries and discharge configurations were investigated to optimize the atomic beam intensity and stability. After the formation of the atomic beam, a travelling-wave Zeeman decelerator was employed to further reduce the longitudinal velocity of hydrogen atoms through time-dependent magnetic fields. Laser-induced fluorescence (LIF) detection at 121.6 nm was used to characterize the hydrogen atomic beam and monitor the deceleration process. Lyman- α radiation [1] was generated through nonlinear frequency conversion of 730 nm to produce the sixth harmonic [2]. The generated slow hydrogen beam is a promising source for precision spectroscopy, laser cooling, and future studies of fundamental physics.



Graph 1: Schematic of Lyman- α laser system for H source spectroscopy

- [1] Lyman, T. An extension of the spectrum in the extreme ultra-violet. *Nature* **93**, 241 (1914).
[2] Ahmadi, M. et al. Observation of the 1S–2P Lyman-alpha transition in antihydrogen. *Nature* **561**, 211–215 (2018).

List of Participants

PIs & Guest speakers

Bruder, Lukas

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Colla, Alessandra

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Grant, Edward

University of British Columbia – Department of Chemistry – 2036 Main Mall, Vancouver, BC Canada V6T 1Z1

Hartweg, Sebastian

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Madison, Kirk

University of British Columbia – Department of Physics & Astronomy – 325 – 6224 Agricultural Road

Momose, Takamasa

University of British Columbia – Department of Chemistry – 2036 Main Mall, Vancouver, BC Canada V6T 1Z1

Sansone, Giuseppe

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Schätz, Tobias

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Schilling, Tanja

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Schneider, Jale

Fraunhofer Institute for Solar Energy Systems – Heidenhofstraße 2 – 79110 Freiburg

Stienkemeier, Frank

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Thumm, Uwe

Kansas State University – Department of Physics – 212 Cardwell Hall – 1228 N. Martin Luther Jr. Drive, Manhattan, KS 66506-2601

von Issendorff, Bernd

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Vrakking, Marc

Max Born Institute – Max-Born-Straße 2A, 12489 Berlin

Doctoral & Postdoctoral Researchers

Alape, Anutthama

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Albalacy, Farouk

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Boulogiannis, Grigorios

Fraunhofer Institute for Solar Energy Systems – Heidenhofstraße 2 – 79110 Freiburg

Demianenko, Aleksandr

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Discher, Samuel

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Döring, Alexander

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Dörr, Frederike

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Ehret, Tim

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Kazemi, Mazyar

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Kurti, Lotar

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Lakhanpal, Nishtha

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Majoni, Simon

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Makos, Ioannis

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Mehrotra, Abhir

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Mondal, Sitanath

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Noort, Collin

University of British Columbia – Department of Chemistry – 2036 Main Mall, Vancouver, BC Canada V6T 1Z1

Pessier, Pascal

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Schmoll, Marvin

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Schütz, Nils-Oliver

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Schwarz, Kevin

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Selz, Felix

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Siemund, Joachim

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Steiner, Benjamin

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Strahinger, Kaleb Julius

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Takouan Tchounga, Steve

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Thalmann, Karin

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Ulahannan, Merline

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Werner, Leonie

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Wouterlood, Brendan

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Zeng, Linda

University of British Columbia – Department of Chemistry – 2036 Main Mall, Vancouver, BC Canada V6T 1Z1

Zhang, Qianqian

University of British Columbia – Department of Chemistry – 2036 Main Mall, Vancouver, BC Canada
V6T 1Z1

Coordination

Ortolf, Simone

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Querfurth, Josefine

University of Freiburg – Institute of Physics – Hermann-Herder-Straße 3 – 79104 Freiburg

Notes

RTG 2717 Annual Convention 2026						
July 27 to July 31						
University of Freiburg, Germany						
	Monday, July 27	Tuesday, July 28	Wednesday, July 29	Thursday, July 30	Friday, July 31	Saturday, August 1
9:00	Arrival & Welcome	PI Lecture Edward GRANT	PI Lecture Jale SCHNEIDER	PI Lecture Takamasa MOMOSE	PI Lecture Uwe THUMM	Start at 8:00 am Excursion "The Three Lakes" Hike Orbey, Alsace (France)
9:30	PI Lecture					
10:00	Alessandra COLLA	PostDoc presentation Ioannis MAKOS	PostDoc presentation Pascal PESSIER	PHD presentation Benjamin STEINER	PHD presentation Karin THALMANN	
10:30	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break	
11:00	PHD presentation Leonie WERNER	PHD presentation Farouk ALBALACY	PHD presentation Nils SCHÜTZ	PHD presentation Greg BOULOGIANNIS	PHD presentation Lotar KURTI	
11:20	PHD presentation Tim EHRET	Aleksandr DEMIANENKO	PHD presentation Felix SELZ	PHD presentation Anutthama ALAPE	PHD presentation Frederike DÖRR	
11:40	PHD presentation Marvin SCHMOLL	PHD presentation Kaleb STRAHRINGER	PHD presentation Maziyar KAZEMI	PHD presentation Brendan WOUTERLOO	Final Remarks	
12:00	Lunch Break	Lunch Break	Lunch Break	Lunch Break	Lunch Break	
02:00	PHD presentation Alexander DÖRING	PHD presentation Joachim SIEMUND	PAC Meetings	PHD presentation Linda ZENG	PAC Meetings	
02:20	PHD presentation Abhir MEHROTRA	PHD presentation Qianqian ZHANG		PHD presentation Sitanath MONDAL		
02:40	PHD presentation Nishtha LAKHANPAL	PHD presentation Steve Takouan Tchounga		PHD presentation Merline ULAHANNAN		
03:00	Coffee Break	Coffee Break		Coffee Break	Coffee Break	
03:30	Lab Tours	Lab Tours	PAC Meetings	Lab Tours	Lab Tours	
	PI Meeting	PAC Meetings		PAC Meetings	PAC Meetings	
05:00		Poster Session				
06:00	Welcome Evening	Free evening	Free evening	Conference Dinner at Caritas Tagungszentrum	Free evening	
7:00	Common Room		PI Dinner at Oma's Küche	After Dinner Talk Marc VRAKKING		
8:00	Arrival day July 26					Departure day Aug 2

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