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DYNAMICS OF CONTROLLED  
ATOMIC AND MOLECULAR  
SYSTEMS



# **BOOK OF ABSTRACTS**

## ***Annual Convention 2023***

### ***RTG DynCAM***

*Dynamics of Controlled Atomic and Molecular Systems*

**August 21 to August 26, 2023**

University of British Columbia  
Vancouver campus  
Vancouver, CA



## Organisation

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## Financial Support



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## Imprint

RTG 2717 / Dynamics of Controlled Atomic and Molecular Systems

Institute of Physics

University of Freiburg

Hermann-Herder-Straße 3

D - 79104 Freiburg

UBC Faculty of Science

Vancouver Campus

2036 Main Mall

Vancouver, BC Canada V6T 1Z1

## General Information

### Duration

Monday, August 21, 2023, 8:45 am – Friday, August 25, 2023, 10 pm

### Location

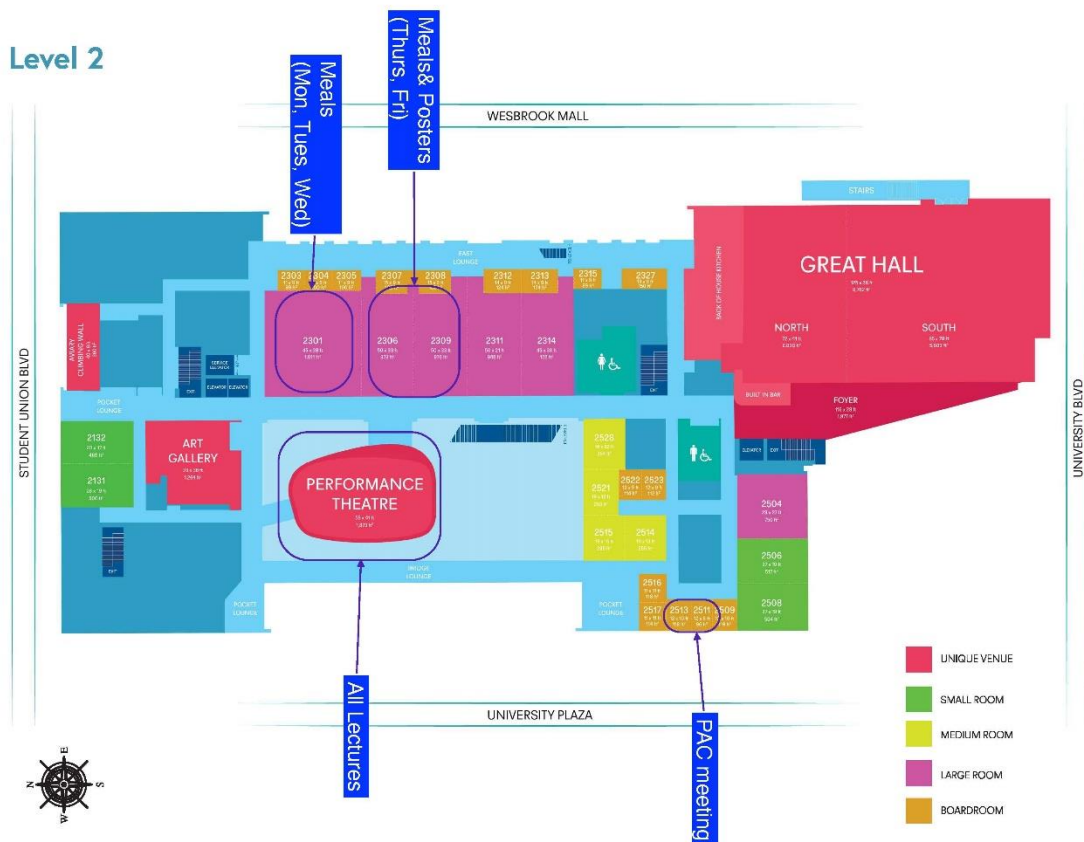
The conference will take place on the UBC campus.

All lectures will be at the Performance Theatre

(2<sup>nd</sup> level of the NEST)

### AMS Student Nest

6133 University Blvd.  
 UBC Campus  
 Vancouver BC, V6T 1Z1





**Accommodation**

We will be housed in the Walter Gage building on the UBC campus, arrival is possible from 3pm.

! The hotel suites include full service housekeeping: Beds made daily, towels changed daily, linens changed weekly. All linens and soap should be included.

! Please find the Walter Gage info sheet with further information on our BSCW server.

Check-in:

**Walter Gage Residence**

Front Desk (4)

5959 Student Union Blvd.  
 Vancouver, B.C. V6T 1K2  
 Tel: 604.822.1020



**WALTER GAGE MAP**

- |                      |  |
|----------------------|--|
| 1. Gage Apartments   | 4. Commonsblock, Front Desk, Mini Mart |
| 2. West Coast Suites | 5. North Tower                         |
| 3. South Tower       | 6. East Tower                          |



## Travel information

### BY TAXI

From the Vancouver International Airport, a taxi will take around 20 minutes to the Walter Gage Residence.

### BY PUBLIC TRANSPORT

Please note that there is no direct bus service from Vancouver International Airport (YVR):

From YVR, take the Canada Line SkyTrain (all routes head north)

Transfer at one of the following stations

- Oakridge Station (41 Ave. & Cambie St.): Take bus #41 or #43
- Broadway City Hall Station (Broadway & Cambie St.): Take bus #99 (B-Line)
- Olympic Village Station (4 Ave. & Cambie St.): Take bus #84

Arrive at UBC. (UBC is final stop)

Vancouver has several Zones determining prices of public transport. You can buy a daily pass which is valid in all three zones, for 11.50 \$ per day. You can find more detailed information under [transit.ca](http://transit.ca).

## Meals & Drinks

Breakfast, coffee breaks and lunch, as well as the burger buffet on Friday evening, will be served in the NEST building, Room 2301 and/or Room 2306/2309.

For the PhD students, the evenings on Monday, Tuesday and Wednesday are free.

On Thursday evening, 24.08., we will have our *Conference Dinner at Cecil's Green Park House*, which is also located on campus.

6251 Cecil Green Park Road  
Vancouver, B.C.  
V6T 1Z1





## Excursion(s)

### St. Mark's Summit Hike

On Wednesday, August 23, we will do the St. Mark's Summit hike, a round trip of 11km.

<https://www.vancouvertrails.com/trails/st-marks-summit/>

It is recommended to pack the following items for the hike: a whistle, a hat, water (at least 1 L), sunglasses, sunblock, lunch, light jacket, fully charged cellphone, flashlight, a change of clothes.

Lunch boxes and water will be provided in the breakfast room before departure from 9:00 am.

### Panorama Ridge Hike

As an additional optional excursion, the Panorama Ridge hike will be offered on Saturday, 26 August. It's a day trip, round trip of 30km and around 1.500 elevation gain.

<https://www.vancouvertrails.com/trails/panorama-ridge/>

It is recommended to pack the following items for the hike: a whistle, a hat, water, snacks & lunch for the day, sunglasses, sunblock, lunch, light jacket, fully charged cellphone, flashlight, a change of clothes.



## WiFi

There is WiFi access throughout the accommodation area and the campus (eg *eduroam*).

## Program

### Monday, August 21, 2023

7:30 – 8:45 a.m.	<b>Breakfast</b> AMS Student Nest, Room 2301
<b>SESSION 1</b>	Chair: <b><i>Kirk Madison</i></b>
8:45 a.m.	Welcome: <u>Takamasa Momose &amp; Frank Stienkemeier</u> AMS Student Nest, Performance Theatre
9:00 a.m.	<u>Tobias Schaetz</u> Experimental Quantum Simulations - each Quantum Matter(s) -
10:00 a.m.	<u>Graziano Amati</u> Signatures of non-Markovianity in a periodically-driven dissipative qubit
10:30 a.m.	<b>Coffee Break</b> AMS Student Nest, Room 2301
11:00 a.m.	<u>Mayara da Silva Santos</u> Probing the electronic structure of reactive transition metal-oxygen species with X-rays
11:20 a.m.	<u>Pranav Kairon</u> The search for a transition: Bayesian extrapolation in Hamiltonian parameter space
11:40 a.m.	<u>Samuel Kellerer</u> Investigation of Correlated Electronic Dynamics by Nonlinear Attosecond Spectroscopy
12:00 a.m.	<b>Lunch</b> AMS Student Nest, Room 2301
<b>SESSION 2</b>	Chair: <b><i>Bernd v. Issendorff</i></b>
2:00 p.m.	<u>Hatsuki Otani</u> Microscopic Superfluidity of Parahydrogen Clusters at 0.4 K
2:20 p.m.	<u>Daniel Hönig</u> Trapping Ion Coulomb Crystals in a 1D Optical Lattice
2:40 p.m.	<u>Max Flach</u> Iron complexes with complete and incomplete first solvation shell investigated by x-ray absorption spectroscopy
3:00 p.m.	<b>Coffee Break</b> AMS Student Nest, Room 2301
3:30 p.m.	<u>Ian MacPhail-Bartley</u> Control of Molecular Rotation in Helium Nanodroplets
3:50 p.m.	<u>Lucas Weitzel Dutra Souto</u> Resonant mode description of open cavities
4:10 p.m.	<u>Arne Morlok</u> Investigation of the homogeneous linewidth of organic molecules in rare-gas clusters
4:30 p.m.	<u>Yilin Li</u> Coherent multidimensional spectroscopy of PTCDAs (3, 4, 9, 10,-perylene tetracarboxylic dianhydride) molecules attached to rare-gas clusters
5:00 p.m.	<b>PI Meeting</b> AMS Student Nest, Performance Theatre
6:00 – 8:45 p.m.	<b>PI Dinner</b> Sage



## Program

Tuesday, August 22, 2023

7:30 – 9:00 a.m.	<b>Breakfast</b> AMS Student Nest, Room 2301
<b>SESSION 3</b>	Chair: <b>Michael Thoss</b>
9:00 a.m.	<u>Valery Milner</u> Rotational Control of Molecules and Rotons in Superfluid Helium
10:00 a.m.	<u>Christina Hofer</u> Field-resolved study of low-energy excitons
10:30 a.m.	<b>Coffee Break</b> AMS Student Nest, Room 2301
11:00 a.m.	<u>Erik Frieling</u> Cross-calibration of atomic sensors for pressure metrology
11:20 a.m.	<u>Carina Hobbs</u> A new ultrahigh-vacuum experiment for simulating surface chemistry and physics of interstellar ices
11:40 a.m.	<u>Nicolai Goelz</u> Rapid Scanning in High-Resolution Coherent Spectroscopy
12:00 a.m.	<b>Lunch</b> AMS Student Nest, Room 2301
<b>SESSION 4</b>	Chair: <b>Roman Krems</b>
2:00 p.m.	<u>Benjamin Steiner</u> Generation and application of high-order harmonic radiation for the investigation of electron-correlation driven processes
2:20 p.m.	<u>Olesya Ablyasova</u> Electronic Structure of the Complete Series of Gas Phase Manganese Acetylacetonates by X-ray Absorption Spectroscopy
2:40 p.m.	<u>Kevin Marroquin</u> Dissipative dynamics of a molecular Rydberg gas: Avalanche to an ultracold plasma state of strong coupling
3:00 p.m.	<b>Coffee Break</b> AMS Student Nest, Room 2301
3:30 p.m.	<u>Philipp Elsaesser</u> Film Growth of Diindenoperylene on aSiO <sub>2</sub>
3:50 p.m.	<u>Fabian Richter</u> Strong-field XUV coherent control
4:10 p.m.	<u>Sudhang Varshney</u> tba
4:30 p.m.	<b>PAC Meetings &amp; Lab Tours</b>
<b>Free Evening</b>	

## Program

Wednesday, August 23, 2023

7:30 – 9:00 a.m.      **Breakfast**  
AMS Student Nest, Room 2301

9:00 a.m.              **Pick up your Lunch Boxes**  
AMS Student Nest, Room 2301

9:30 a.m.              **Departure**  
UBC Bookstore

10:00 a.m. – 6:00  
p.m.                    **St. Mark's Summit Hike**

## Program

Thursday, August 24, 2023

7:30 – 9:00 a.m.	<b>Breakfast</b> AMS Student Nest, 2306/2309
<b>SESSION 5</b>	Chair: <i>Ilsa Cooke</i>
9:00 a.m.	<u>Andreas Buchleitner</u> Many-body wave-particle duality
10:00 a.m.	<u>Ioannis Makos</u> Investigating nuclear dynamics using attosecond photoelectron interferometry
10:30 a.m.	<b>Coffee Break</b> AMS Student Nest, 2306/2309
11:00 a.m.	<u>Rysa Greenwood</u> tba
11:20 a.m.	<u>Kevin Schwarz</u> Improvements to the setup for photoelectron spectroscopy studies of gas phase acene anion clusters
11:40 a.m.	<u>Karin Thalmann</u> Electronic structure and electron transfer in singlet fission donor-acceptor complexes
12:00 a.m.	<b>Lunch</b> AMS Student Nest, 2306/2309
<b>Session 6</b>	Chair: <i>Lukas Bruder</i>
2:00 p.m.	<u>Anja Seegebrecht</u> Work, Heat and Internal Energy in Open Quantum Systems: A Comparison of Four Approaches
2:20 p.m.	<u>Amirhossein Rashidi</u> Trapping Ammonia Molecules Using a Fabry-Perrot MW Cavity
2:40 p.m.	<u>Aaron Ngai</u> Method of Kinetic Energy Reconstruction from Time-of-Flight Spectra
3:00 p.m.	<b>Coffee Break</b> AMS Student Nest, 2306/2309
3:30 p.m.	<u>Sarang Dev Ganashamendiram</u> A setup for extreme ultraviolet wave packet interferometry using tabletop high harmonic generation
3:50 p.m.	<u>Giorgio Ciliberto</u> Quantum Information in Analogue Black Holes
4:10 p.m.	<u>Avinash Deshmukh</u> A Model for Quantum Diffractive Heating and Measurements of Quantum Diffractive Universality
4:30 p.m.	<b>PAC Meetings &amp; Lab Tours</b>
6:00 – 8:45 p.m.	<b>Conference Dinner</b> Cecils Green Park House
7:45 – 8:30	<b>After Dinner Talk:</b> <u>Ilya Averbukh</u> Echoes in space and time



## Program

Friday, August 25, 2023

7:30 – 9:00 a.m.	<b>Breakfast</b> AMS Student Nest, 2306/2309
<b>SESSION 7</b>	Chair: <b>Frank Stienkemeier</b>
9:00 a.m.	<u>Yan Alexander Wang</u> The Art of Converging Self-Consistent Field Calculations and Achieving Chemical Accuracy for DFT Calculations
10:00 a.m.	<u>Sebastian Hartweg</u> Ultrafast dynamics of highly-excited isolated tetracene molecules
10:30 a.m.	<b>Coffee Break</b> AMS Student Nest, 2306/2309
11:00 a.m.	<u>Barbara Merzuk</u> Attosecond time-resolved coincidence spectroscopy of atoms and small molecules
11:20 a.m.	<u>Ruoxi Wang</u> Local dissipation drives global relaxation in a molecular ultracold plasma with on-site disorder and long-range dipolar interactions
11:40 a.m.	<u>Rudolf Smorka</u> Chirality-Induced Spin Selectivity in Electron Transport through Chiral Molecules: The Role of Vibrationally Assisted Spin-Orbit Coupling
12:00 a.m.	<b>Lunch</b> AMS Student Nest, 2306/2309
<b>SESSION 8</b>	Chair: <b>Ed Grant</b>
2:00 p.m.	<u>Elham Torabian</u> How to find the optimum quantum ansatz for quantum kernels?
2:20 p.m.	<u>Brendan Wouterlood</u> Photoelectron Photoion Multicoincidence Study of Micro-Solvated Thymine Molecules
2:40 p.m.	<u>Andreas Woitzik</u> Quantum State Preparation in a Micromaser
3:00 p.m.	<b>Coffee Break</b> AMS Student Nest, 2306/2309
3:30 p.m.	<u>Joachim Siemund</u> Energy-Dependence of Feshbach Resonances in a Hybrid Atom-Ion System
3:50 p.m.	<u>Yun-wen Mao</u> Efficient interpolation of molecular entropy across chemical space
4:10 p.m.	<u>Takamase Momose &amp; Frank Stienkemeier</u> Final Remarks
4:30 p.m.	<b>PAC Meetings &amp; Lab Tours</b>
6:00 – 8:45 p.m.	<b>Poster &amp; Burger Session</b> Room 2306/2309

## PAC Meetings

### PAC Meetings on Tuesday, August 22, 2023

- 4:30 p.m. **Arne Morlok**, Frank Stienkemeier, Lukas Bruder (Room 2511)
- 4:30 p.m. NN (Room 2513)
- 4:30 p.m. NN (Performance Theatre)
- 5:15 p.m. **Hatsuki Otani & Chie Nakayama** Takamasa Momose, Frank Stienkemeier (Room 2511)
- 5:15 p.m. NN (Room 2513)
- 5:15 p.m. NN (Performance Theatre)

### PAC Meetings on Thursday, August 24, 2023

- 4:30 p.m. **Ian MacPhail-Bartley**, Valery Milner, Frank Stienkemeier (Room 2511)
- 4:30 p.m. **Lucas Weitzel**, Andreas Buchleitner, Tobias Schätz (Room 2513)
- 4:30 p.m. NN (Performance Theatre)
- 5:15 p.m. **Karin Thalmann**, Michael Thoss, Frank Stienkemeier (Room 2511)
- 5:15 p.m. NN (Room 2513)
- 5:15 p.m. NN (Performance Theatre)

### PAC Meetings on Friday, August 25, 2023

- 4:30 p.m. **Joachim Siemund**, Tobias Schätz, Kirk Madison (Room 2511)
- 4:30 p.m. **Rudolf Smorka**, Michael Thoss (Room 2513)
- 4:30 p.m. NN (Performance Theatre)
- 5:15 p.m. **Brendan Wouterlood**, Frank Stienkemeier (Room 2511)
- 5:15 p.m. NN (Room 2513)
- 5:15 p.m. NN (Room 2513)

PAC meetings will take place in Room 2511, Room 2513, and the Performance Theatre.

# ABSTRACTS



## Experimental Quantum Simulations

### - each Quantum Matter(s) -

T. Schaetz

*Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3a, 79104 Freiburg, Germany,*

Direct experimental access to some of the most intriguing and puzzling quantum phenomena is difficult due to their fragility to noise. Their efficient simulation on conventional computers might be impossible, since quantum behaviour is not efficiently translatable in classical language. However, to reach beyond the capabilities of very powerful numerical methods and approximations, leading theorists of the field demand more than one-dimensional systems linked via interactions at long range and the study of complex quantum dynamics, respectively. In these systems, we could still gain deeper insight into complex quantum behaviour via experimentally simulating it in another quantum system. Here, not all but the relevant parameters and interactions might be controlled and robust effects detected sufficiently well.

Trapped atomic ions are among the most promising candidates to provide a platform for experimental quantum simulations, featuring unique control as well as operational fidelities in one-dimensional systems of few-ions. We aim to scale this system to larger size and dimensionality while preserving the unique controllability via trapping individual ions (atoms) at individual sites of arrays - on the one hand, by trapping above radio-frequency surface traps with electrodes of the micrometer scale, on the other hand, by confining them within optical lattices (potentially combining them with atoms).

After a general introduction to the field, we will present our recent results on selected experimental realisations. We will discuss in detail the challenges/limitations and prospects of the field.

## Signatures of non-Markovianity in a periodically-driven dissipative qubit

G. Amati

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

Dissipation is a fundamental phenomenon occurring in the dynamics of quantum systems that classify as open, in the sense that they are allowed to interact with an external environment. Dissipative dynamics are often labeled as non-Markovian, in contrast to Markovian memory-less evolution. Non-Markovian effects can be quantified by measuring the loss of distinguishability between two copies of a quantum system prepared in maximally distinguishable states. The trace distance is a well defined metric which allows to measure dynamically this feature and to quantify signatures of non-Markovianity. Another relevant approach to quantum dissipation is the Nakajima-Zwanzig formalism. This framework allows to express the dynamics of an open quantum system in terms of an integro-differential equation of motion which depends on its own past via a memory kernel. The timescale to relaxation of the kernel provides an alternative measurement of non-Markovianity comparable with the trace-distance approach. In my talk I will discuss how to quantify dissipation from these methods by studying the numerically exact solution of the driven-dissipative dynamics of a qubit coupled to an external periodic field and in contact with a bosonic bath. I will also discuss how the presence of the drive affects the loss of coherence in the qubit, and the related consequences on the measurements of non-Markovianity.

## Probing the electronic structure of reactive transition metal-oxygen species with X-rays

Mayara da Silva Santos<sup>1,2</sup>, Robert Medel<sup>3</sup>, Simon Kruse<sup>1,4</sup>, Max Flach<sup>1,2</sup>, Olesya S. Ablyasova<sup>1,2</sup>, Martin Timm<sup>1</sup>, Bernd von Issendorff<sup>2</sup>, Konstantin Hirsch<sup>1</sup>, Vicente Zamudio-Bayer<sup>1</sup>, Tony Stüker<sup>3</sup>, Sebastian Riedel<sup>3</sup>, J. Tobias Lau<sup>1,2</sup>

*1 Abteilung für Hochempfindliche Röntgenspektroskopie, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany*

*2 Physikalisches Institut, Universität Freiburg, Germany*

*3 Institut für Chemie und Biochemie–Anorganische Chemie, Freie Universität Berlin, Germany*

*4 Institut für Physik, Humboldt Universität zu Berlin, Germany*

Discovering compounds that present transition metals with unusual oxidation states or reactive oxygen species (superoxide, peroxide and oxygen-centered radical) is of great scientific and technological interests, as they have key applications as oxidizing agents, catalysts, or reaction intermediates, and can improve the performance of various materials.[1,2]

Here, we use X-ray absorption spectroscopy (XAS) at the oxygen K and metal L3, M3 or N3 edges of gas-phase [MOn]<sup>+</sup> systems (M = transition metal, n = integer) to identify the spectroscopic signatures of oxygen ligands and assign the oxidation state of the metal.[3] The cationic species are mass selected and accumulated in the cryogenic ion trap. X-ray absorption spectra are then recorded in partial ion yield mode.[4] Our ion trap is installed at the undulator beamline UE52-PGM at the Berlin synchrotron radiation facility BESSY II operated by the Helmholtz-Zentrum Berlin.

Reactive species, such as oxygen-centered radicals and species containing high-valent transition metals, are analyzed in stable conditions in the ground state inside the cryogenic ion trap. This method is here demonstrated to be an important tool to identify the character of oxygen ligands, offering direct access to element specific electronic structures.

[1] Y. X. Zhao, et al., Phys. Chem. Chem. Phys. 13 (2011) 1925–1938

[2] S. Riedel and M. Kaupp, Coord. Chem. Rev. 253 (2009) 606–624

[3] M. da S. Santos, et al., Angew. Chem. Int. Ed. (2022) e202207688

[4] K. Hirsch, et al., J. Phys. B: At., Mol. Opt. Phys. 42 (2009) 154029



## The search for a transition: Bayesian extrapolation in Hamiltonian parameter space

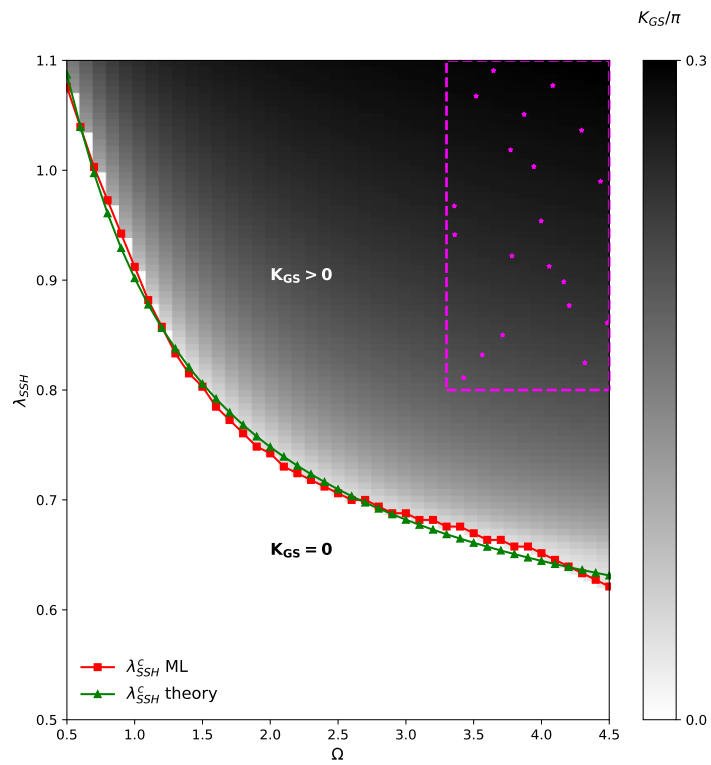
Pranav Kairon<sup>a),c)</sup>, Roman V. Krems<sup>b),c)</sup>

*a) Department of Physics and Astronomy, University of British Columbia, Vancouver, B.C., Canada*

*b) Department of Chemistry, University of British Columbia, Vancouver, B.C., Canada*

*c) Stewart Blusson Quantum Matter Institute, Vancouver, B.C., Canada*

Despite notable progress in numerical approaches to study strongly correlated electron systems, limitations such as exponential scaling in system size and challenges in the identification of emerging phases still present themselves as major bottlenecks. In this paper, we use data-driven Machine Learning (ML) models to address the outlined drawbacks of numerical methods. Previously, we demonstrated how to extrapolate quantum observables across a phase transition [1]. Here, we extend our work to tackle a higher dimensional problem of extrapolating the physics of polarons under generalized couplings in phonon frequency space using ML. We obtain the data in the adiabatic regime using Generalized Green's function Cluster Expansion (GGCE) [2]. We investigate the interplay between prediction accuracies and training regimes (pink shaded region) and showcase the effectiveness of our approach by accurately predicting sharp transitions at lower phonon frequencies. We use automatic model building method as described in [1] to select the best kernels for the gaussian process regression model using Bayesian Information Criterion as our model selection criteria. Furthermore, we comment on the existence of sharp transition in the extreme adiabatic regime for the Peierls polaron, where variational quantum Monte Carlo methods such as GGCE fail to converge. We also use multi-fidelity gaussian process regression to obtain converged polaron dispersions by training on un-converged or lower fidelity calculations of the same dispersions in combination with few high fidelity training points. This provides a way to ease the computational cost of these calculations which often run for days at a time on supercomputing clusters. In summation, this work not only underscores the limitations of existing numerical methodologies in exploring correlated electron systems but also charts an innovative trajectory through the fusion of data-driven Machine Learning models and quantum physics. We show that ML-based predictions can guide our understanding of the polaron physics in extreme adiabatic regime which plays a crucial role in the study of high-temperature superconductivity.



#### References

- [1] Vargas-Hernández, R. A., Sous, J., Berciu, M., & Krems, R. V. *Physical review letters*, *121*(25), 255702 (2018)
- [2] Carbone, M. R., Reichman, D. R., & Sous, J. *Physical Review B*, *104*(3), 035106. (2021).

## Investigation of Correlated Electronic Dynamics by Nonlinear Attosecond Spectroscopy

S. Kellerer<sup>1</sup>, I. Makos<sup>1</sup>, D. Schomas<sup>1</sup>, D. Busto<sup>1,2</sup>, S. Majoni<sup>1</sup>, R. Moshhammer<sup>3</sup>, C. D. Schröter<sup>3</sup>, T. Pfeifer<sup>3</sup>, A. Nayak<sup>4</sup>, T. Csizmadia<sup>4</sup>, Z. Divéki<sup>4</sup>, K. Varju<sup>4</sup>, F. Frassetto<sup>5</sup>, L. Poletto<sup>5</sup>, P. Tzallas<sup>6</sup>, D. Charalambidis<sup>6</sup> and G. Sansone<sup>1</sup>

<sup>1</sup>Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

<sup>2</sup>Division of Atomic Physics, Lund University, Professorsgatan 1, S-22363 Lund, Sweden

<sup>3</sup>Max-Planck-Institut für Kernphysik Heidelberg, Saupfercheckweg 1, D-69117 Heidelberg, Germany

<sup>4</sup>ELI-ALPS, Wolfgang Sandner utca 3, H-6728 Szeged, Hungary

<sup>5</sup>CNR-IFN Padova, via Trasea 7, I-35131 Padova, Italy

<sup>6</sup>IESL-FORTH Hellas, P.O. Box 1527, GR-711 10 Heraklion, Greece

The investigation of ultrafast processes like electronic dynamics in small quantum systems such as atoms or molecules demands for the generation and control of laser pulses with durations comparable, or even shorter, than the timescale of the processes under investigation. By utilizing the process of high-order harmonic generation (HHG) extreme ultraviolet (XUV) pulses with attosecond duration can be produced [1]. The combination of an attosecond source and a photoelectron/photoion coincidence spectrometer offers the possibility to investigate in detail the photoionization process, providing information on the role played by electronic correlation in the case of multiple ionization or on correlated electronic-nuclear dynamics in molecules [2].

Combining intense attosecond pulses and coincidence spectroscopy is challenging due to the requirements on the laser source driving the HHG process. Coincidence spectroscopy requires long-term measurements calling for high repetition rates attosecond sources, in order to obtain enough statistics in a reasonable amount of time, while high XUV peak intensities are necessary for observing multi-photon processes.

These requirements will be fulfilled by using the SYLOS-driven Compact beamline at the laser facility Extreme Light Infrastructure Attosecond Light Pulse Source (ELI-ALPS) located in Szeged, Hungary [3]. As an end-station at this beamline we will install a photoelectron/photoion apparatus that will be used for coincidence spectroscopy (Reaction Microscope, ReMi) [4].

Utilizing a split-and-delay unit, which will divide the XUV beam into two parts with variable relative temporal delay, we plan to apply the intense trains and isolated attosecond pulses generated on the SYLOS-driven Compact beamline to perform XUV-pump-XUV-probe on helium and hydrogen.

The main goal of this project is to investigate the electronic correlation in simple quantum systems. One of the experiments will be measurements on the two-photon double-ionization (TPDI) of helium, where different pathways can lead to double-ionization (see Fig. 1) and has been discussed in several theoretical papers [5]. So far gaining reliable experimental data on this problem is demanding and corresponding measurements are still missing. These experiments are expected to be possible by using our ReMi as an end-station at the beamline at ELI-ALPS.

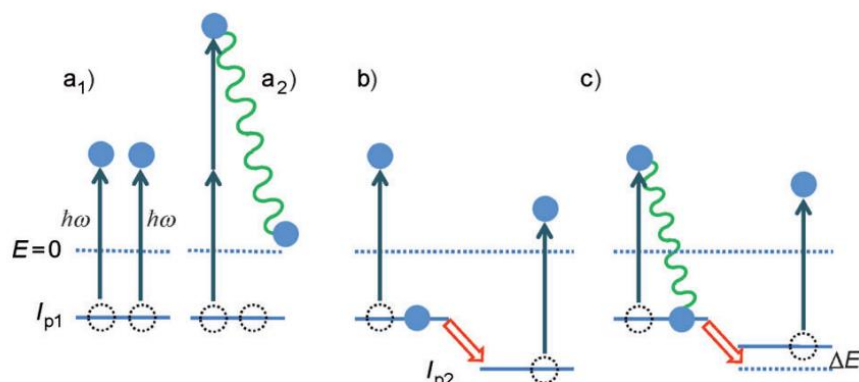


Figure 1: Schematic view of double ionization induced by absorption of two XUV photons  $\hbar\omega$ . a) Non-sequential TPDI described by independent interaction of the two electrons with the external field (a1) or by interaction of a single electron with the external field and involving electron correlation (a2) (shown as a wavy line). b) Sequential TPDI described by independent interaction of the electrons with the external field at different time instants. c) Sequential TPDI characterized by electron correlation leading to the population of shake-up states.  $I_{p1}$  and  $I_{p2}$  are the first and second ionization potentials, respectively.  $\Delta E$  is the energy difference between the shake-up state and the ionic ground state. [6]

- [1] F. Krausz, and M. Ivanov, *Reviews of Modern Physics* 81, 163 (2009).
- [2] L. Cattaneo et al., *Nature Physics* 14, 733 (2018).
- [3] Sergei Kühn et al, *J. Phys. B: At. Mol. Opt. Phys.* 50 (2017).
- [4] J. Ullrich et al., *J. Phys. B: At. Mol. Opt. Phys.* 30, 2917 (1997)
- [5] Y. Li et al, *J. Phys. B: At. Mol. Opt. Phys.* 49 (2016).
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## Microscopic Superfluidity of Parahydrogen Clusters at 0.4 K

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The existence of superfluidity in hydrogen molecules has been a subject of controversy ever since the proposal by Ginzburg and Sobyenin [1]. Despite numerous efforts, the supercooling of liquid hydrogen to transition temperatures of superfluidity has not yet been achieved. In this study, we investigated the nature of small clusters of parahydrogen ( $p\text{-H}_2$ ) molecules embedded in helium droplets. The parahydrogen molecule is an ideal candidate for realizing superfluidity because it is a spinless composite boson molecule with the smallest mass.

In order to detect the microscopic superfluidity of parahydrogen molecules, we embedded  $\text{CH}_4\text{-(}p\text{-H}_2\text{)N}$  clusters with  $N = 2 - 20$  inside helium droplets at 0.4 K, and observed vibration-rotation transitions of  $\text{CH}_4$  within the parahydrogen clusters. In a previous study, we reported the remarkably narrow linewidth of the bending mode of  $\text{CH}_4$  in helium droplets [2]. This narrow linewidth enabled us to distinguish the rotation-vibration transitions of  $\text{CH}_4$  at different  $p\text{-H}_2$  cluster sizes.

Analysis of the rotational constant of  $\text{CH}_4\text{-(}p\text{-H}_2\text{)N}$  at different cluster sizes revealed almost free rotation of  $\text{CH}_4$ . This free rotation is attributed to the almost perfect slip of the  $(p\text{-H}_2)\text{N}$  clusters relative to the rotation of  $\text{CH}_4$ . However, a more in-depth analysis indicated that the cluster size dependence of the rotational constant cannot be solely explained by the slip effect.

Through the use of path-integral Monte Carlo (PIMC) simulations, we found that the cluster size dependence can be adequately explained by the density of individual  $\text{H}_2$  molecules, without any exchange of wavefunctions with other  $\text{H}_2$  molecules, or the normal fluid density. Our analysis strongly suggests that small parahydrogen clusters exhibit significant microscopic superfluidity at 0.4 K.

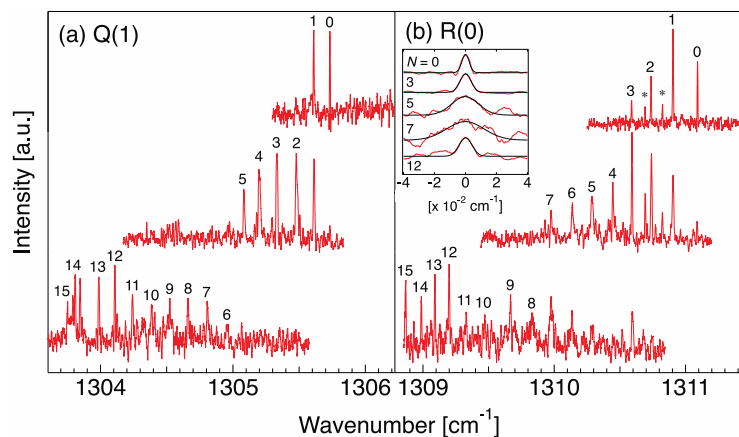


Fig. 1 The rotationally resolved IR spectra of  $\text{CH}_4-(p\text{-H}_2)_N$  clusters in helium droplets for (a) Q(1), and (b) R(0) rotational branches. Each peak is labeled by  $N$ .

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## Trapping Ion Coulomb Crystals in a 1D Optical Lattice

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The long-range Coulomb interaction between ions and the dependence of the trapping potential on the internal electronic state of the ions make optically trapped ion Coulomb crystals an interesting platform for quantum simulations. Optical lattices further extend this platform by providing arrays of individual microtraps for the ions.

In the past, we reported the successful trapping of a single ion in a one-dimensional optical lattice as well as of ion Coulomb crystals in a single-beam optical dipole trap. In this talk, we present recent advancements in trapping  $^{138}\text{Ba}^+$  ions in a one-dimensional optical lattice at a wavelength of 532 nm and the first successful trapping of linear ion Coulomb crystals ( $N \leq 3$ ) in such a trap array. The observed eigenfrequencies of the ions in the lattice and the increased robustness against axial electric fields provide evidence for the single-site confinement of the ions at individual lattice sites.

As optical lattices are extendable in size and dimension, they might allow for the realization of ion-microtrap structures in 2D and 3D. This could enable new pathways towards analog quantum simulation of systems incorporating long-range interactions. Additionally, the absence of micromotion in optical traps could give them an edge over rf-traps in applications, where heating and decoherence induced by micromotion become limiting factors. This includes the study of atom-ion interactions at ultracold temperatures, as well as the creation and study of coherent superpositions of structural Coulomb crystal phases and their entanglement.

## Iron complexes with complete and incomplete first solvation shell investigated by x-ray absorption spectroscopy

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Water plays an essential role as a solvent in chemical processes in biological, catalytic and atmospheric chemistry. In these fields a good understanding of interaction between transition metal complexes and water molecules is of major interest<sup>[1-4]</sup>. The interaction between water molecules and transition metal complexes has been subject of various studies on liquid and gas phase samples focused on the changes in electronic<sup>[5,6]</sup>, geometrical structures<sup>[7,8]</sup> and bond properties<sup>[9]</sup>. However the interaction of water molecules and transition metal complexes is still not fully understood especially the changes in the electronic structure with respect to the number of water molecules bonding to a transition metal complex. Oxygen 1s x-ray absorption spectra pre-edge features are known to originate from water-metal d interaction<sup>[5]</sup>, but how the electronic structure and furthermore how these spectral features depend on the number of water molecules bonding to a transition metal complex is not yet understood. In this study we contribute to this question by providing x-ray absorption spectra (XAS) of the iron L- and oxygen K-edge of iron complexes  $[\text{Fe}(\text{H}_2\text{O})_6]^{2+}$  and  $[\text{FeOH}(\text{H}_2\text{O})_n]^+$  ( $n=0-3$ ) in the gas phase. The measured spectra are compared to simulated ones from time-dependent density functional theory (TD-DFT). As we can well resolve the oxygen K-edge we are able to observe excitation energy shifts of the pre-edge features with respect to the contribution of the number of water molecules to the LUMO orbital in the iron hydroxide series. The amount of these excitation energy shifts correlates with how strongly the water molecules participate in the LUMO Fe-OH hybrid orbital. A comparison between the oxygen K-edge of  $[\text{Fe}(\text{H}_2\text{O})_6]^{2+}$  and  $[\text{FeOH}(\text{H}_2\text{O})_n]^+$  shows low energy features are present in  $[\text{FeOH}]^+$  as well as in  $[\text{Fe}(\text{H}_2\text{O})_6]^{2+}$  at similar energies but are narrower in the  $[\text{Fe}(\text{H}_2\text{O})_6]^{2+}$  spectrum. Compared to literature these oxygen K-edge low energy features are also at similar energies but less distinct for the literature liquid phase spectra. The iron L-edge spectra show less changes as in all our samples iron is in the oxidation state 2+ as expected. However a comparison of the iron L3-edge of gas phase  $[\text{Fe}(\text{H}_2\text{O})_6]^{2+}$  with liquid phase XAS of 1M  $\text{FeCl}_2$  in  $\text{H}_2\text{O}$  reveals a broadening from the gas phase to the liquid phase. These preliminary results are part of an on going study on the way to provide deeper insight in the interaction of water molecules with transition metal complex.

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## Control of Molecular Rotation in Helium Nanodroplets

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Carbon disulphide molecules embedded in helium nanodroplets are cooled down below 0.4 K, after which a short laser pulse can non-adiabatically excite a broad distribution of rotational energy levels. Monitoring the alignment as molecules rotate can resolve spectral lines due to strong rotational coherence, though strongly excited states transfer angular momentum into the droplet too quickly for quantum revivals to be observed. The CS<sub>2</sub> coupling to the helium results in a “band” of similar frequencies that can be modelled by greatly enhanced centrifugal distortion [1]. Experimental results and prospects of controlling the excitation by applying a second laser pulse to reduce (or enhance) the population of specific energy levels are discussed, as well as how future experiments with a double pulse system could be used to investigate the timescale of how angular momentum transfers from the dopant to the the droplet.

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## Resonant mode description of open cavities

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In the usually employed theoretical approaches for open resonator QED systems, one considers a quantum emitter - such as an atom - in a cavity which interacts with a few discrete electromagnetic cavity modes. Models that employ this treatment, as is the case for the seminal Jaynes-Cummings model and its generalizations, have been tremendously successful in describing experiments. Losses and leakage from the cavity are then introduced as a (weak) interaction with the environment. Mathematically, the system's time evolution is depicted via a Lindblad master equation. However, all of these descriptions are intrinsically phenomenological and it is not known if they hold in all situations, as underlying approximations are still unclear. For instance, in the case of strongly leaking systems, such as plasmonic cavities, the weak-coupling assumption is not valid anymore and the theoretical line of attack needs to be reassessed. We hence try to answer the following question: is it possible to construct from first principles a description of leaky cavities by few broadened modes, in the spirit of the Jaynes-Cummings model and compatible with a Lindblad master equation? This will extend our theoretical understanding of more general systems or, in the case of a negative answer, lead to a no-go theorem.



## Investigation of the homogeneous linewidth of organic molecules in rare-gas clusters

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Two-dimensional spectroscopy (2DES) is a powerful method to study dynamics of atoms and molecules with a high spectro-temporal resolution. In our group, we apply the technique to doped cluster beams, which are generated with supersonic expansion of rare gases (Fig. 1a)) [1,2].

Rare gases are chosen for the spectroscopic matrix as they act as miniature cryostats for the dopants and provide an environment of low interaction. Still, even rare-gas clusters have a residual system-bath interaction, which influences the spectroscopic properties of the dopant. 2DES is commonly used to analyze system-bath interactions as the non-linear measurement scheme makes detailed studies of the underlying physics possible.

Previous 2DES experiments on phthalocyanine (Pc, inset Fig. 1b)) on neon clusters (Fig. 1b)) allowed resolving the homogeneous linewidth of Pc which provided some insight into the binding configurations [3]. We extended this investigation in varying the cluster species and improving the data acquisition scheme (Fig. 1c)), since the previous measurements were limited by long acquisition times. First results are presented, which suggest differences in the homogenous linewidth and the molecular dynamics depending on the cluster species.

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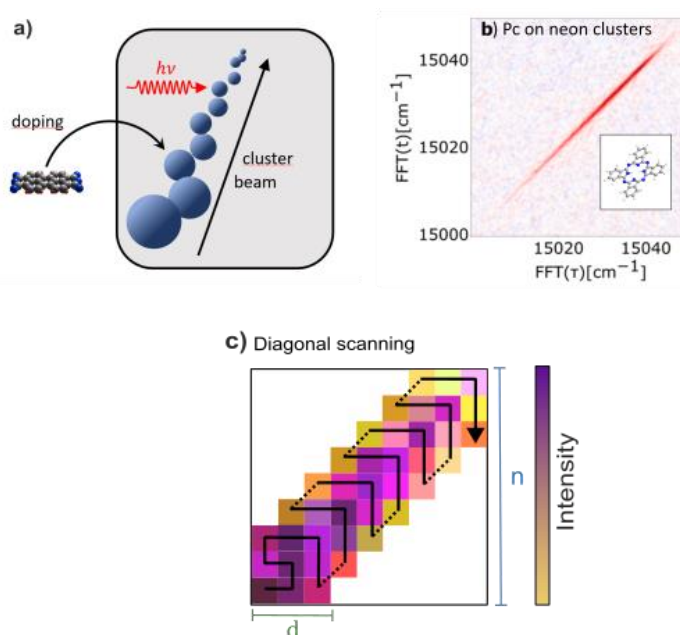


Figure 2: a) Schematic of the doping of a cluster beam and the interaction with the light pulses. b) 2D spectrum of Pc on neon clusters with the structure of a Pc molecule as an inset. c) Schematic of an improved data acquisition scheme.

## Coherent multidimensional spectroscopy of PTCDA (3, 4, 9, 10,-perylene tetracarboxylic dianhydride) molecules attached to rare-gas clusters

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Coherent multidimensional spectroscopy is a versatile technique enabling further insights into intra- and inter-molecular couplings on ultrashort time scales. We have extended the method to molecular nanosystems prepared in the gas phase [1,2]. Recently we started analyzing 2D beating maps to obtain information about the electronic and vibrational coherences in the systems [3], which are otherwise covered by linebroadening mechanisms. We were able to observe a slight difference of the vibrational beating frequency between electronic ground and excited states (Fig. 1(a)), and a low vibrational frequency (Fig. 1(b)). Both observations have not been reported before to our knowledge. To compare the influence of different environments on the molecule, we also measured 1D and 2D spectra of PTCDA attached to hydrogen clusters and in the liquid phase. First results will be presented.

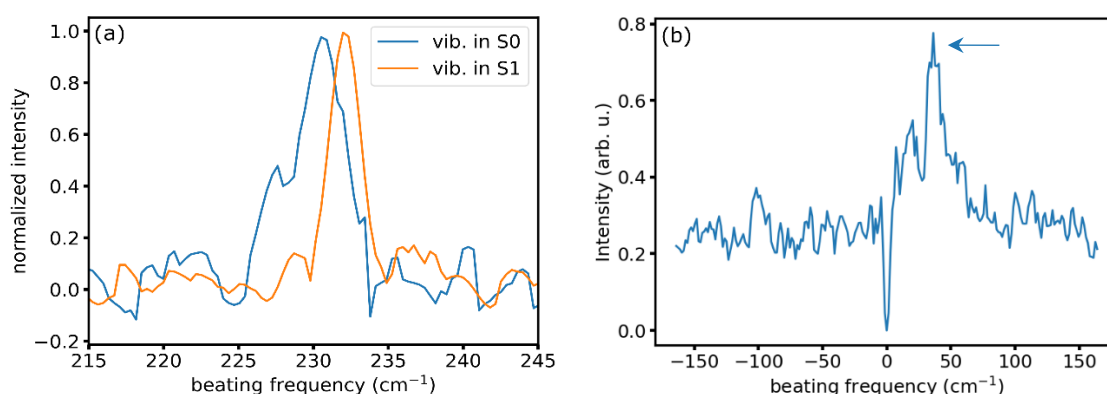


Fig.1 (a) 2D beating maps can separate the contribution of vibrational coherences from electronic ground and excited states [3]. The beating map analysis of PTCDA molecules attached to argon clusters shows a slight difference of the vibrational beating frequency around 230 cm<sup>-1</sup> (in-plane A<sub>g</sub> ν<sub>c-c</sub> along long axis [4]) in the electronic ground (blue) and excited states (orange). (b) 2D beating map analysis of PTCDA molecules attached to argon clusters reveals a slow vibrational mode between 30 cm<sup>-1</sup> and 40 cm<sup>-1</sup>, which is relatively weak and hidden below the broadening of the zero-phonon line in the 1D absorption spectrum.

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## Rotational Control of Molecules and Rotons in Superfluid Helium

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Molecules immersed in liquid helium are excellent probes of superfluidity. Their electronic, vibrational and rotational dynamics provide valuable clues about the superfluid at the nanoscale. We present an experimental study of the laser-induced rotation of helium dimers inside the superfluid  $^4\text{He}$  bath at variable temperature. The coherent rotational dynamics of  $\text{He}_2$  is initiated in a controlled way by ultrashort laser pulses, and tracked by means of time-resolved laser-induced fluorescence. We detect the decay of rotational coherence on the nanosecond timescale and investigate the effects of temperature on the decoherence rate. The observed temperature dependence suggests a non-equilibrium evolution of the quantum bath, accompanied by the emission of the wave of second sound. The method offers new ways of studying superfluidity with molecular nano-probes under variable thermodynamic conditions [1].

A Superfluid  $^4\text{He}$  is a very dense system of strongly interacting quasiparticles (phonons, maxons and rotons), which determine the fascinating properties of this quantum liquid. Quasiparticle properties are deduced from experiment, predominantly with neutron scattering, and controversies over their description still remain, notably regarding the nature of rotons and their binding into roton pairs. We developed a method of studying roton pairs in superfluid helium after exciting them with either a femtosecond laser pulse or a shaped pulse known as an optical centrifuge. By tracking the non-equilibrium dynamics of the laser-induced two-roton states on a picosecond timescale, we observe an ultrafast cooling of hot roton pairs as they thermalize with the colder gas of other quasiparticles. We show that the thermalization rate increases with increasing temperature of the helium bath, with no detectable dynamics above the superfluid transition. We also demonstrate that the angular momentum of the roton pair can be controlled with an optical centrifuge [2,3].

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## Field-resolved study of low-energy excitons

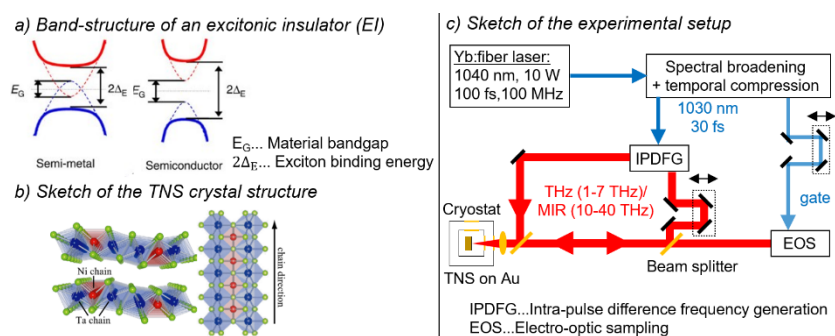
Christina Hofer<sup>a),b)</sup>, Sydney K. Y. Dufresne<sup>a),b)</sup>, Bradley G. Guislain<sup>a),b)</sup>,  
Ziliang Ye<sup>a),b)</sup> and David J. Jones<sup>a),b)</sup>

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In solids, electrons can bind with an associated hole into an exciton: a quasi-particle with atom-like properties. Typically, excitons have low binding energies and are short-lived at room temperature. Exfoliating materials to single atomic layers reduces the Coulomb screening seen by the excitons. As a result, their binding energy increases into the mid-infrared and even visible spectral regions along with an increased lifetime. One manifestation of exciton formation is an excitonic insulator (EI). An EI is a quantum many-body state that is theoretically predicted to occur in small bandgap semiconductors or semimetals with small band overlap and low Coulomb screening. In such materials, excitons with a binding energy larger than the bandgap can exist without optical excitation, thus forming a new ground state (see Fig. a) [1]).  $\text{Ta}_2\text{NiSe}_5$  (TNS) is one host candidate for this exotic quantum state (see Fig. b) [2]), with a phase transition at the critical temperature  $T_c = 328$  K. Below  $T_c$ , the optical bandgap and exciton binding energy is  $\sim 160$  meV [1]. Transient changes in the (1-3 THz) phonon modes of TNS were observed using near-infrared photoexcitation and time-resolved reflectivity [3-5]. Recent time- and angle-resolved photoemission spectroscopy experiments investigated the role of electron-electron interactions for maintaining the insulating state after photoexcitation [6]. However, whether the phase transition is mainly driven electronically or structurally remains uncertain and contradictory results have been observed.

Here, we present an electric field-resolved spectrometer for the comprehensive study of the formation of the EI phase in TNS. The instrument is based on an Yb: fiber laser (see Fig. c)), which drives intra-pulse difference frequency generation in GaP, SiC and GaSe nonlinear crystals to generate few-cycle waveforms covering the frequency range between 1-40 THz (4-160 meV). The 1-7 THz radiation resonantly drive individual structural modes. In addition, the higher-frequency MIR radiation is resonant with electronic transitions, avoiding parasitic phonon excitations. This spectral coverage uniquely enables probing the evolution of the bandgap while potentially driving a structural transition into the EI phase. "Electro-optic sampling" (EOS) [7] is used for field-resolved characterization of the transmitted THz and MIR waves. In EOS, shifting the detection to the near-infrared via nonlinear interaction with a sub-cycle gate pulse and the ability to temporally filter the sample response benefit the detection sensitivity and dynamic range. The field measurement gives access to the instantaneous complex



dielectric sample response, which was previously used to disentangle electronic and structural orders in a different material [8]. Scanning the pump-probe delay results in a spectrogram of the complex sample response, that tracks the evolution of the bandgap and can reveal changes in the spectral weight of the exciton binding energy. This spectrometer promises unprecedented capabilities to drive phonon and electronic modes on resonance and probe them phase-coherently and with high sensitivity. A separation of electron and phonon contributions to the EI formation as well as their couplings promises to resolve existing contradictions and open questions on the nature of the phase transition. In addition, recent progress in the exfoliation of TNS monolayers also allows to isolate the electronic degrees of freedom and benefits from the instruments measurement sensitivity when sample sizes are limited.

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## Cross-calibration of atomic sensors for pressure metrology

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Sensors based on single atoms have shown great promise for density and pressure metrology in the high, ultra-high, and extremely-high vacuum regimes. Specifically, the density of background gas particles in vacuum can be determined by measuring the collision rate between the particles and an ensemble of sensor atoms. This requires preparing the sensor atoms in a particular quantum state (both internal and external), observing the rate of changes of that state, and using the cross section coefficient for state-changing collisions to convert the rate into the corresponding density. The cross section can be known by various methods including by theoretical calculation, calibration of the sensor atom at a known density, or measurements of the post-collision sensor-atom momentum recoil distribution. Discovering systematic errors in these methods can be aided by direct comparisons of the methods. Alternatively, measurements of the same background gas with different sensor atoms offers another point of comparison free of many systematics inherent with other methods. Here, we present such measurements for two sensor atoms  $^{87}\text{Rb}$  and  $^6\text{Li}$  for a variety of both atomic and molecular background gases including  $\text{H}_2$ ,  $\text{N}_2$ ,  $\text{Ar}$ ,  $\text{Ne}$ ,  $\text{Kr}$  and  $\text{Xe}$ . This work demonstrates the utility of sensor-atom cross-calibration experiments to check the validity of theoretical computations to extend and enhance the performance of cold atom based pressure sensors. In addition, it provides a model-free method for transferring the primacy of one atomic standard to another sensor atom.



## A new ultrahigh-vacuum experiment for simulating surface chemistry and physics of interstellar ices

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Astrochemistry concerns the formation, nature, and abundance of molecules in the interstellar medium (ISM) and star-forming regions. These astrophysical objects are of interest as they contain the chemical material from which new planets and solar systems are formed. Nearly 300 molecules have been detected in the ISM, with the rate of new detections still growing. It is anticipated that many of these molecules, particularly the so-called complex organic molecules (COMs), are formed on or in icy mantles on interstellar dust grains.<sup>1</sup> The formation of these molecules in ices, their subsequent chemical evolution and their transport to the gas-phase remains poorly constrained. Quantitative laboratory measurements of processes on ices, including activation energies, product yields and branching ratios, are critical to explaining the presence of these molecules in astrophysical regions.

The design and construction, as well as proof-of-concept measurements, of a new ultra-high vacuum (UHV) chamber at UBC, will be presented. To simulate processes in astrochemical ices, Fourier-transform infrared spectroscopy (FTIR) will be used to detect parent molecules and their products in situ in the ice, as well as temperature-programmed desorption (TPD) combined with photoionisation reflectron time-of-flight mass spectrometry (ReTOF-MS) to detect molecules upon their sublimation. Additionally, this chamber will be fitted with a hydrogen discharge lamp to produce continuum and Lyman-alpha VUV light to simulate interstellar radiation. This setup has been designed to study the formation and diffusion of radicals on ice surfaces, as well as the evolution of COMs during energetic and non-energetic processing of the ice. This research is particularly timely, with the recent launch of the James Webb Space Telescope (JWST), as the data collected during these experiments at UBC will be used to support new observations of ices from JWST, in addition to observations from terrestrial telescopes.

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## Rapid Scanning in High-Resolution Coherent Spectroscopy

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Coherent multidimensional spectroscopy (CMDs) is a powerful ultrafast spectroscopic technique to study dynamics of matter with a high spectro-temporal resolution otherwise only accessible in disjunct experiments. Extending the method to weakly perturbed molecular and cluster species in the gas phase permits very high spectral resolution [1].

Previous experiments have revealed valuable insights such as the homogeneous line profile of chromophores solvated in nanoclusters [2]. However, in this case, the attainable resolution is limited by the acquisition time. To solve this problem, we have implemented a rapid-scanning method developed by the Ogilvie group [3] which reduces the acquisition time by up to two orders of magnitude (Fig. 1). First results are presented which demonstrate the potential of the rapid scanning approach.

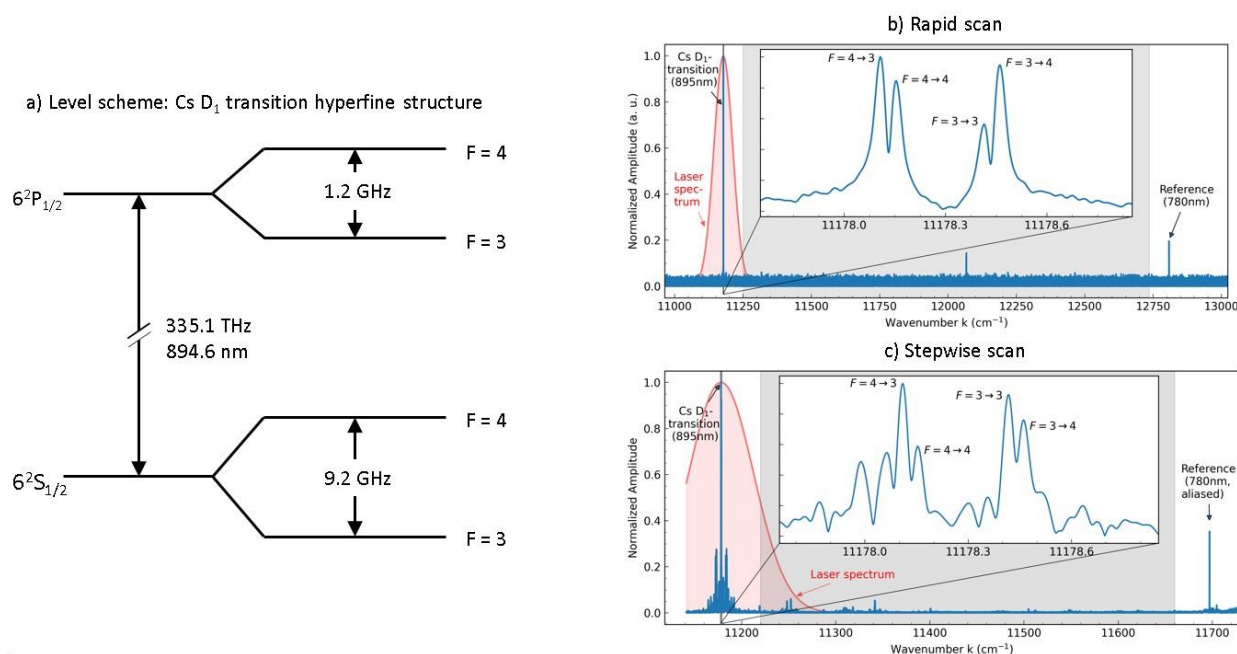


Figure 1: a) Level scheme of the Cs D<sub>1</sub> transition hyperfine structure. b) Wave packet interferometric (WPI) measurement of the Cs D<sub>1</sub> transition using the rapid scanning approach (2 minutes measurement time). c) Stepwise WPI measurement in 15 hours measurement time.

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## Generation and application of high-order harmonic radiation for the investigation of electron-correlation driven processes

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The time-resolved investigation of ultrafast processes like the electron dynamics in the valence and core shells of atoms and molecules requires time resolution ranging from the femtosecond down to the attosecond domain. For these investigations, attosecond laser pulses in the extreme ultraviolet (XUV) spectral range are available and are obtained by the process of high-order harmonic generation (HHG).

The excitation of electronic-correlation driven processes, such as the Auger decay in krypton [1] or single photon double ionisation in helium [2], requires a minimum photon energy, typically in the range around 60 to 100 eV. Since the goal of this project is to investigate these processes using electron-electron-ion coincidence, the first challenge is to extend the cutoff energy in the HHG process to reach the desired energy range.

To drive the HHG process, laser pulses from a commercially available Yb-based laser system need to be temporally compressed using a multi-pass cell, since such cells offer an excellent power throughput of up to 95 % [3] when compared to the usually employed hollow-core fiber setups. Consequently, high enough peak intensities can be reached to efficiently drive HHG in neon, which allows the generation of sufficiently high energetic XUV photons of 60 eV and above.

The obtained attosecond XUV pulses will then be employed in the already existing attosecond coincidence spectrometer in Freiburg for the time-resolved investigation of electron dynamics occurring during the above-mentioned processes.

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## Electronic Structure of the Complete Series of Gas Phase Manganese Acetylacetonates by X-ray Absorption Spectroscopy

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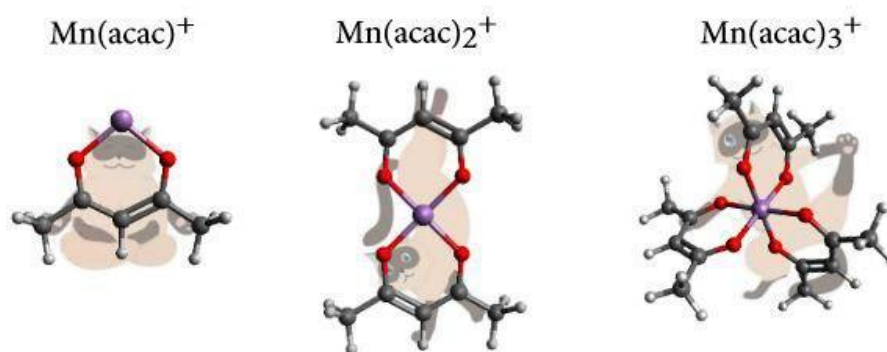
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Transition metal-ligand complexes have attracted a lot of attention as a promising redox active molecule for redox flow batteries[1], as a potential complex for aqueous synthesis of metal-organic-frameworks [2] and as fascinating single-molecule magnets[3]. One classical example of such complexes is manganese acetylacetonate  $\text{Mn}(\text{acac})_n$ , where manganese is involved into OEC reaction and acetylacetonate is one of the most valuable ligands in coordination chemistry. However, the application of that complex in industry would profit from a thorough understanding of its electronic structure  $\text{Mn}(\text{acac})_n$ . [4] In particular, connection of oxidation state and (under-)coordination of these complexes will play a crucial role in the following investigation of that complex application in industry.

We have performed X-ray absorption spectroscopy (XAS) in ion yield mode at the manganese L-edge and oxygen and carbon K-edge on a series of gas-phase mass-selected manganese Mono-, Bis, and Trisacetylacetonate ions. The experiments were performed at the BESSY II synchrotron source with the IonTrap end-station. Accompanied with RAS/DFT calculation and CFM/CTM modeling, we are able to extract information about the geometry, electronic structure, spin and oxidation state of the  $\text{Mn}(\text{acac})_n^+$ . Obtained results were compared with theoretically predicted electronic state of  $\text{Mn}(\text{acac})_n^+$ [5]. During this comparison we explain the correlation between coordination and electronic state of complex.



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## Dissipative dynamics of a molecular Rydberg gas: Avalanche to an ultracold plasma state of strong coupling

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Spontaneous avalanche to plasma splits the core of an ellipsoidal Rydberg gas of nitric oxide. Ambipolar expansion first quenches the electron temperature of this core plasma. Then, long-range, resonant charge transfer from ballistic ions to frozen Rydberg molecules in the wings of the ellipsoid quenches the ion/Rydberg-molecule relative velocity distribution. This sequence of steps gives rise to a remarkable mechanics of self-assembly, in which the kinetic energy of initially formed hot electrons and ions drives an observed separation of plasma volumes. These dynamics adiabatically sequester energy in a reservoir of mass transport, starting a process that anneals separating volumes to form an apparent glass of strongly coupled ions and electrons. Short-time electron spectroscopy provides experimental evidence for complete ionization. The long lifetime of this system, particularly its stability with respect to recombination and neutral dissociation, suggests that this transformation affords a robust state of arrested relaxation, far from thermal equilibrium. We see this most directly in the absorption spectrum of transitions to states in the initially selected Rydberg series, detected as the long-lived signal that survives a flight time of 400  $\mu\text{s}$  to reach an imaging detector. The initial density of electrons produced by prompt Penning ionization, which varies with the selected initial principal quantum number and density of the Rydberg gas, determines a balance between the rising density of ions and the falling density of Rydberg molecules. This Penning-regulated ion - Rydberg molecule balance appears necessary as a critical factor in achieving the long ultracold plasma lifetime to produce spectral features detected after very long delays.

## Film Growth of Diindenoperylene on aSiO<sub>2</sub>

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Film growth is of high technological importance in the context of growing single crystals, coating surfaces and producing films. However, the processes involved in film growth pose many fundamental challenges, both in experiment and theory. While there is by now a good understanding of the growth of films consisting of atoms, molecular films behave partially in different ways.

Diindenoperylene (DIP) is an organic semiconductor, which is a candidate for organic solar cells or OLEDs. For this quasi two dimensional molecule with one long axis, it has been found in experiments, that it undergoes different phases during film growth [1].

We have investigated the growth of DIP on an amorphous SiO<sub>2</sub> substrate. We performed MD simulations with the polymer-consistent force field - interface force field (PCFF-IFF) [2]. We have studied the clustering of single DIP molecules on amorphous SiO<sub>2</sub>, as well as the molecular orientations of larger structures close to the surface of the substrate.

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## Strong-field XUV coherent control

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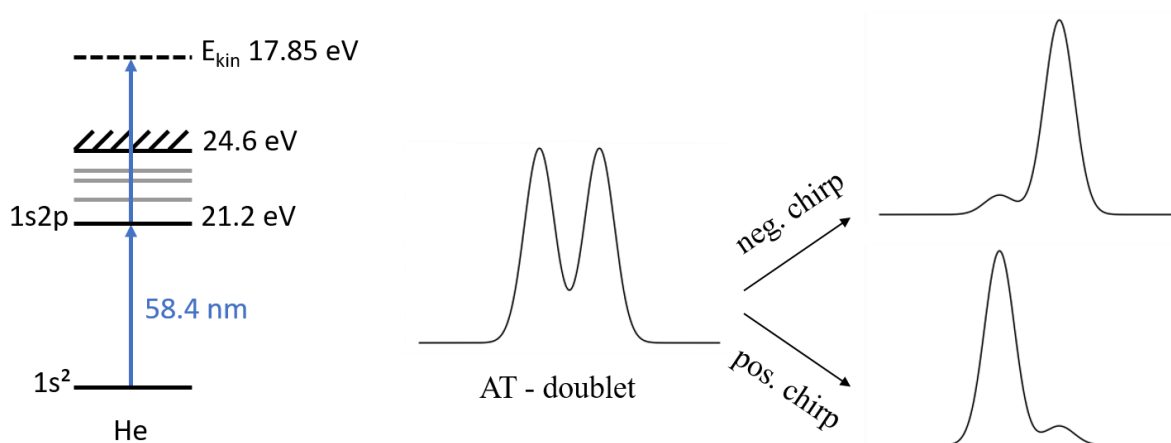
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Coherent control drew a lot of interest in recent years spanning over various fields of research regarding the promising abilities for quantum computing, precision measurements and various other applications. Coherent control extended to the strong field regime shows particular promise in the manipulation of matter and controlling photochemical reactions [1]. In this work, we develop a scheme to extend strong-field coherent control to the XUV domain. With intense XUV pulses, we induce Rabi oscillations in atoms and atomic clusters, leading to Autler-Townes level splittings in the photoelectron spectra (see Fig.) [2]. In the near infrared domain, the feasibility to coherently control the population of the Autler-Townes doublet has been shown, based on chirp manipulation of the laser pulses [3,4]. To establish comparable schemes in the XUV domain, we implement chirp control of the XUV pulses from the free electron laser FERMI. By manipulating the chirp of the XUV pulses in a controlled way, we achieved a strong-field coherent control of Autler-Townes states in the XUV domain.



We will present simulations of the expected Autler-Townes splitting as well as preliminary results from our beamtime at FERMI.



**Figure:** Level scheme of helium with relevant states, their corresponding energies and the laser energy, with the resulting kinetic energy of the electrons (left). Coherent control scheme of the respective Autler-Townes states upon chirped pulses (right).

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## *Dependence of Rubidium Molecule formation on Magneto-Optical-Trap settings*

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Measuring the electric dipole moment (EDM) with high precision will pave way to understanding physics Beyond-the-Standard-Model (BSM). To that end, proposals are underway to use ultracold molecules since they have the potential to provide signals far beyond current state-of-the-art measurements. Using polar molecules can amplify the effects of BSM physics, enabling order of magnitudes improvement in sensitivity. A scientific goal is therefore the assembly of the ultracold polar molecules FrAg, which has a octupole-deformed nucleus, from a quantum degenerate gas of Fr and Ag atoms.

To that end, it is desired to understand the scattering properties of both atoms, as well as the dimer. Control over scattering rates is necessary to perform the standard techniques of evaporative or sympathetic cooling used to create ultracold molecules. For this control, knowledge of the relevant molecular and atomic spectra is required. This can be done using single and two photon photo-association (PA) spectroscopy, which uses tunable lasers to drive transition from free, colliding pair of atoms to bound states in an electronically excited molecular potential.

Preliminary PA studies in a Rubidium magneto-optical-trap (MOT) have indicated that the PA rate is sensitive to the MOT depth. Molecule formation may also be blocked by a shielding effect due to the cooling lasers. We report PA spectroscopy in a MOT with the well-studied system of Rubidium, which has properties analogous with Fr.

## Many-body wave-particle duality

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Wave-particle duality is the key feature of quantum mechanics: The statistics of granular, i.e. particle-like measurement events which individually respond to (experimental) „Yes or no?“ questions exhibit wave-like interference contributions — which undermines the imagination of mutually exclusive, distinct paths taken by a single particle, ergo: tertium datur! And it is also experimentally very well verified: Whenever „which-way information“ becomes available in the environment, i.e. when environmental degrees of freedom get entangled with those interrogated by the experimental set-up, the interference contrast gradually fades away. The trade-off between which-way information and interference contrast can be cast in the form of an inequality and also considered a corner stone of our modern understanding of decoherence. Yet, wave-particle duality and its relation to decoherence theory hitherto are mostly debated in a single or, at best, two-particle context, while a panoply of intricate interference phenomena emerges on the level of many-body quantum dynamics, and nowadays becomes accessible in experiments with ever increasing resolution - from photonic circuitry over quantum gas microscopes to the realm of atto science. The talk will give an introduction to our current understanding of many-body interference phenomena, and lift wave-particle duality to the many-body level.

## Investigating nuclear dynamics using attosecond photoelectron interferometry

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Attosecond photoelectron interferometric techniques have been utilized, over the past decade, to investigate dynamics in molecular systems following photoionization. These techniques have provided valuable insights into electron correlation effects and coupled electronic-nuclear dynamics [1–3]. 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 [4,5].

In this study, we investigate photoionization dynamics in a gas mixture of methane ( $\text{CH}_4$ ) and deuteromethane ( $\text{CD}_4$ ), utilizing attosecond photoelectron coincidence spectroscopy. The absorption of an extreme ultraviolet (XUV) photon originating from an attosecond pulse train populates a manifold of cationic states. An additional absorption or emission of an infrared (IR) photon gives rise to a two-color photoionization spectrogram. A collinear configuration is used to control the relative delay between the XUV and the IR pulses, which are co-propagating in a reaction microscope where they interact with the gas target [6].

The investigation of the mixture of  $\text{CH}_4$  -  $\text{CD}_4$  using attosecond photoelectron interferometry give access to the nuclear response of the two isotopologues, since the electronic properties of the two molecular systems are not significantly affected by the two-color field [7]. Looking into the amplitude and the contrast of the oscillations of the photoelectron peaks, we obtain information regarding the nuclear dynamics upon photoionization, as well as the effect of nuclear motion on the correlated electronic-nuclear dynamics [8].

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## *Probing Excitons in Organic Semiconductors using TR-ARPES*

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In organic semiconductors photoexcitation generates an electron-hole pair strongly bound together by Coulomb interaction. This electron-hole pair is called an exciton and often recombine quickly (10's- 100's of femtoseconds). To achieve efficient charge separation in these materials, it is necessary to drive the dissociation of the exciton. The mechanisms that result in efficient charge separation in these materials are still not well understood. Therefore, to better advise device design it is necessary to gain a deeper understanding of the dynamics that occur post photoexcitation with femtosecond resolution and the extent of delocalization of the excitonic states.

While the ultrafast-response of organic semiconductors have been studied using all-optical techniques for a number of years [1], a lack of momentum resolution has limited their interpretation. Time-resolved, angle-resolved photoemission spectroscopy (TR-ARPES) is a powerful technique that allows a user to visualize the energy-momentum landscape of a material and monitor how the material responds to photoexciton with femtosecond resolution. Only in the last few years has much attention has been placed on using TR-ARPES (or similar techniques) to investigate organic semiconductors because of its capability to directly map the momentum dependent dispersion of the excitonic states with high temporal resolution [2-4].

Here, I show the capability to probe the excitonic states in  $C_{60}$ , a prototypical organic photovoltaic material, using TR-ARPES. We have been able to track the dynamics of the excitonic states with sub picosecond resolution. We have also been able to resolve the momentum dependent dispersion of the excitonic states with angular resolution unachieved so far. With this improved angular resolution, we hope to access the extent of delocalization of the excitons in the  $C_{60}$  lattice.

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## Improvements to the setup for photoelectron spectroscopy studies of gas phase acene anion clusters

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Organic semiconductors like acene molecules show interesting properties and keep being of interest across science and technology. They are used, for instance, in organic solar cells.

To get a better understanding of those molecules, they are investigated in the gas phase by photo electron spectroscopy (PES) to gain knowledge on the different electronic and vibrational modes of the molecules, especially from electronic relaxation processes giving information about the dynamics within the molecules.

Continuing with my project, improvements to the setup have been and will continue to be developed, including an automated control of the valve to keep the pressure and gas flow of molecules and clusters as constant as possible via a PID regulation.

Furthermore, temperature-resolved studies are of high interest due to changes in the vibrational modes accessible to the clusters, so a further improvement to the setup and to increase the resolution of the photoelectron spectra include adding a radio frequency ion trap into the setup, which will be introduced.

## Electronic structure and electron transfer in singlet fission donor-acceptor complexes

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July 25, 2023

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Singlet fission (SF) is a spin-allowed process in organic materials transforming a singlet exciton to two triplet excitons [1]. Since SF has the ability to multiply charge carriers, SF could be utilised in solar cells to circumvent the Shockley-Queisser limit [2,3]. To investigate future applications, we link a molecule exhibiting SF to an electron acceptor. In detail, we consider the complex of two covalently linked diazadiborane chromophore units as the SF exhibiting donor and tetracyanoquinodimethane as the acceptor molecule.

We use ab-initio multireference perturbation theory techniques to determine the electronic structure, in particular the electronically excited states including the locally excited, charge transfer, and multiexcitonic states. Furthermore, quantum dynamical simulations are carried out to analyse the electron and energy transfer in the complex.

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## Work, Heat and Internal Energy in Open Quantum Systems: A Comparison of Four Approaches

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We compare definitions of the internal energy of an open quantum system and strategies to split the internal energy into work and heat contributions as given by four different approaches from the autonomous system framework. Our discussion focuses on methods that allow for arbitrary environments (not just heat baths) and driving by a quantum mechanical system. As a simple application we consider an atom as the system of interest coupled to an oscillator field mode as the environment and analyse three different types of interaction. We discuss ambiguities in the definitions and highlight differences that appear if one aims at constructing environments that act as pure heat or work reservoirs. Further, we identify different sources of work (e.g. coherence, correlations, or frequency offset), depending on the underlying framework. Finally, we give arguments to favour the approach based on minimal dissipation.



## Trapping Ammonia Molecules Using a Fabry-Perrot MW Cavity

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This project aims to trap pre-decelerated ammonia molecules using an alternating electrical field formed by resonating microwaves between two concave mirrors, creating what is known as a Fabry-Perrot cavity. This approach relies on the principle that the rotational states of a polar molecule undergo non-degeneracy when subjected to an external electric field. The electric field can be applied through two methods: the direct current (DC) approach utilizing electrodes with distinct electrical potentials or an alternating current (AC) strategy using an electromagnetic wave that inherently carries an alternating electrical field. In this study, we utilize the AC electric field by introducing microwave (MW) radiation into a Fabry-Perrot cavity to generate an intense standing wave.

For trapping, we focus on the  $|JK\rangle=|1,1\rangle$  rotational state of ammonia,  $\text{NH}_3$ . Due to inversion tunneling motion between two pyramidal structures, the  $J=1$  state splits into two states with a spacing of  $0.79 \text{ cm}^{-1}=23.7 \text{ GHz}$ . This inversion transition in the  $J=1$  rotational state can effectively trap  $\text{NH}_3$  within a cavity. The behavior of inversion states in the AC field within the MW cavity depends on the frequency detuning, which refers to the difference between the applied MW frequency and the resonance frequency between the inversion doublet. For instance, a blue detuning (slightly higher MW frequency than the resonance frequency) causes the lower level of the inversion doublet to become a high-field seeking (HFS) state. As a result,  $J=1$  ammonia molecules can be trapped at the maximum electric field point of the MW standing wave within a cavity under the blue detuning condition. To further enhance the electric field within the cavity, we coated the cavity surface with PbSn and cooled it to achieve superconductivity [1]. The ongoing status of the MW trapping experiment will be discussed.

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## Method of Kinetic Energy Reconstruction from Time-of-Flight Spectra

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We present a method for the reconstruction of ion kinetic energy release (KER) distributions from ion time-of-flight (TOF) mass spectra, using ion trajectory simulations and is applicable also to complicated spectrometer geometries with largely anisotropic ion collection efficiencies. A calibration procedure using a single ion mass peak allows the accurate unique determination of parameters related to the spectrometer calibration, experimental alignment and instrument response function, which increases the agreement between simulations and experiment. The calibrated simulation extrapolates to a set of energy-dependent TOF basis functions, which allows the transformation to KER distributions through least-squares and regularization methods. We demonstrate this reconstruction method on a recent XUV-UV pump-probe experiment [1] on helium nanodroplets performed at the LDM endstation of the Fermi FEL [2] and retrieve time-resolved ion-KER spectra for the ions from ion-TOF spectra. We will also discuss how several simplifications to this procedure lead to inaccurate reconstructions, which are not obvious to see in the resulting KER spectra but can be seen in the calibration procedure.

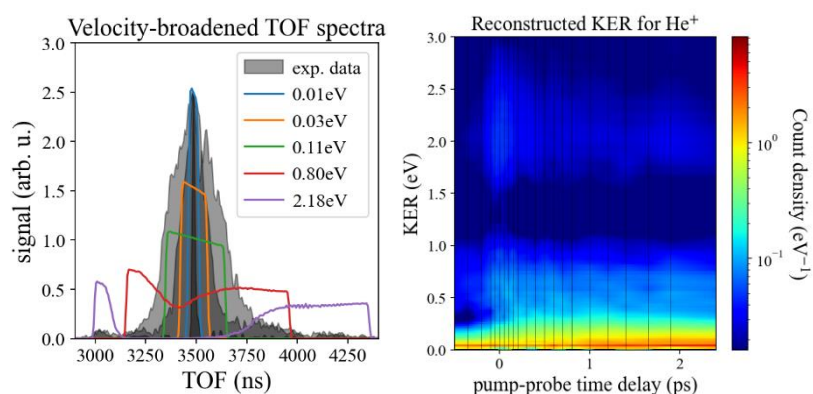


Figure: (Left) Simulated basis functions for different (isotropic) ion KER. The three-shaded regions represent ion TOF spectra taken at three different pump-probe time-delays (between the excitation and ionization lasers) showing characteristic broadening around the He<sup>+</sup> peak from coulomb explosion of Helium nanoclusters. (Right) Reconstructed ion-KER distributions from the left figure for He<sup>+</sup> at different pump-probe time-delays.

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## A setup for extreme ultraviolet wave packet interferometry using tabletop high harmonic generation

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Quantum interference techniques such as wave packet interferometry (WPI) in the extreme ultraviolet (XUV) regime set the basis for establishing advanced nonlinear spectroscopy methods in this wavelength regime [1]. These methods are however very difficult to implement at short wavelengths due to the required high phase stability and sensitivity. We are exploring methods based on acousto-optical phase modulation (PM) to solve these problems. First results from applications in seeded FELs and tabletop high-harmonic generation (HHG) are promising [2,3]. We designed, built and characterized a special compact interferometer [figure 1] that can be operated at intense laser conditions ( $\sim 5\text{mJ}$  per pulse) at  $800\text{nm}$ . Despite the strong angular dispersion induced by the ‘large’ AOM crystals, the setup is used successfully for the generation of higher harmonics up to  $\sim 26\text{ eV}$  (17H) in Argon [figure 2]. Here, we will present the characterization of the setup and an in-depth analysis of its application in HHG. Further, we will also show an outlook to the planned (PM-WPI) experiments in the XUV.

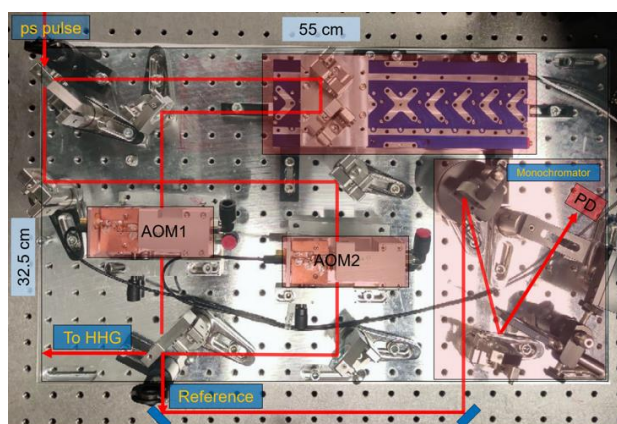


Figure 3

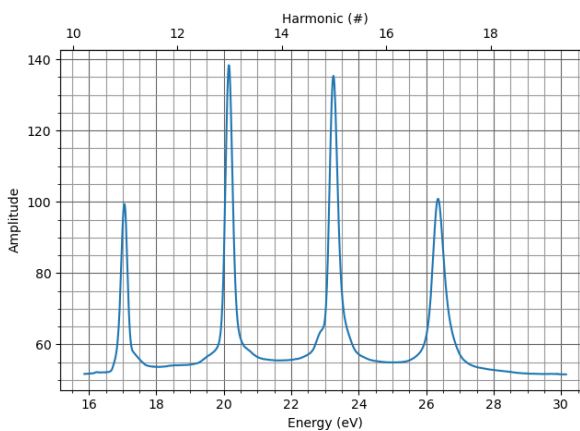


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## Quantum Information in Analogue Black Holes

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In an acoustic analogue system, as the ones obtained in BECs, a transonic fluid flow (i.e. a flow which is supersonic in a region of space and subsonic elsewhere), can be experimentally implemented in order to model a gravitational black hole. Quantum fluctuations of the sound field induce emission of Hawking quanta away from the acoustic horizon. This radiation is correlated and entangled to a "partner" which falls inside the analogous black hole. Here we study the entanglement in such systems by defining pseudo-spins for continuous variables in order to test the violation of Bell's inequalities in an acoustic black hole configuration.

## A Model for Quantum Diffractive Heating and Measurements of Quantum Diffractive Universality

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Collisions between trapped cold atoms and thermal background gases cause ensemble heating; the energy distribution and particle number of the trapped gas change with time. Heating presents a major challenge in analyzing trapped gases, and it must be characterized and accounted for to have accurate measurements. We propose a model that describes how the energy distribution of a trapped gas changes in time, and we demonstrate agreement between the model and experimental measurements for a trapped Rubidium gas subject to collisions from a thermal Argon background. We also show that this model demonstrates Quantum Diffractive Universality for several background gases, that the evolution for a trapped Rubidium ensemble subject to different background gases is identical under a rescaling of the energy. We then use this energy scaling to extract ratios of the velocity averaged cross-section  $\langle\sigma(v)v\rangle$  from experimental measurements, and we compare the results to those obtained from numerical quantum scattering calculations.

## Echoes in Space and Time

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Echo phenomena are widespread in physics, spanning NMR, plasma physics, nonlinear optics, cavity quantum electrodynamics, cold atoms physics, and more. We've recently identified possibly the simplest classical system that displays echoes—a group of randomly oriented free rotors with randomly distributed rotational velocities. After being excited by delayed impulsive kicks, the ensemble's mean orientation/alignment shows multiple full and fractional echoes. These echoes result from kick-induced filamentation of the rotational phase space, and I will present a simple toy model explaining this phenomenon at the high school level.

Alignment echoes, as predicted, were first observed optically in a CO<sub>2</sub> gas exposed to femtosecond laser pulses. We also employed the Coulomb explosion technique to analyze these echoes in various ways. The mechanism behind echo formation has broad applicability and implications across different physics fields. Notably, SLAC's demonstration of efficient high harmonic generation (up to the 75th) in tailored electron beams within free-electron lasers shares similarities with high-order fractional echoes seen in our molecular experiments. Alignment echoes are already proving helpful in exploring collisional relaxation in dense molecular gases.

We've recently expanded this concept to single quantum systems, exploring echoes in a single vibrating molecule (observed in 2020) and a single quantum Kerr-nonlinear oscillator—a paradigmatic model in cavity and circuit quantum electrodynamics and quantum optomechanics. Lastly, I'll discuss how our quest for echoes in single quantum systems has led us to propose a new form of spectroscopy for Gravitational Quantum States (GQS) of ultra-cold neutrons, atoms, and anti-atoms bouncing in the Earth's gravitational field.

## The Art of Converging Self-Consistent Field Calculations and Achieving Chemical Accuracy for DFT Calculations

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Self-consistent field (SCF) algorithm is at the very center of density functional theory (DFT) and Hartree-Fock methods in quantum chemistry. In practical calculations, SCF often encounters slow convergence and even failure. In this talk, we present a series of new methods to accelerate SCF convergence by utilizing linear-expansion shooting techniques (LIST) [1–4], which outperform Pulay's DIIS [5] and its recent improvements, including EDIIS and ADIIS [6–9].

On the other hand, the fundamental challenge of DFT is to design universally applicable, highly accurate exchange-correlation (XC) density functionals (DFs), but this goal is out of reach even after nearly 100 years of development with more than 200 XC DFs published [10,11]. In this talk, we present a transparent approach to this problem based on vector analysis of the functional space spanned by the 200 plus popular XC DFs in the literature [10,11]: the resulting combinatorial DFs can achieve chemical accuracy (*e.g.*, error in energetics < 1 kcal/mol or 0.04 eV) outperforming all existing XC DFs (including the best  $\omega$ B97M-V and M06-L DFs) across the board [12].

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## Ultrafast dynamics of highly-excited isolated tetracene molecules

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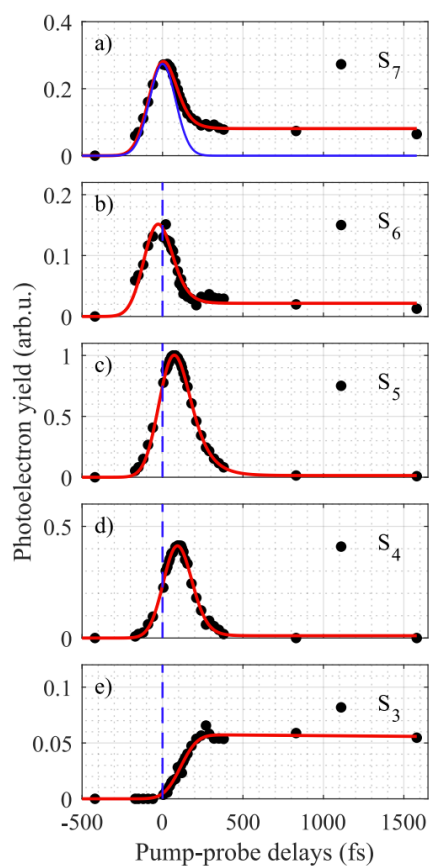
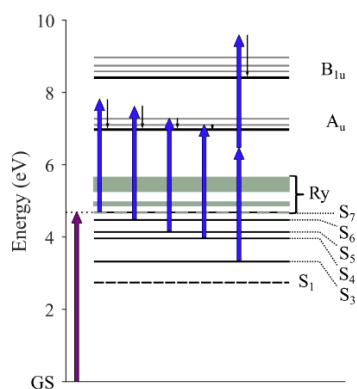
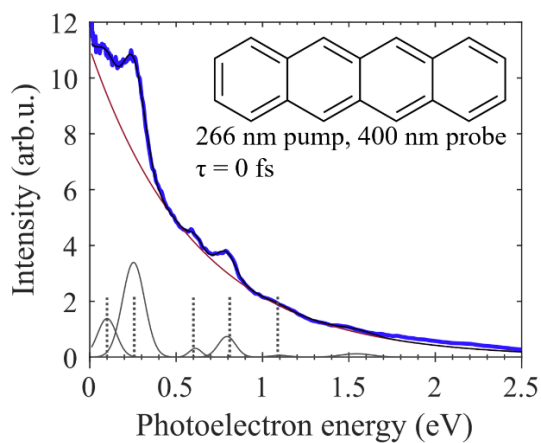
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Acenes, specifically tetracene and pentacene, are promising candidates for applications in organic photovoltaics since ensembles of these molecules can undergo singlet fission to produce two triplet excitations from a single singlet excitation. This process may thus allow to produce multiple charge carriers from a single absorbed photon, and therefore might help overcome fundamental limitations of the efficiency of solar cells. The potential applications motivate the fundamental study of the ultrafast excitation dynamics of these molecules and their aggregates to provide a fundamental understanding of the underlying processes and energetics.

I will present results of two spectroscopic studies of tetracene addressing a bright electronic transition of tetracene in the ultra-violet range of the electromagnetic spectrum. High-resolution fluorescence spectroscopy can provide detailed information on the vibronic structure of molecules as well as some insights into the relaxation dynamics, the method is limited to transitions of non-zero oscillator strength. Femtosecond pump-probe photoelectron spectroscopy on the other hand provides more detailed information on the relaxation dynamics without limitation to bright states, while lacking energy resolution. Our experimental work highlights the complementary nature of both techniques, in unravelling the relaxation of highly excited tetracene through a series of dark states. The experimentally obtained electronic structure including dark and bright states will be compared to CASPT2 calculations.

In addition, I will present initial data of femtosecond photoelectron spectroscopy of tetracene embedded in liquid helium nanodroplets. While the doping of organic molecules into superfluid helium nanodroplets offers a promising path to extend spectroscopic studies from isolated molecules to molecular clusters and aggregates, it also imposes additional challenges related to the interactions of photoelectrons with the superfluid helium environment.





## Attosecond time-resolved coincidence spectroscopy of atoms and small molecules

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Studying photoionization dynamics and characterising the time delays associated with the photoemission of an electron wave packet can unveil important characteristics of electronic correlations in atoms [1] and coupled electronic-nuclear dynamics in molecular systems [2, 3]. Especially in the latter case, attosecond photoelectron spectroscopy in combination with electron-ion coincidence detection is beneficial or even necessary since this allows disentangling the different photoionization and dissociation channels. Additionally, attosecond coincidence spectroscopy of the dissociative pathways may give access to the orientation of the molecule at the instant of photoionization.

In the first part of this work, we investigate the photoionization dynamics in C<sub>2</sub>H<sub>4</sub> molecules. Since C<sub>2</sub>H<sub>4</sub> is the smallest alkene, it is a good starting point to investigate this family. Our experimental setup consists of an attosecond beamline, based on high-order harmonic generation working at 50 kHz repetition rate. The attosecond pulse train source is combined with an ultrastable interferometer and a reaction microscope [4]. We perform RABBIT (Reconstruction of Attosecond Beating By Interference of Two-photon transitions) [5] measurements while detecting photoelectrons and photoions in coincidence. In the second part, we perform measurements using a slightly modified beamline to generate attosecond pulse trains using two colour laser fields. With these XUV fields we perform streaking-like [6,7] measurements in argon.

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## Local dissipation drives global relaxation in a molecular ultracold plasma with on-site disorder and long-range dipolar interactions

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The nitric oxide ultracold plasma evolves to form a disordered ensemble of dipoles populating a wide distribution of Rydberg and excitonic states concentrated in an energy interval within a few hundred GHz of the ionization threshold, doped by a trace population of more deeply bound Rydberg molecules. This residual population of lower- $n$  molecules includes a fraction that retains the selected principal quantum number,  $n_0$ . Electron-Rydberg,  $l$ -mixing collisions drive this population to non-penetrating states of high- $l$ . Excitation by mm-wave radiation tuned to resonance with  $n_0/(2)$  to  $(n_0 \pm 1)d(2)$  transitions depletes the plasma signal to an amplitude near zero, even though delayed selective field ionization spectra show that the distribution of states evolves by then to contain fewer than one percent in the  $n_0$  level resonant with the mm-wave field. Reading the nature of this coupling in the linewidths and depths of these depletion resonances, we see direct evidence that predissociation, which transfers population from the spectroscopically active  $(n_0 \pm 1)d(2)$  states to a system of free  $N(^4S) + O(^3P)$  atoms, bridges the closed plasma ensemble to a thermal continuum, in effect creating an open quantum system that combines the plasma with the reservoir of free atoms. We approximate these dynamics using a Markovian approach that applies the Lindblad master equation to a one-dimensional model of eleven spins with disorder and one dissipative site.

## Chirality-Induced Spin Selectivity in Electron Transport through Chiral Molecules: The Role of Vibrationally Assisted Spin-Orbit Coupling

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*July 30, 2023*

The chirality-induced spin selectivity effect, which is the preferential transmission of electrons based on their spins through chiral materials, has attracted considerable interest due to its potential applications in spintronics, electrochemistry, optoelectronics, as well for providing a deeper understanding of spin-selective chemical reactions and biological processes. This effect has been experimentally validated across various materials, such as organic molecules like double-stranded DNA, and setups, such as spin-dependent single-molecule conductance measurements. From a theoretical perspective, the CISS effect arises from the interplay between geometrical helicity and spin-orbit interactions and is a nonequilibrium phenomenon. While existing model Hamiltonians reproduce experimental observations, they often rely on unrealistic spin-orbit interaction parameters, possibly due to neglecting electron correlations arising due to Coulomb and electron-vibrational interactions. To address this, we present initial results investigating the impact of vibrationally assisted spin-orbit coupling on spin-dependent quantum transport. We employ a combination between hierarchical equations of motion with Ehrenfest dynamics. As part of future work, we plan to explore alternative approaches beyond Ehrenfest to gain a deeper understanding of the chirality-induced spin selectivity effect.

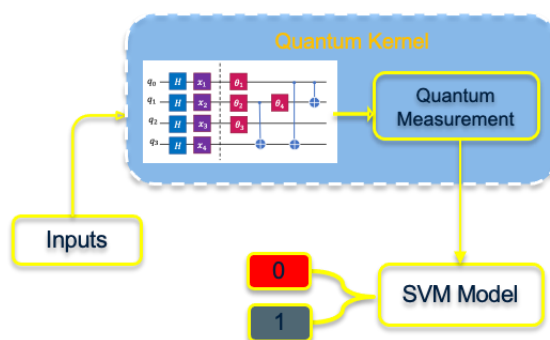
## How to find the optimum quantum ansatz for quantum Kernels?

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The potential of quantum computing for enhancing machine learning (ML) has been acknowledged, but creating quantum ML models that surpass classical ML models remains an unanswered challenge <sup>[1]</sup>. A solution is presented in the form of a Bayesian algorithm aimed at constructing quantum kernels for support vector machines (SVM). This novel approach involves tailoring quantum gate sequences to fit the data <sup>[2]</sup>. The algorithm encodes the original data to the quantum space and then employs a gradual augmentation of quantum circuits by adding quantum gates. These gates are chosen based on a Bayesian information criterion used as a metric for circuit selection. Furthermore, the algorithm fine-tunes the parameters of the locally most efficient quantum circuits using Bayesian optimization. The outcome of this methodology is particularly noteworthy: the quantum models developed exhibit markedly superior performance compared to optimized classical models that employ traditional kernels. In essence, the study presents a pioneering Bayesian algorithm that optimizes quantum kernel construction for support vector machines. This algorithmic innovation outpaces the capabilities of classical models with standard kernels in solving classification problems. In addition, this compositional algorithm can be applied to optimize the ansatz for kernel-based machine learning tasks behind SVM such as Gaussian Process and other ansatz-dependent algorithms such as Variational Quantum Eigensolvers (VQE).



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## Photoelectron Photoion Multicoincidence Study of Micro-Solvated Thymine Molecules

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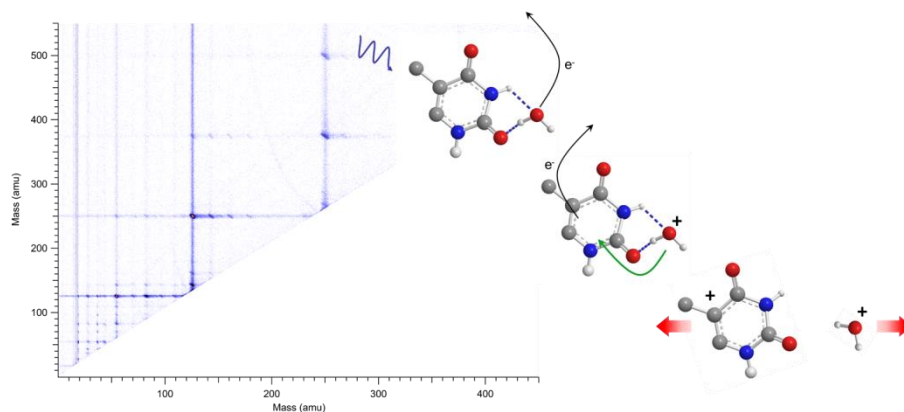
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The study of small biomolecules, such as amino acids and nucleobases, and their interactions with each other and the surrounding solvent molecules, is highly important, since intermolecular interactions often define their biological function [1]. Studying biomolecules in the gas phase allows unparalleled detail and fundamental insights into energetics and dynamics at the molecular level, due to the simplicity and isolation of the system. However, *in-vivo* bio-molecular systems exist mostly in the condensed phase, specifically in aqueous systems. These environments can affect not only ionisation energies [2, 3], but also cationic fragmentation and relaxation pathways. Photoelectron spectroscopy is of particular interest for such studies, due to its sensitivity to the sometimes subtle effects of the environment on the electronic structure as well as on the relaxation pathways and dynamics. The created photoelectrons and secondary electrons created during post-ionisation relaxation are important for the field of radiation chemistry since low energy electrons can trigger processes and reactions damaging biological material.

A prominent example for such a relaxation pathway is intermolecular Coulombic decay (ICD) [4], see figure 1, where after the ionisation of an inner valence shell electron, the created vacancy is filled by an outer valence shell electron. The excess energy is removed via the emission of an additional electron from a neighbouring molecule. This creates an energetically low lying dicationic state with the two positive charges spatially separated. The study of clusters over a wide size range with double imaging photoelectron photoion coincidence (i2PEPICO) spectroscopy [3] can be exploited to bridge the gap between the gas phase and the condensed phases for bio-relevant systems where ion-ion coincidence allows for easy identification of signals arising from non-local auto-ionisation processes of clusters such as ICD. Additionally, the disentanglement of signal contributions arising from varying cluster sizes and their fragmentation pathways can be achieved.

This talk will present preliminary results of a photoelectron photoion (multi) coincidence study of small water clusters  $(\text{H}_2\text{O})_n$  ( $n=1-10$ ) and water-thymine complexes. The advantage of filtering photoelectron spectra by not only a single ionisation channel (i2PEPICO) but also in coincidence with double ionisation events (i2PEPIPICO) will be demonstrated in the context of identification of fragmentation pathways with and without the involvement of ICD processes.



**Figure 1.** Ion-ion coincidence map of micro-solvated thymine ionised at a photon energy of 40 eV. To the right, an ICD process of a thymine water complex is illustrated.

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## Quantum State Preparation in a Micromaser

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Quantum algorithms process information encoded into quantum states via an appropriate unitary transformation. Their purpose is to deliver a sought-after target state that represents the solution of a predefined computational problem. From a physical perspective, this process can be interpreted as a quantum control problem, where a given target state is to be prepared through an optimally tailored unitary transformation. In this talk we adopt the one-atom (or micro-) maser as a model to study the transfer of quantum information in state space. We consider a string of atoms that interact sequentially with a cavity mode, to understand the relation between the cavity's convergence towards a given target state and the entanglement content of the injected atomic string.



## Energy-Dependence of Feshbach Resonances in a Hybrid Atom-Ion System

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We investigate the inelastic loss dynamics around Feshbach resonances between neutral atoms and ions depending on the collision energy. By immersing a single  $^{138}\text{Ba}^+$  ion in an ultracold cloud of  $^6\text{Li}$ , we have demonstrated the enhancement of both two- and three-body interactions through changes in the ion's electronic state and motional energy. Currently, we probe the atom-ion interaction rate while tuning the ion's kinetic energy and atomic cloud temperature. We observe features such as the suppression of inelastic loss processes for higher collisional energies on resonance. This energy dependence could provide insight into the nature of the interaction dynamics.

## Efficient interpolation of molecular entropy across chemical space

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Chemical space refers to the theoretical space that encompasses all possible chemical compounds, molecules, and structures. It is a multidimensional space, where each dimension represents a unique chemical property. Owing to the immense size of this chemical space, researchers interested in a target application concentrate on a subspace. The quest for an optimal molecule within a chemical subspace can still be demanding, exemplified by an estimated range of  $10^{23}$  to  $10^{60}$  molecules possessing medicinal properties. [1]. Moreover, the substantial costs associated with experiments and theoretical calculations impose limitations on the comprehensive exploration of the entire space. The vast chemical space and limited data underscore the need for a tool to guide chemists efficiently and precisely. The astonishing advancement of data-driven methods over the past decade presents a viable solution to the small-data chemical space interpolation problem. Indeed, numerous publications on data-driven models for chemical space interpolation have increased in recent years. [2-7].

In the present work, we consider the interpolation of the entropy of molecules within the chemical subspace defined by the QM9 dataset [8], which comprises 133,885 small organic molecules. The process of constructing a data-driven model to interpolate the chemical subspace is broken down into three steps: (1) dataset preparation, (2) creation of a chemical descriptor, and (3) model selection. In this work, we place emphasis on the latter two aspects.

A chemical descriptor is a carefully designed input to a data-driven model, which concentrates the most important physical attributes in the most concise manner possible, in order to maximize the predictive capability of the model while minimizing the computational cost [9]. An interpretable model not only permits the justification of outcomes but also serves as the key to unveiling the underlying physics. In this work, we developed the nine dimensional CM-GC descriptor with embedded physical insights inspired by Coulomb matrix descriptor [2] and the Gershgorin circle theorem [10, 11].

Different molecular properties exhibit vastly different variation across chemical space. Therefore, the most data-efficient predictions are based on models tailored to the specific molecular properties. We implemented Bayesian information criterion (BIC) [12] to choose the optimal kernel for the Gaussian process regression (GPR) [13] model for interpolating entropy space.

In conclusion, we created a novel low-dimensional chemical descriptor and tailored a data-driven model targeting entropy predictions. We employed the optimized GPR model in conjunction with the 9D CM-GC descriptor to accurately interpolate the entropy subspace with chemical accuracy using only 40 training points. This work not only contributes to chemical space interpolation using a interpretable descriptor, but also highlights the importance model selection especially for small data problems.

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<p align="center"><b>RTG 2717 Annual Convention 2023</b>  <b>August 21 to 26</b>                      UBC Vancouver, Canada</p>							
	Monday, August 21	Tuesday, August 22	Wednesday, August 23	Thursday, August 24	Friday, August 25	Saturday, August 26 6am to 9pm	
9:00	Arrival & Welcome <b>Momose &amp; Stienkemeier</b>	PI Lecture Valery MILNER	Excursion - St. Mark's Summit Hike	PI Lecture Andreas BUCHLEITNER	PI Lecture Yan Alexander WANG	Panorama Ridge Hike	
	PI Lecture Tobias SCHAETZ				PostDoc presentation Ioannis MAKOS		PostDoc presentation Sebastian HARTWEG
10:00	PostDoc presentation Graziano AMATI	PostDoc presentation Christina HOFER			Coffee Break		Coffee Break
	Coffee Break	Coffee Break			PHD presentation Rysa GREENWOOD		PHD presentation Barbara MERZUK
11:00	PHD presentation Mayara da SILVA SANTOS	PHD presentation Erik FRIELING			PHD presentation Kevin SCHWARZ		PHD presentation Ruoxi WANG
	PHD presentation Pranav KAIRON	PHD presentation Carina HOBBS			PHD presentation Karin THALMANN		PHD presentation Rudolf SMORKA
	PHD presentation Samuel KELLERER	PHD presentation Nicolai GOELZ			Lunch Break		Lunch Break
12:00	Lunch Break	Lunch Break			PHD presentation Anja SEEGBRECHT		PHD presentation Elham TORABIAN
	PHD presentation Hatsuki OTANI	PHD presentation Benjamin STEINER			PHD presentation Amirhossein RASHIDI		PHD presentation Brendan WOUTERLOOD
	PHD presentation Daniel HOENIG	PHD presentation Olesya ABLYSOVA			PHD presentation Aaron NGAI		PHD presentation Andreas WOITZIK
	PHD presentation Max FLACH	PHD presentation Kevin MARROQUIN			Coffee Break		Coffee Break
03:00	Coffee Break	Coffee Break			PHD presentation S D GANESHAMANDIRAM		PHD presentation Joachim SIEMUND
03:30	PHD presentation Ian MacPHAIL-BARTLEY	PHD presentation Philipp ELSAESSER			PHD presentations Giorgio CLUBERTO		PHD presentations Yun-wen MAO
	PHD presentation Lucas WEITZEL	PHD presentation Fabian RICHTER			PHD presentation Avinash DESHMUKH		Final Remarks Momose & Stienkemeier
	PHD presentation Arne MORLOK	PHD presentation Sudhang VARSHNEY			Lab Tours		Lab Tours
04:30	PHD presentation Yilin LI (?)				PAC Meetings		PAC Meetings
05:00	PI Meeting	Lab Tours			Lab Tours		Lab Tours
06:00					Conference Dinner & After Dinner Talk: Ilya Averbukh		Poster Session
7:00	PI Dinner	Free evening		Free evening			
8:00							