

**ANNUAL CONVENTION 2018**

**IRTG CoCo**

*Cold Controlled Ensembles in Physics and Chemistry*

# BOOK OF ABSTRACTS

## 4<sup>th</sup> CoCo Annual Convention

**July 23 – 27, 2018**

**Stadthotel Freiburg/University of Freiburg  
Freiburg, Germany**

**DFG**



**UNI  
FREIBURG**

## Impressum

IRTG 2079 / Cold Controlled Ensembles in Physics and Chemistry

Institute of Physics

University of Freiburg

Hermann-Herder-Straße 3

79104 Freiburg

<http://www.irtg-coco.uni-freiburg.de>



## Organisation

THE ANNUAL CONVENTION IS AN IMPORTANT PART OF THE STRUCTURED GRADUATE PROGRAM OF THE IRTG 2079. THE RESEARCHERS FROM UBC/VANCOUVER AND UNIVERSITY OF FREIBURG MEET TO DISCUSS THEIR RESEARCH, PLAN FURTHER PROJECTS AND PUBLICATIONS, AND STRENGTHEN THE NETWORK BETWEEN BOTH UNIVERSITIES.

## Organisation

### **IRTG 7079 „Cold Controlled Ensembles in Physics and Chemistry“**

#### Organizers

Frank Stienkemeier, University of Freiburg

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## Financial Support





## General Information

### Duration

Monday, July 23, 2018, 9:00 a.m. – Friday, July 27, 2018, 8:00 p.m.

### Location

Talks of doctoral researchers, postdoctoral researchers and PIs as well as meals:

Stadthotel Freiburg, Karlstraße 7, 79104 Freiburg

Meetingroom: Feldberg/Tüniberg

Lab tours, Poster sessions and PAC meetings:

University of Freiburg

Institutsviertel

Poster sessions: Physics Highj Rise Building, Foyer 1<sup>st</sup> Floor.

### Travel Information – Individual Journeys

From Frankfurt Main Airport: train to Freiburg Hauptbahnhof; can be booked online [www.db.de](http://www.db.de)

From Zurich Airport: train to Freiburg Hauptbahnhof directly or via Basel SBB; can be booked online unter [www.sbb.ch](http://www.sbb.ch)

In Freiburg from Main Railway Station to Stadthotel Freiburg: approx. 15 minutes walking distance or by tram #4 from Freiburg Hauptbahnhof to Siegesdenkmal (direction -> Zähringen; one way ticket costs 2,30 €). For more details, please see the map on the page 3.

### Accommodation

Doctoral researchers and PIs from UBC will be accommodated in Stadthotel Freiburg (if not otherwise agreed).

Stadthotel Freiburg

Karlstraße 7

79104 Freiburg

### Meals & Drinks

For all participants: meals and drinks during the scientific program as well as lunches and dinners are included. Lunches and dinners will take place in Hotel Restaurant in the form of a buffet. For lunches: water and apple juice included; for dinners: 2 drinks (softdrinks, beer or wine) included. For participants accommodated in Stadthotel Freiburg, breakfast is included too.

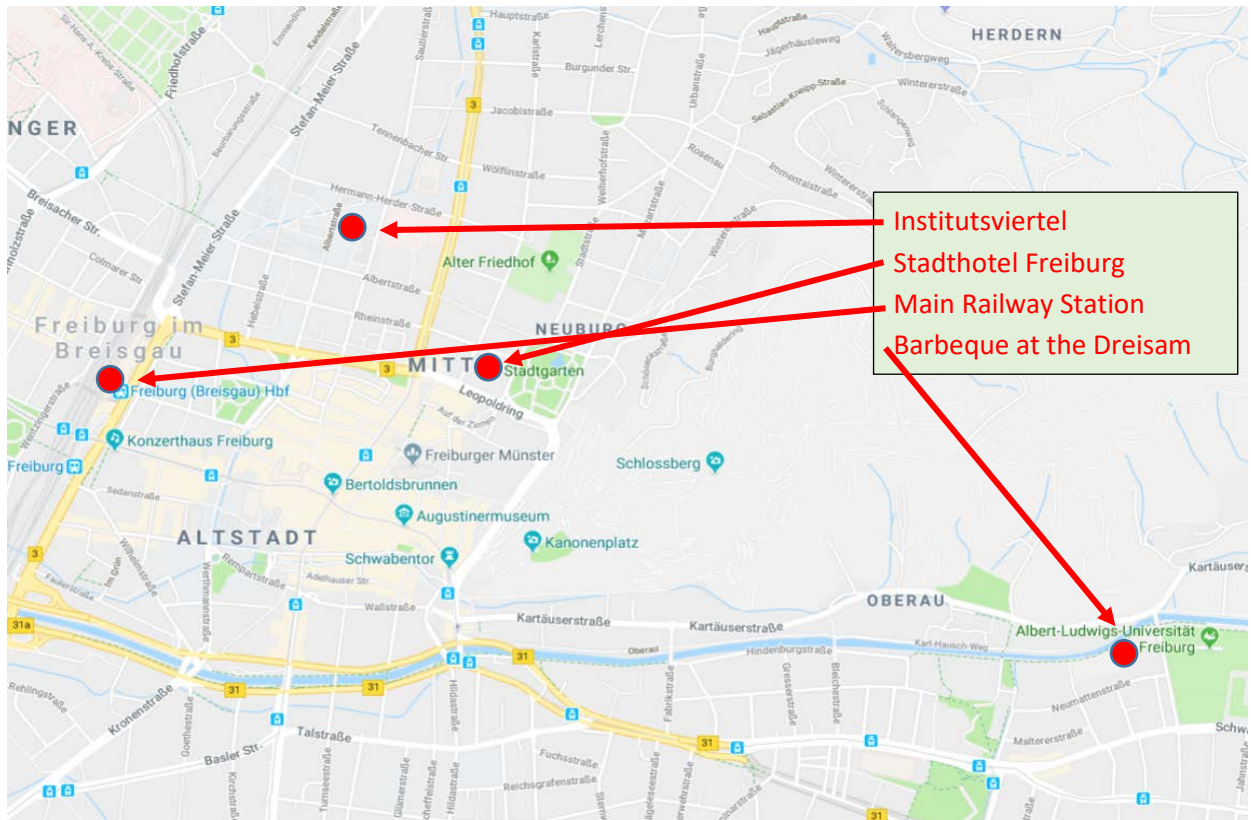
### Excursion / Group activities

On Monday, July 23, 2018, a soccer match and the barbecue at the Draisam river will be organized. A hiking trip will take place on Wednesday, July 25, 2018. Please bring appropriate clothes and shoes!

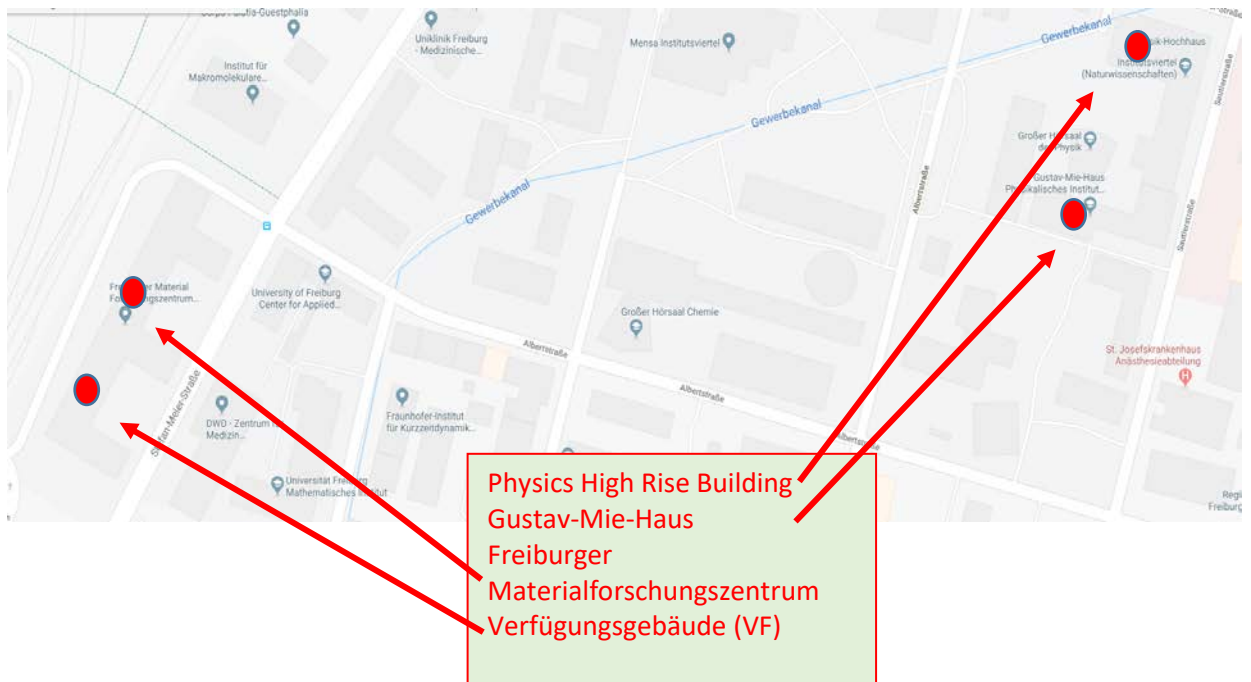
### WiFi

Eduroam will be available throughout the Institutsviertel. Free WiFi will be available during lectures and talks in the Stadthotel Freiburg.

## Freiburg City Map



## Map of Institutsviertel





## Scientific Program

Monday, July 23, 2018

|            |  |
|------------|--|
| 9:00 a.m.  | Frank Stienkemeier, Takamasa Momose:<br>Opening remarks  |
| 9:05 a.m.  | Michael Thoss:<br>"Quantum dynamics in molecular systems and condensed matter: Theory and applications to photoinduced processes"            |
| 10:00 a.m. | Matthias Bohlen:<br>"Spectroscopy of perylene diimide and oligoacenes on rare gas clusters"  |
| 10:30 a.m. | Coffee Break   |
| 11:00 a.m. | Fumika Suzuki:<br>"Toward the Separation of Enantiomers by the Casimir-Polder Force"   |
| 11:30 a.m. | Andreas Wituschek:<br>"Stable platform for phase-modulation of seed lasers facilitating all-XUV coherent nonlinear time-domain spectroscopy" |
| 12:00 p.m. | Pascal Weckesser:<br>"Building a fast deterministic single ion source for an atom-ion experiment"  |
| 12:30 p.m. | Lunch Break  |
| 1:30 p.m.  | Reyhaneh Ghassemizadeh:<br>"Ab Initio study on molecular charge transport and conformational analysis via IR-Raman spectroscopy"             |
| 2:00 p.m.  | Kariman Elshimi:<br>"Photoelectron spectroscopy of size-selected clusters at free electron lasers"   |
| 2:30 p.m.  | Jordan Fordyce:<br>"Molecular superrotors in helium nanodroplets"  |
| 3:00 p.m.  | PAC Meeting 1<br>Coffee Break  |
| 4:00 p.m.  | PAC Meeting 2  |
| 5:00 p.m.  | Soccer Match   |
| 7:00 p.m.  | Barbecue at the Dreisam  |

Tuesday, July 24, 2018

|            |   |
|------------|---|
| 8:30 a.m.  | PI Meeting  |
| 9:30 a.m.  | Kirk Madison:<br>"Ultra-cold reactions of Li dimers and using quantum measurement to realize a primary and self-defining UHV pressure standard" |
| 10:30 a.m. | Coffee Break  |
| 11:00 a.m. | Manish Vashishta:<br>"Study of collisional processes of magnetically trapped cold methyl radicals"  |
| 11:30 a.m. | Pinrui Shen:<br>"A primary, self-defining UHV standard based on universal van der Waals scattering"   |



|            |   |
|------------|---|
| 12:00 p.m. | Janine Franz:<br>"Macroscopic QED study of the interatomic Coulombic decay"   |
| 12:30 p.m. | Lunch Brak  |
| 1:30 p.m.  | Jonas Grzesiak:<br>"Reactive scattering between metastable helium atoms and ultracold lithium atoms"                                |
| 2:00 p.m.  | Oliver Stauffert:<br>"Electron - phonon coupling with density functional theory including environment effects and polaron dynamics" |
| 2:30 p.m.  | Aghigh Jalehdoust:<br>"Construction of a new source for organic cluster generation"   |
| 3:00 p.m.  | Coffee Break  |
| 4:00 p.m.  | PAC Meeting 3<br>Lab Tour: von Issendorff   |
| 5:00 p.m.  | PAC Meeting 4<br>Lab Tour: Stienkemeier   |
| 6:00 p.m.  | Poster Session  |
| 7:00 p.m.  | Dinner / Pls' Dinner  |

## Wednesday, July 25, 2018

|           |           |
|-----------|-----------|
| 9:00 a.m. | Excursion |
| 7:00 p.m. | Dinner    |

## Thursday, July 26, 2018

|            |  |
|------------|--|
| 9:00 a.m.  | Giuseppe Sansone:<br>"Multi-color pulse shaping at Free Electron Lasers"   |
| 10:00 a.m. | Markus Debatin:<br>"Cold interactions between Lithium and Barium"  |
| 10:30 a.m. | Coffee break   |
| 11:00 a.m. | Brendan Moore:<br>"Infrared spectroscopy of alanine water clusters and water aggregation in solid parahydrogen"  |
| 11:30 a.m. | Luke Melo:<br>"Integration of Confocal Raman and interferometric scattering microscopies for the analysis of nanoscale complex and biological specimens" |
| 12:00 p.m. | Sebasitan Fuchs:<br>"Collective enhancement of the Casimir-Polder potential"   |
| 12:30 p.m. | Lunch Break  |
| 1:30 p.m.  | Ulrich Bangert:<br>"Many-body resonances in dilute gas-phase systems"  |
| 2:00 p.m.  | Simon Dold:<br>"Time-dependent X-Ray diffraction imaging of metal clusters"  |



|           |  |
|-----------|--|
| 2:30 p.m. | Jun Dai<br>"Possible research projects"                          |
| 3:00 p.m. | Coffee Break   |
| 4:00 p.m. | PAC Meeting 5<br>Lab Tour: Schätz                                |
| 5:00 p.m. | PAC Meeting 6<br>Lab Tour: Sansone                               |
| 6:00 p.m. | Poster Session   |
| 7:00 p.m. | Dinner   |
| 8:00 p.m. | Takamasa Momose:<br>"Spectroscopy of hydrogen and antihydrogen " |

Friday, July 27, 2018

|            |  |
|------------|--|
| 9:00 a.m.  | Roman Krems:<br>"Applications of machine learning for quantum dynamics"  |
| 10:00 a.m. | Audrey Scognamiglio:<br>"Photo-ionization and electron-impact-ionization-TOF spectrometry for the detection of large organic molecules embedded in cluster beams"                    |
| 10:30 a.m. | Coffee break   |
| 11:00 a.m. | Tobias Brünner:<br>"Signatures of indistinguishability in bosonic many-body dynamics"  |
| 11:30 a.m. | Julian Schmidt:<br>"Optical trapping of ion crystals and ion-atom ensembles"   |
| 12:00 p.m. | Daniel Uhl:<br>"Photoelectron two-dimensional coherent spectroscopy"   |
| 12:30 p.m. | Lunch Break  |
| 1:30 p.m.  | Meral Ari:<br>"Computational screening of tetra thiophenyl-substituted phthalocyanines as bulk heterojunction solar cell materials and comparison with the phenoxy-substituted form" |
| 2:00 p.m.  | Marcel Binz:<br>"Coherent multidimensional spectroscopy of dilute gas-phase nanosystems"   |
| 2:30 p.m.  | Rodrigo Vargas-Hernández:<br>"Machine learning for many-body quantum physics"  |
| 3:00 p.m.  | Coffee Break   |
| 4:00 p.m.  | PAC Meeting 7<br>Labtour: Dulitz   |
| 5:00 p.m.  | PAC Meeting 8  |
| 6:00 p.m.  | PAC Meeting 9  |
| 7:00 p.m.  | Dinner   |





PAC Meetings

## PAC meetings

PAC Meetings on Monday, July 23, 2018

- 3:00 p.m. Andreas Wituschek, Frank Stienkemeier, David Jones
- 3:00 p.m. Fumika Suzuki, Takamasa Momose, Stefan Buhmann
- 4:00 p.m. Kariman Elshimi, Bernd von Issendorff, David Jones
- 4:00 p.m. Jordan Fordyce, Valery Milner, Frank Stienkemeier
- 4:00 p.m. Reyhaneh Ghassemizadeh, Michael Walter, Takamasa Momose

PAC Meetings on Tuesday, July 24, 2018

- 4:00 p.m. Janine Franz, Stefan Buhmann, Ed Grant
- 4:00 p.m. Mathhias Bohlen, Frank Stienkemeier, David Jones
- 4:00 p.m. Manish Vashishta, Takamasa Momose, Marcel Mudrich, Katrin Dulitz
- 5:00 p.m. Pinrui Shen, Kirk Madison, Frank Stienkemeier
- 5:00 p.m. Aghigh Jalehdoost, Bernd von Issendorff, David Jones
- 5:00 p.m. Jonas Grzesiak, Marcel Mudrich, Katrin Dulitz, Takamasa Momose

PAC Meetings on Thursday, July 26, 2018

- 4:00 p.m. Ulrich Bangert, Frank Stienkemeier, Takamasa Momose
- 4:00 p.m. Sebastian Fuchs, Stefan Buhmann, Roman Krems
- 4:00 p.m. Luke Melo, Ed Grant, Bernd von Issendorff
- 5:00 p.m. Oliver Stauffert, Michael Walter, Roman Krems
- 5:00 p.m. Brendan Moore, Takamasa Momose, Frank Stienkemeier
- 5:00 p.m. Pascal Weckesser, Tobias Schätz
- 5:00 p.m. Simon Dold, Bernd von Issendorff, Ed Grant

PAC Meetings on Friday, July 27, 2018

- 4:00 p.m. Rodrigo Vargas-Hernández, Roman Krems, Tobias Schätz
- 4:00 p.m. Marcel Binz, Frank Stienkemeier, Valery Milner
- 4:00 p.m. Meral Ari, Michael Walter
- 5:00 p.m. Julian Schmidt, Tobias Schätz, Kirk Madison
- 5:00 p.m. Audrey Scognamiglio, Frank Stienkemeier, Valery Milner
- 5:00 p.m. Jun Dai, Roman Krems
- 6:00 p.m. Markus Debatin, Tobias Schätz
- 6:00 p.m. Daniel Uhl, Frank Stienkemeier, Roman Krems



Notes

Notes



## Abstracts – Pls' Lectures

(in alphabetical order)



## Applications of machine learning for quantum dynamics

Roman Krems and Rodrigo Vargas-Hernandez

*Department of Chemistry, University of British Columbia, Vancouver, Canada*

Machine learning is becoming a new tool for physics and chemistry research. This presentation will discuss how quantum theory of molecular dynamics can benefit from machine learning. In particular, it will be argued that combining machine learning with quantum dynamics calculations allows one to ask new questions and may help solve problems generally considered unfeasible.

The main focus of this presentation will be on the inverse scattering problem in chemical reaction dynamics. I will illustrate a machine-learning approach that can be used to build global potential energy surfaces (PES) for reactive molecular systems based on feedback from quantum scattering calculations. The method is designed to correct for the uncertainties of quantum chemistry calculations and yield potentials that reproduce accurately the reaction probabilities in a wide range of energies. These surfaces are obtained automatically and do not require manual fitting of the ab initio energies with analytical functions. The PES are built from a small number of ab initio points by an iterative process that incrementally samples the most relevant parts of the configuration space. Using the dynamical results of previous authors as targets, we show that such feedback loops produce accurate global PES with 30 ab initio energies for the three-dimensional  $\text{H} + \text{H}_2 \rightarrow \text{H}_2 + \text{H}$  reaction and 290 ab initio energies for the six-dimensional  $\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$  reaction [1]. We also introduce a method that quickly converges to an accurate PES without the a priori knowledge of the dynamical results.

In the second part of the talk, I will illustrate how machine learning can be used for extrapolation of properties of complex quantum systems. I will describe a machine-learning method for predicting sharp transitions in a Hamiltonian phase diagram by extrapolation [2]. The method is based on Gaussian Process regression with a combination of kernels chosen through an iterative procedure maximizing the predicting power of the kernels. The method is capable of extrapolating across the transition lines. The calculations within a given phase can be used to predict not only the closest sharp transition, but also a transition removed from the available data by a separate phase. This method is thus particularly valuable for searching phase transitions in the parts of the parameter space that cannot be probed experimentally or theoretically.

[1] R. A. Vargas-Hernández, Y. Guan, D. H. Zhang, R. V. Krems, „A machine-learning approach for the inverse scattering problem in quantum reaction dynamics“, arXiv: 1711.06376.

[2] R. A. Vargas-Hernández, J. Sous, M. Berciu, R. V. Krems, „Extrapolating quantum observables with machine learning: inferring multiple phase transitions from properties of a single phase“, arXiv: 1803.08195.



## **Ultra-cold reactions of Li dimers and using quantum measurement to realize a primary and self-defining UHV pressure standard**

Kirk W. Madison

*Center for Research on Ultra-Cold Systems (CRUCS), University of British Columbia, 6221 University Blvd., Vancouver, BC, V6T 1Z16221 University Blvd., Vancouver, BC, V6T 1Z1, Canada*

We report recent measurements of state dependent ultra-cold chemical reactions of  $\text{Li}_2$  in the lowest lying triplet potential. These dimers are formed by STIRAP of Feshbach molecules in a nearly quantum degenerate atomic gas. The measurements reveal that the dominant loss channel of the lowest lying state in the triplet potential, a predicted barrierless trimer reaction<sup>1</sup>, proceeds near the unitarity limit. This is the work of Gene Polovy, Erik Frieling, Denis Uhland, and K.W. Madison.

We also discuss how quantum diffractive collisions can be observed with cold atoms exposed to a room temperature background gas<sup>2</sup>, and we discuss a recent discovery that these collisions, by virtue of the quantum measurement that they induce of the sensor atom, can be used to create a self-defining, primary, quantum pressure standard for ultra-high vacuum. This is the work of Pinrui Shen, James L. Booth, Roman Krems, Rodrigo Vargas, and K.W. Madison

[1] Michal Tomza, Kirk W. Madison, Robert Moszynski, Roman V. Krems, Phys. Rev. A 88, 050701(R) (2013)

[2] David E. Fagnan, Jicheng Wang, Chenchong Zhu, Pavle Djuricanin, Bruce G. Klappauf, James L. Booth, and Kirk W. Madison, Phys. Rev. A 80, 022712 (2009).



## Spectroscopy of hydrogen and antihydrogen

Takamasa Momose

*Department of Chemistry, The University of British Columbia, 2036 Main Mall, Vancouver BC,  
CANADA*

Spectroscopy of hydrogen atom has played a central role in the development of theories of fundamental physics, including quantum mechanics and quantum electrodynamics. Antihydrogen, the bound state of an antiproton and positron, is the antimatter of hydrogen atom, and has only recently been created at CERN by a few collaborations. In the last two years, the ALPHA (Antihydrogen Laser PHysics Apparatus) Collaboration at CERN has made a significant progress in antihydrogen formation, resulting in hundreds of trapped anti-atoms available for spectroscopy. With these trapped antihydrogen, ALPHA was able to record the 1S hyperfine transition, 1S-2S forbidden transition, and 1S- 2P allowed transition for the first time. Precision measurements of these transitions will provide tests of fundamental symmetries between matter and antimatter. In this talk, I will provide an overview of history of hydrogen spectroscopy and its antimatter counterpart.



## Multi-color pulse shaping at Free Electron Lasers

Giuseppe Sansone

*Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

The generation of intense, multicolor fields in the extreme ultraviolet spectral range at Free Electron Lasers (FELs) opens new perspectives for the characterization and control of nonlinear processes in atoms and molecules. In particular, these sources give access to the high intensities required for the observation and investigation of nonlinear processes, and, using suitable delay lines, they can be used for the implementation of XUV-pump-XUV-probe experiments.

The seeded FEL FERMI (Trieste, Italy) offers the possibility to synthesize multicolor coherent fields, whose amplitudes and relative phases can be independently controlled. Recently the first experiment demonstration of the coherent control of the photoionization process in neon atoms was reported [1]. In the temporal domain, the coherent superposition of two or more coherent harmonics leads to a complex temporal structure, whose characteristics depend on the relative phases between the harmonics.

I will also present experimental data on the complete temporal characterization of attosecond pulse trains with only a partial synchronization with an external laser field. I will describe also the possibility to completely shape the temporal characteristics of multicolor fields in the XUV and X-ray spectral range using FELs.

[1] K. Prince *et al* Nature Phot. **10**, 176-179 (2016).



## Quantum dynamics in molecular systems and condensed matter: Theory and applications to photoinduced processes

Michael Thoss

*Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

The accurate theoretical treatment and simulation of dynamical processes in many-body quantum systems is a central goal in chemical and condensed matter physics. In this talk, I will discuss our recent work in this area. After an introduction to the topic and an overview of different dynamical methods, I will focus on time-dependent multiconfiguration methods as an example for basis-set approaches to quantum dynamics. Applications of the methodology to photoinduced electron transfer processes are presented, including electron transfer in donor-acceptor complexes and electron injection at dye-semiconductor interfaces. Moreover, recent studies of intramolecular singlet fission are discussed.





**Abstracts – Doctoral and Postdoctoral Researchers' Talks**  
(in alphabetical order)



## Computational screening of tetra thiophenyl-substituted phthalocyanines as bulk heterojunction solar cell materials and comparison with the phenoxy-substituted form

Meral Ari

*Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

Tetra thiophenyl-substituted phthalocyanines were screened computationally as bulk heterojunction organic solar cell materials of phthalocyanines (Pcs) with the aim of finding more efficient products. The electronic absorption spectrum and the molecular orbital properties of peripherally and non-peripherally tetrasubstituted Pcs were investigated by DFT/TDDFT calculations and substitution effect was screened. The screened compounds were found to be promising for providing good performance on BHJ solar cells with their small band gaps, red-shifted absorption bands in near infrared region, deep HOMO energy levels and high electron mobilities. Furthermore, the model of Scharber et al. [1] was used for open-circuit voltage (Voc) prediction for Pcs as the donor moiety and [6,6]-phenyl-C<sub>61</sub>-butyric acid methyl ester (PCBM) as the acceptor moiety. Peripheral Pc provides higher calculated eVoc value of 0.47. Calculated absorption bands are compared with the experimental wavelength values. Finally, all the results are compared with the results for the tetra phenoxy-substituted Pcs from the previous study [2] to see the effect of thio-oxy difference.

[1] M.C. Scharber, D. Mühlbacher, M. Koppe, P. Denk, C. Waldauf, A.J. Heeger and C.J. Brabec, *Adv. Mater.* **18**, 789 (2006).

[2] M. Ari, 1st International Conference in Computing, Information Technology and Business Applications (ICCITBA), Durres, Albania, 2017.



## Many-body resonances in dilute gas-phase systems

Ulrich Bangert<sup>1</sup>, Lukas Bruder<sup>1</sup>, Marcel Binz<sup>1</sup>, Markus Schulz-Weiling<sup>2</sup> and Frank Stienkemeier<sup>1</sup>

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

<sup>2</sup>*Department of Chemistry, University of British Columbia, Vancouver British Columbia, Canada V6T*

1Z1

We investigate the collective behavior of atomic gases at low density and ambient temperature. In this regime, interatomic interactions are small and collective effects are masked by inhomogeneous broadening. Therefore, collective signatures are hard to detect with frequency domain methods. To this end, we have developed a highly efficient time-domain detection method based on a nonlinear femtosecond pump-probe excitation scheme [1]. With this method, we detected, for the first time, four-body resonances in a rubidium vapor at densities down to  $10^8 \text{ cm}^{-3}$ . Furthermore, we observe phase shifts in the absorption spectrum that are connected to the hyperfine levels of the system. Our findings are surprising considering the weak interparticle interaction present at the studied conditions, which has triggered some interest from theory to explain our results [2,3].

Recently, we further investigated these effects using pump-probe pulses with orthogonal polarization. In this way, we suppress strong linear signals, which could induce experimental artifacts. Additionally, we reduce so-called build-up effects by using a new laser system with a lower repetition rate (First experiments: 80 MHz, Recent experiments: 200 kHz). The new results confirm the physical nature of our signals.

[1] L. Bruder, M. Binz, and F. Stienkemeier, Phys. Rev. A 92, 053412 (2015)

[2] S. Mukamel, J. Chem. Phys. 145, 041102 (2016)

[3] Z.-Z. Li, L. Bruder, F. Stienkemeier, and A. Eisfeld, Phys. Rev. A 95, 052509 (2017)



## Coherent multidimensional spectroscopy of dilute gas-phase nanosystems

M. Binz, U. Bangert, D. Uhl, L. Bruder and F. Stienkemeier

*Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

The helium nanodroplet isolation (HENDI) technique is a well-established powerful method to perform spectroscopic studies at very low temperatures. Due to the low target densities in doped droplet beam experiments, coherent time-resolved spectroscopy of such systems has remained a challenging task. In this context, we are investigating the phase-modulation technique established by Marcus et al. [1]. The combination of continuous acousto-optical phase-modulation with lock-in detection greatly improves the signal-to-noise ratio and the sensitivity in this scheme [2].

Recently, we have performed the first two-dimensional electronic spectroscopy (2DES) study of isolated, cold molecular nanosystems prepared with the HENDI technique [3]. The used experimental setup and technique will be introduced and the first results will be presented.

For this study, we synthesized weakly-bound high-spin Rb<sub>2</sub> and Rb<sub>3</sub> molecules on the surface of the helium nanodroplets as a test bench system. Our method shows an unprecedented sensitivity and resolution which allows us to precisely analyze the photodynamics in Rb<sub>2</sub> attached to the droplet surface and the interaction dynamics of the Rb<sub>3</sub>-helium droplet system.

- [1] P.F. Tekavec, T. R. Dyke, and A. H. Marcus, J. Chem. Phys. **125**, 194303 (2006).
- [2] L. Bruder, M. Mudrich, and F. Stienkemeier, Phys. Chem. Chem. Phys. **17**, 23877 (2015).
- [3] L. Bruder, U. Bangert, M. Binz, D. Uhl, R. Vexiau, N. Bouloufa-Maafa, O. Dulieu, and F. Stienkemeier, arXiv:1806.08314, (2018).



## Spectroscopy of perylene diimide and oligoacenes on rare gas clusters

M. Bohlen<sup>1</sup>, S. Izadnia<sup>1</sup>, C. A. Rice<sup>1</sup>, A. C. LaForge<sup>1</sup>, F. Stienkemeier<sup>1</sup>, Y. Xu<sup>2</sup> and W. Jäger<sup>2</sup>

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

<sup>2</sup>*Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada*

The semiconducting character of  $\pi$ -conjugated molecules, such as perylene-derivates or polyacenes are quite promising due to widespread applications of organic electronics. Here we report on spectroscopy of monomers and dimers of perylene diimide (PDI) embedded in helium nanodroplets and adhered to the surface of rare gas clusters. We observed the  $S_1 - S_0$  electronic transition of PDI molecules using laser-induced fluorescence (LIF) as a function of excitation wavelength. The spectrum shows several vibrational transitions as well as dimer contributions, that could be verified by investigations of dependences of the respective features to the PDI partial pressure.[1]

Furthermore, the collective effects of oligoacenes regarding fluorescence lifetime and intensity adhered to Neon clusters were already investigated using nanosecond laser-excitations.[2] Those measurements should be extended in two directions: Firstly, we will address faster timescales using femtosecond laser-excitation and Time-Dependent Single Photon Counting (TDSPC) to detect radiative decays of oligoacenes, and secondly, the interaction with the substrate should be clarified by deposition of chromophores to the surface of argon clusters and comparison with previous measurements. We present the implementation of the technical improvements as well as first results.

[1] S. Izadnia, M. Bohlen, C. A. Rice, A. C. LaForge, F. Stienkemeier, Y. Xu, W. Jäger in preparation

[2] S. Izadnia, D. Schönleber, A. Einfeld, A. Ruf, A. C. LaForge, F. Stienkemeier *J. Phys. Chem. Let.* 8, 2068-2073 (2017).



## Signatures of indistinguishability in bosonic many-body dynamics

T. Brünner, G. Dufour, A. Rodríguez, A. Buchleitner

*Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

Many-body interference occurs as a fundamental process during the evolution of a quantum system consisting of two or more indistinguishable particles. The (measurable) consequences of this interference, as a function of the particles' mutual indistinguishability, was so far mainly studied for noninteracting photons transmitted through beam-splitter arrays, while the role of many-body interference in the dynamics of interacting particles, e.g. cold atoms in optical lattices, had remained unclear. We identify a quantifier of the particles' mutual indistinguishability attuned to time-continuously evolving systems of (interacting) particles, which predicts the dynamical behaviour of observables influenced by genuine few-body interference. Our measure allows a systematic exploration of the role of many-body interference in the non-, weakly, and strongly interacting regimes.

[1] T. Brünner, G. Dufour, A. Rodríguez, and A. Buchleitner Phys. Rev. Lett. 120, 210401 (2018).



## Possible research projects

Jun Dai

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Starting with a good research project is vital for my PhD studies that I begin this September. This talk will combine a quick review of my undergraduate research on simulating the Ising model with magnetic field, and my experience from the visits with each IRTG research group, to understand the experiments in cold controlled molecules and atoms. I will outline a few possible research projects I might pursue following these interactions. This talk will ask for feedback to guide me to ideas for applying quantum simulations for understanding the physics of cold atoms, molecules, and beyond.



## Cold interactions between Lithium and Barium

Markus Debatin

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We investigate interactions between laser-cooled neutral Li atoms and Ba + ions. A magneto-optical trap (MOT) of Li is overlapped with laser-cooled Ba ions trapped in a Paul trap. In this configuration we observe state-dependent inelastic collision rates. For a detailed investigation of collisions at even lower temperatures we are currently setting up optical dipole traps for the ions [1] and neutral atoms. This will eventually allow us to reach temperatures low enough to resolve individual angular momentum contributions or even reach the s-wave regime. First optical trapping of ions is observed in our new Ba-Li setup. In the talk I will present the setup together with the first results.

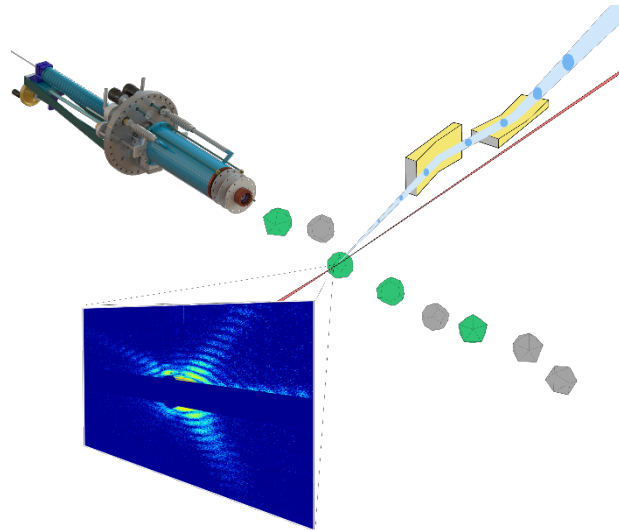
[1] A. Lambrecht et al., *Nature Photonics* **11.11** 704 (2017)



## Time-dependent X-Ray diffraction imaging of metal clusters

Simon Dold

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Wide angle X-Ray diffraction has been proven a viable tool to determine the 3D structure of metal clusters[1]. Our goal is to utilize ultrashort X-Ray pulses as a tool to resolve ultrafast processes in nanoscale systems by imaging structure in a time-dependent manner.

Diffraction experiments on metal clusters in gas-phase require high intensities of both, clusters and X-ray beam to vanquish low cross-sections for these scattering processes. To overcome this difficulties a carefully taylored source for clusters has to be set up. I will present the current status of an improved variant of a gas-aggregation source of Haberland sputter source type[2] as well and the current status of the experiments.

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## Photoelectron spectroscopy of size-selected clusters at free electron lasers

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Investigation of nanoscopic systems using photoelectron spectroscopy at free electron lasers not only will contribute to a better understanding of the electronic structure, and the resulting physical and chemical properties of nanoscale matter, but also will enable deep insights into the many-particle dynamics by exposing finite quantum systems to high-energy and high-intensity radiation. Small clusters with up to few hundreds of atoms exhibit quantum-size effects and they can be considered as ideal model systems for the study of fundamental physical phenomena. [1, 2]

Therefore, the aim of this project is to provide a specialized spectrometer system for studying the electronic structure and the dynamics of free mass-selected and temperature-controlled clusters at Free-electron laser (FEL). This spectrometer system involves a high-resolution magnetic bottle type photoelectron spectrometer, a high-resolution electron hemispherical analyzer, and an ion time-of-flight mass spectrometer. These three spectrometers are adapted to both the intense cluster beams as well as to the specific parameters imposed by FEL. The first two spectrometers will provide detailed investigations on the electronic structure and relaxation in well-defined nanosystems in quantum-size-regime, while the ion time-of-flight mass spectrometer is used to monitor the cluster size and photo-fragmentation.

The whole machine is designed and built in a collaboration with the group of Prof. Meiwes-Broer in Rostock. One aspect of this development is the design and the construction of the magnetic bottle type photoelectron spectrometer based on experience gained in a similar experiment at FLASH. One challenge of this spectrometer is to achieve very low pressure down to  $10^{-12}$  mbar in order to minimize the background signal. For this purpose, first, a cold head near the active region is attached. Second, two benders and several differential pumping stages are used in order to prevent direct buffer gas beam coming out of the trap to reach the active region. Regarding the ion optics of the machine, comprehensive simulations have been done and used for the spectrometer design. In this talk, our newly constructed spectrometer is presented. More details about challenges we have encountered while designing and constructing the new spectrometer system are given.

[1] J. Bahn, P. Oelßner, M. Köther, C. Braun, V. Senz, S. Palutke, M. Martins, E. Rühl, G. Ganteför, T. Möller, B. von Issendorff, D. Bauer, J. Tiggesbäumker and K.-H. Meiwes-Broer, *New J. Phys.* **14**, 075008 (2012)

[2] V. Senz, T. Fischer, P. Oelßner, J. Tiggesbäumker, J. Stanzel, C. Bostedt, H. Thomas, M. Schöffler, L. Foucar, M. Martins, J. Neville, M. Neeb, T. Möller, W. Wurth, E. Rühl, R. Dörner, H. Schmidt-Böcking, W. Eberhardt, G. Ganteför, R. Treusch, P. Radcliffe, and K.-H. Meiwes-Broer, *Phys. Rev. Lett.* **101**, 138303 (2009).

## Molecular superrotors in helium nanodroplets

Jordan Fordyce<sup>1</sup>, Ian MacPhailBartley<sup>1</sup>, Valery Milner<sup>1</sup> and Frank Stienkemeier<sup>2</sup>

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<sup>2</sup>Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

The aim of the project is to study the critical behaviour of fast rotating molecules with super-fluid helium, more specifically, the interaction of molecular “superrotors” with helium nanodroplets. Droplets ideally capture single dopant gas molecules and are then exposed to two laser beams. The first beam, a combination of two chirped circularly polarized pulses, called an “optical centrifuge”, excites them to the extreme rotational states. The second beam, a femtosecond “probe”, ionizes the molecules. The recorded velocity map ion image is analyzed to determine the rotational state, or orientation, of the molecules.

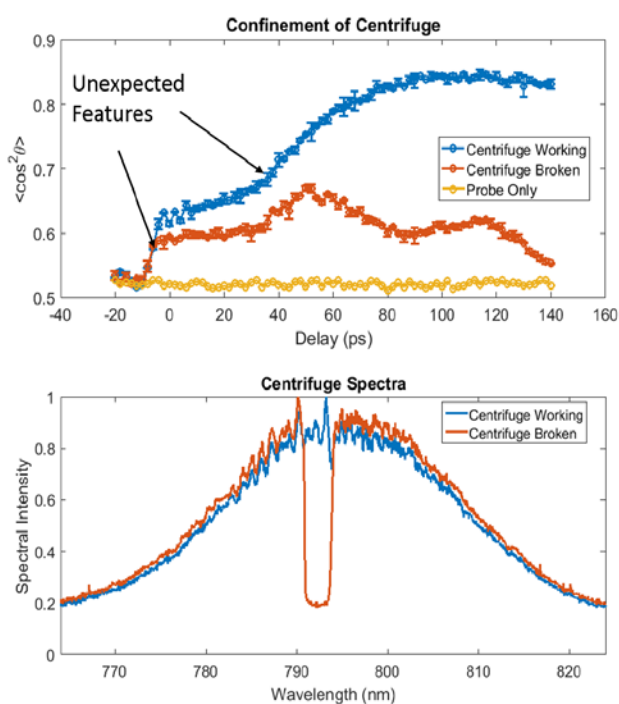


Figure 1: (Top) Effect of confinement from the probe arriving before the centrifuge (negative times) and after the centrifuge (positive times). A value of 1 would be perfectly confined to a line while 0.5 would be an isotropic circle. (Bottom) The corresponding spectra of the centrifuge to the upper plots. The notch in the spectra means the adiabaticity criteria to catch and rotate molecules is broken, making the centrifuge ineffective.

pulse, which was not anticipated but can be explained by investigating the shape of the pulses. This new understanding of the behaviour of the rotation dynamics will help interpret the effect of the helium matrix with the rotation of molecular superrotors.

Because the molecules are anticipated to rotate with a speed well above Landau’s velocity inside the droplets, it is anticipated that the helium could couple to the rotor, changing its rotational properties. Therefore, if helium couples strongly to the rotor then very weak confinement to the rotational plane is expected and would require a high degree of sensitivity to be detected.

As well, the time dynamics of the free dopant gas molecules were carefully studied to better characterize the onset of confinement to the rotational plane from the optical centrifuge, as shown in Figure 1. Confinement is characterized by  $\langle \cos^2 \theta \rangle$ , which is the average value of the angle between the probe polarization and the projection of the ion velocity vector onto the detector screen. It was found that the broken centrifuge exhibited some degree of confinement during the optical centrifuge pulse and that maximum confinement was not reached until the end of the centrifuge



## Macroscopic QED study of the interatomic Coulombic decay

Janine Franz

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Interatomic Coulombic decay is a double ionization process similar to Auger decay: an inner-shell ionized atom relaxes by filling a vacancy with an electron from a higher energy level. The emitted photon that carries the energy difference is then absorbed by a second atom and ionizes it. This is in contrast to Auger decay where the same atom absorbs the photon and is ionised in an additional shell, leaving the atom doubly ionized. The process typically occurs in weakly bound atomic van-der-Waals clusters and is highly relevant in a biological context since the emitted electron in the secondary process typically exhibits energies, which have been shown to be harmful to DNA. Using macroscopic quantum electrodynamics, we have derived a general expression for the interatomic Coulombic decay rate in arbitrary dielectric environments. Two different approaches, namely time-dependent and time-independent perturbation theory yield contradicting predictions for this decay rate, in the talk I will discuss the theory leading to these expressions.



## Collective enhancement of the Casimir-Polder potential

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The Casimir-Polder potential can be enhanced by replacing the single atom in front of a surface by an atomic ensemble. If the extension of the cloud of identical atoms is smaller than the atomic transition frequency, it can be treated as one single atom of equidistant energy states, which is called the “Dicke approximation”.

We study this effect by combining the Dicke model with the theory of macroscopic quantum electrodynamics. To this purpose, we show a connection between the Dicke states and the atomic dipole moments with the surface-dressed collective decay rates. Moreover, the central assumption of the Dicke model, the long-wavelength approximation, is checked for two atoms and the effect of the distance on the total emission rate is analyzed. The presence of the surface plays a crucial role in the enhancement of the dynamics of the emission. Finally, we present a Casimir-Polder potential for an atomic ensemble showing a very pronounced peak in time-domain [1].

[1] S. Fuchs, S. Y. Buhmann, arXiv: 1804.01265 (submitted to NJP).



## **Ab Initio study on molecular charge transport and conformational analysis via IR-Raman spectroscopy**

Reyhaneh Ghassemizadeh, Michael Walter, Takamasa Momose

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Rapid development in technology of Organic PhotoVoltaic (OPVs) and their application in green industry over the past couple of decades, attracts many attentions to study on efficiency enhancement of such devices. Motion of polarons through organic donor-acceptor pairs is a fundamental process in order to have an efficient charge transfer (CT) procedure. Polarons refers to CT excitons which could overcome the strong Coulomb binding energy and create separated electrons and holes. Therefore, studying the interaction between electron distribution and molecular vibrations can be useful to continuously follow up polarons through the materials. Experimentally, e.g. by applying an external DC-bias, the amount of charge transfer has been estimated from changes in vibrational properties measured via SERS (surface enhanced Raman spectroscopy) or SEIRAS (surface enhanced infrared absorption spectroscopy).

We are interested to study on properties of the system of molecules carrying fractional charges using Density Functional Theory (DFT). A polymer in contact to an oxidizer molecules is a case to observe fractional charge transport. We have modeled this situation by calculating the molecular pair between PCPDTBT and F4TCNQ. The amount of charge transfer is obtained by the occupation of Kohn-Sham orbitals via DFT and by a bader analysis. We have also assigned the Raman shifts of PCPDTBT in presence of the oxidizer which is the fingerprint of fractional charge transport in this polymer blend.

We have also calculated the IR spectroscopic signatures of Zwitterion beta-alanine and simulate it's stability in water. Amino-acids have many applications in bio-science and astronomy. The spectroscopic properties of Beta-alanine has been widely invested. However, the spectroscopic features of the zwitterionic form of beta-alanine have not yet been explored. Beta-alanine is stable in vacuum. Adding water molecules, leads to proton transfer form a zwitterion beta-alanine. Within the DFT frame, we could calculate the stability of zwitterion beta-alanine surrounded by more than 3 water molecules. The energy barrier of this process is under study. Finding the global minimum structure for the solution of water and zwitterion beta-alanine, computationally is so expensive and so hard to achieve. However, using minima-hopping method and simulating many different possibilities of water molecules around the zwitterion beta-alanine, we could achieve a stable configuration with the lowest energy comparing to many other configuraitons. In the next step, we have obtained the IR- spectra. Assigning IR peaks of a molecule in solution is much more difficult than in vacuum because of mixing of the modes happens due to water-molecule interactions. With the comparison of our calculated spectra to the experiment, we have observed a peak which possibly can be assigned to zwitterion beta-alanine.



## Reactive scattering between metastable helium atoms and ultracold lithium atoms

Jonas Grzesiak<sup>1</sup>, Simon Hofsäss<sup>1</sup>, Vivien Behrendt<sup>1</sup>, Frank Stienkemeier<sup>1</sup>, Marcel Mudrich<sup>2</sup>, and Katrin Dulitz<sup>1</sup>

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The experimental observation of quantum effects in Penning ionization reactions has recently attracted a lot of attention [1]. Our goal is to study such processes in a quantum-state-controlled manner at low collision energies, e.g., to study the influence of electron-spin polarization on the reaction rate. For this, we use an experimental setup which is composed of a magneto-optical trap for ultracold lithium atoms and a discharge source for the production of supersonic beams of metastable helium atoms. In this contribution, I will present a novel detection scheme which allows for the mass-selected detection of the ionic reaction products at improved energy resolution and we will discuss the influence of elastic collisions on the reaction rate measurements. I will also discuss the influence of the electronically excited  $^2P_{3/2}$  state in lithium on the reaction, as a first step of gaining control over the quantum states involved.

[1] A. B. Henson, S. Gersten, Y. Shagam, J. Narevicius, E. Narevicius, *Science* **338**, 234 (2012).



## Construction of a new source for organic cluster generation

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Organic semiconductors are a new class of semiconductors with a lot of capabilities in new technologies and worth studying the physics behind them more deeply.<sup>1</sup> Generation of organic clusters and studying their electronic dynamics is the goal of this project, because by studying the clusters, one can find how the physical properties evolve from molecular state to bulk state.<sup>2</sup> For this purpose, a new molecular cluster source has been designed and constructed. This source is a high temperature pulsed valve that makes possible to generate molecular clusters by supersonic expansion.<sup>3</sup> The important features of this valve are that it could operate at very high temperatures (like 600°C) and also has a much better sealing in compare to the similar designs.<sup>4,5</sup> First, the operation of the valve was tested at room temperature with generation of CO<sub>2</sub> clusters. After that the heating and cooling parts were added in order to generate organic clusters, which needs high temperatures.

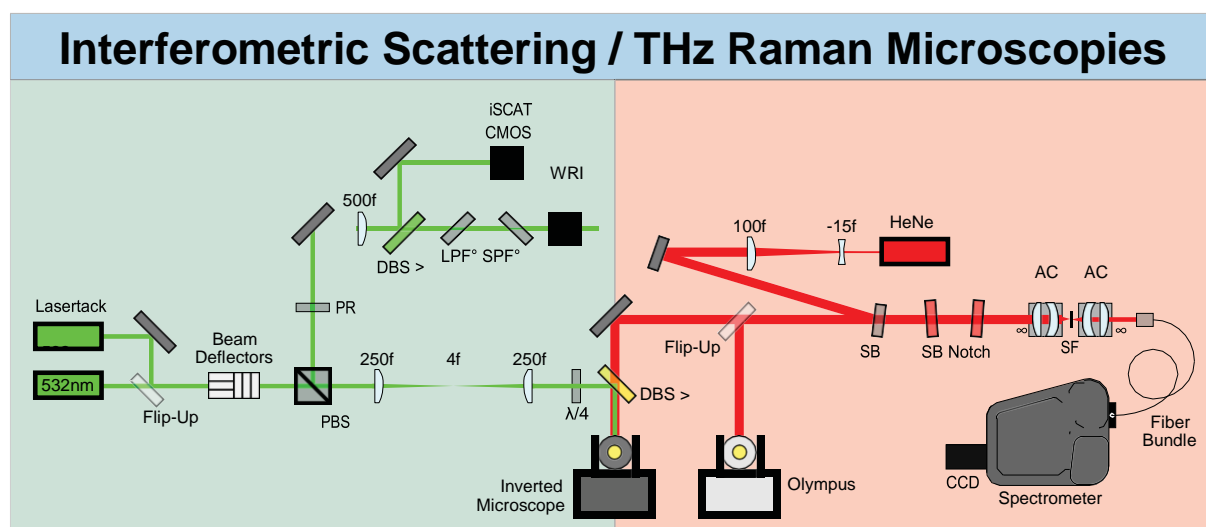
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- [3] O. F. Hagen, Rev. Sci. Instrum. **63**, 4 (1992).
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## Integration of Confocal Raman and interferometric scattering microscopies for the analysis of nanoscale complex and biological specimens

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The integration of confocal Raman microscopy with wide-field interferometric scattering (iSCAT)<sup>1</sup> microscopy offers a novel advance in the analysis of complex and bio-materials.<sup>2</sup> Raman spectroscopy provides information about the chemical morphology of samples; however instruments typically lack the ability to quickly render wide-field images capable of detecting sub-diffraction limited features. iSCAT produces wide-field maps of sample refractive index morphology with video frame-rates at the diffraction limit or better.<sup>3</sup> Collinear iSCAT and confocal Raman rapidly and reliably provide complementary information about sample chemistry and morphology, conveniently integrated into a single instrument. Additionally, interference between reflected and back-scattered light provides relative phase information from which 3-D reconstructions may be rendered. Applications include *Saccharomyces cerevisiae* cells, graphene and gold/silver nanoparticles.

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[3] Cole, D.; Young, G.; Weigel, A.; Sebesta, A.; Kukura, P. *ACS Photonics* **2017**



## Infrared spectroscopy of alanine water clusters and water aggregation in solid parahydrogen

Brendan Moore, ShinYi Toh, Ying-Tung Angel Wong, Pavle Djuricanin, Takamasa Momose

*Department of Chemistry, The University of British Columbia, 2036 Main Mall, Vancouver, BC, Canada*

The formation of gas phase  $\beta$ -alanine zwitterions has been studied using solid *para*-H<sub>2</sub> FT-IR matrix-isolation spectroscopy.  $\beta$ -alanine was co-deposited with mixtures of H<sub>2</sub>O/ *para*-H<sub>2</sub> to observe the stabilization effect of water molecules on the zwitterion form of  $\beta$ -alanine. Through a comparison with theoretical computations, as well as with crystalline  $\beta$ -alanine FT-IR spectra, the characteristic NH<sub>3</sub> N-H bending vibrational frequency for the zwitterionic form was identified. Analysis of the spectral peak temporal behavior shows that other proposed zwitterion peaks behave similarly to the characteristic NH<sub>3</sub> spectral peak. In agreement with theoretical studies, it has been shown that water can stabilize the zwitterionic form of gas phase amino acids, causing the zwitterion to form preferentially over the neutral form under certain conditions.

The  $\beta$ -alanine zwitterion formation rate may be attributed to aggregation of small water clusters in the solid *para*-H<sub>2</sub> matrix. The aggregation of small water clusters occurs due to diffusion of water molecules in the solid *para*-H<sub>2</sub> matrix. The diffusion of water monomers, as well as dimers, is observed at temperatures as low as 4K. As solid *para*-H<sub>2</sub> is a quantum crystal, the behavior of diffusion in this solid differs from classical solid state diffusion. A comparison between the diffusion of water molecules in the *para*-H<sub>2</sub> matrix and diffusion of impuritons in a quantum crystal is made. As the size of water cluster increases, the aggregation rate displays some similar behavior to the formation rate of  $\beta$ -alanine zwitterions. It is proposed that water clusters of size  $n > 5$  are responsible for the stabilization of  $\beta$ -alanine in the zwitterionic form in the *para*-H<sub>2</sub> matrix.



## Optical trapping of ion crystals and ion-atom ensembles

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Studying the chemistry of individual atoms on the quantum level, ideally with full control of the initial states and with the possibility to resolve the product states, is a long-standing goal in atomic and molecular physics, which is predicted to have applications beyond quantum chemistry, e.g. for simulating quantum many-body systems. In order to reach the quantum regime, the thermal energies of the reactants should be low enough to suppress the contributions by higher angular momentum scattering waves. For atom-ion ensembles, where the interactions are long-ranged and follow a  $1/r^4$  scaling, the onset of this s-wave regime is expected at temperatures between 50 nK (for  $\text{Ba}^+ + \text{Rb}$ ) and tens of  $\mu\text{K}$  (for  $\text{Yb}^+ + \text{Li}$ ) [1]. So far, such temperatures remain out of reach in hybrid traps – which consist of a radiofrequency trap for the ion and an optical or magnetic trap for the atoms – due to an intrinsic micromotion heating effect [1].

Some quantum many-body systems can also be studied with trapped ion crystals in Paul traps with high accuracy thanks to the extensive control over the electronic and motional states of the ions [2]. One-dimensional systems can readily be implemented with ion chains in linear Paul traps. In two-dimensional systems, it has been proposed theoretically to study structural quantum phase transitions at the transition from 1D to 2D crystals [3]. However, this remains a major experimental challenge due to the intrinsic micromotion when the ions are displaced from the axis of the linear Paul trap [4].

In my talk, I will present an overview of our recent work on optical trapping of single ions and ion crystals without radiofrequency fields, which avoid the limiting effects stemming from micromotion [5,6]. I will also discuss our recent progress towards the investigation of atom-ion interactions. In our approach, both the atoms and ions are loaded into an optical trap.

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- [5] A. Lambrecht et al., Nat. Phot. **11**, 704-707 (2017)
- [6] J. Schmidt et al., Phys. Rev. X **8**, 021028 (2018)



## Photo-ionization and electron-impact-ionization-TOF spectrometry for the detection of large organic molecules embedded in cluster beams

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The isolation of atoms, molecules and molecular complexes in rare-gas cluster beams, and particularly in helium nanodroplets, offers a versatile method for the study of energetic and dynamical properties of these systems, because it provides low-temperature conditions with minimal perturbation by the environment <sup>[1]</sup>. Femtosecond pump-probe spectroscopy as well as frequency-domain spectroscopy will be used to disentangle the effect of the helium droplet environment from the properties of the molecular system itself. For the detection and mass selection of the needed high mass range, as well as to give insights into the mass and charge distribution, it is advantageous to use a combination of electron-impact ionization, photo-ionization and time-of-flight (TOF) spectrometry in a collinear arrangement to the cluster beam.

On the one hand, we have combined an electron gun with a TOF spectrometer in order to provide a versatile ionization method and a good mass resolution. On the other hand, due to the possible absorption and/or relaxation to the several rotational and vibrational states of large molecules, such as polyaromatics and fullerenes ( $C_{60}$ ), these systems should be photo-excited with energetic photons. This will be achieved by generating the third harmonic of 400 nm light, which will produce 9 eV photons <sup>[2]</sup>.

In this presentation, preliminary results using different molecular species will be discussed. The characteristics of the electron gun and of the experimental setup, including the VUV generation scheme, will be detailed as well.

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## **A primary, self-defining UHV standard based on universal van der Waals scattering**

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The van der Waals or London dispersion force between neutral particles arises from quantum zero-point fluctuations of the electromagnetic field and plays a fundamental role in a vast array of fields including chemistry, biology, and physics. We experimentally show here that this ubiquitous and immutable law of nature also makes a stationary neutral atom an ideal and self-defining absolute particle flux sensor for vacuum. In brief, the passage of a particle through the collision cross section of the sensor atom is detected by the momentum transfer to it, and the incident particle flux is the single particle collision rate divided by the total cross section. Crucial to this application, we show that the scattering of the sensor atom into momentum states that exceed some value can be measured from the loss rate of a trap of finite depth and follows a universal scaling law that depends only on the mass of the sensor atom and the total cross section for velocity-averaged elastic collisions. The scaling has implications for all neutral particle scattering and allows the total cross section and particle density to be found by a measurement of trap loss as a function of trap depth.



## Electron - phonon coupling with density functional theory including environment effects and polaron dynamics

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In order to investigate on novel materials, we describe electronic structures for organic molecules, with density functional theory (DFT) and their excited states with time dependent DFT. In terms of excitations, we are especially interested in coupling of electronic and nuclear degrees of freedom. In this respect, we study photoexcitation in molecules that can be described by the Franck-Condon (FC) principle, or the related excitons in solid state physics. We present a study on pentacene (Pc), where the calculated FC factors from our simulations are in excellent agreement to vibrationally resolved experimental spectra recorded in the Stienkemeier group. A main part of the study includes hereby the influences of the environment on the spectra. In the experimental setup, Pc is investigated in helium droplets or neon clusters as ultra-cold environments, which has to be included in the DFT simulations. The vibrational lines in the helium droplet experiment match the vacuum FC factors, which indicates that there is almost no coupling to the environment. In contrast, there is substantial vibrational coupling to the neon cluster surface. These couplings give rise to a broadening of the spectrum as well as the appearance of an additional peak, the so called „butterfly mode“. Further we describe a method to investigate polaron phenomena with DFT. Polarons in the Su-Schrieffer-Heeger (SSH) Hamiltonian model have been thoroughly investigated in terms of the electron phonon coupling [1]. We use DFT calculations to obtain the SSH parameters in order to explore a set of possible materials representing strong electron-phonon coupling. Hereby linear chain molecules based on polyacetylene are investigated. Our results predict an increase of the coupling parameter through stretching of the chain or by substitution of the hydrogens by other side groups. With the new insight gained in the electron phonon coupling within these simple chains, one might improve the understanding of polarons in more complex materials and take a step towards the direction of high temperature superconductors.

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## Toward the separation of enantiomers by the Casimir-Polder force

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Many molecules are chiral which can exist in left- and right-handed forms (i.e., non-superimposable mirror images). These two forms of a chiral molecule are known as enantiomers. Distinguishing two types of enantiomers is of great practical importance. For example, in designing pharmaceuticals, it is necessary to choose the right enantiomer to obtain the desired effects. In this project, we propose a method for the analysis and separation of chiral molecules using the Casimir-Polder force in the framework of macroscopic quantum electrodynamics (QED) [1]. In [2], it was found that there exists a chiral component of the Casimir-Polder force which is sensitive to the handedness of the objects concerned and can be attractive or repulsive depending on their chirality. The force could hence be used to differentiate enantiomers of opposite handedness. However it is often the case that the electric component of the force which is not discriminatory with respect to enantiomers dominates over their chiral component and the chiral contribution to the interaction is too small to distinguish between them.

Here we study the Casimir-Polder force experienced by a chiral molecule in a planar cavity consisting of two chiral mirrors such that the chiral part would be enhanced and symmetric configurations selectively cancel the electric part but not the chiral part, as a consequence of nondiscriminatory and discriminatory nature of electromagnetic and chiral components respectively. Since the chiral component changes its sign depending on chirality of molecules and mirrors, it would be possible to identify the handedness of the chiral molecule by measuring enhancement or reduction of the force and possibly set up a Stern–Gerlach type discriminator for enantiomers.

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## Photoelectron two-dimensional coherent spectroscopy

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Two-dimensional electronic spectroscopy (2DES) is a powerful tool to explore coherences and correlations on ultrafast time scales. Until now, 2DES studies have mostly been conducted in the condensed phase. We have built a setup to perform 2DES experiments on molecular and cluster beams in the gas phase. To achieve sufficiently high sensitivity for our gas-phase studies, we have adapted the phase modulation technique developed by Marcus et al. [1]. Our setup can additionally be combined with an energy-resolved photoelectron detection, which basically adds an additional dimension to the 2D spectra. For this purpose, we have built a magnetic bottle spectrometer to combine photoionization with energy-selective detection of photoelectrons. Binding energies are thus deduced from the time-of-flight, processed in a gating module and combined with a lock-in detection to increase the sensitivity.

Signal gating at high trigger rates (> 100kHz) can be realized by commercially available boxcar averagers. However, devices reaching this high trigger rates are expensive. We have developed a cost-effective solution for gating applications implemented in a field programmable gate array (FPGA).

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## Machine learning for many-body quantum physics

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Solving the Schrodinger equation (SE) for many-body systems has been the main challenge for quantum physicists over the last century. In this talk, I will illustrate how with machine learning it may be possible to reduce the number of times the SE needs to obtain physical results. In the first part of my talk I will explain the application of kernel methods of machine learning for fitting potential energy surfaces (PES) of polyatomic molecules. In particular, I will illustrate the application of Bayesian optimization with Gaussian processes as an efficient method for sampling the configuration space of poly- atomic molecules. In the second part of my talk I will discuss the possibility to extrapolate quantum observables with machine learning to discover phase transitions for condensed matter systems.

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- [2] R. A. Vargas-Hernández, Y. Guan, D. H. Zhang, R. V. Krems, A machine-learning approach for the inverse scattering problem in quantum reaction dynamics; arXiv:1711.06376 (2017).
- [3] A. Kamath, R. A. Vargas-Hernández, R. V. Krems, T. Carrington Jr., and S. Manzhos, Neural Networks vs Gaussian Process Regression for Representing Potential Energy Surfaces: a Comparative Study of Fit Quality and Vibrational Spec- trum Accuracy; J. Chem. Phys. 148, 241702, (2017).



## Study of collisional processes of magnetically trapped cold methyl radicals

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Study of cold atoms and molecules have been grown rapidly in the last few decades. Atoms have been cooled to nK temperatures which lead to the first ever Bose Einstein condensates. Apart from this, cooled atoms have been subjected to various collisional studies. Cold atomic collisions have been characterized by known interatomic potentials, and various quantum effects such as resonance scattering have been explained by the standard scattering theories. On the other hand, collisions of cold molecules, especially those of reactive molecules, have been studied less than those of atoms due to the difficulties in making cold molecules, and information is still lacking to fully understand cold collisional processes of molecules with complex internal structures. Recently, we demonstrated that methyl radicals, one of the fundamental and important reactive intermediates, can be trapped in a magnetic trap at 200 mK. Those trapped cold radicals are subjected to various collisional studies with foreign atoms and molecules.

Methyl radicals are trapped inside a permanent magnetic trap after they have been slowed down with a molecular decelerator using magnetic fields. The temperature of methyl radicals inside the trap is below 200 mK. At this temperature, introduction of different gases inside the trap region will have different collision dynamics because of their varying interaction potentials. We determine the collision cross section of these gases with the trapped methyl radicals by measuring the loss rate of methyl radicals from the trap. Our latest results will be discussed.

Yang Liu, Manish Vashishta, Pavle Djuricanin, Sida Zhou, Wei Zhong, Tony Mittertreiner, David Carty, and Takamasa Momose. "Magnetic Trapping of Cold Methyl Radicals" *Phys. Rev. Lett.* **118**, 093201 (2017).



## **Building a fast deterministic single ion source for an atom-ion experiment**

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The interplay of ultracold atoms and ions has recently gained interest in the atomic community [1], due to its wide applications in quantum chemistry [2,3] and quantum control [4]. In order to control the atom-ion interaction by means of Feshbach resonances [5] it is necessary to prepare the mixture at ultracold temperatures. At those energies the dynamics of the interaction can be solely described by a single quantum state, known as s-wave scattering.

Optical trapping of ions [6,7,8] provides a new pathway to achieve ultracold atom-ion mixtures in the s-wave regime, as it overcomes the intrinsic micromotion heating effects of a conventional Paul trap [9] currently limiting experiments to collision energies on the order of a few mk.

In order to investigate atom-ion interactions it is necessary to precisely prepare both the atoms and the ions. In this talk I will present our new deterministic loading scheme for the barium ions, combining the principles of laser ablation and optical trapping of ions allowing to load individual ions within 1 second. Important dependencies of the ion loading rate will be presented and discussed.

I further present a short outlook on how to design a new bichromatic optical dipole trap in order to combine both the atoms and the ions in the ultracold regime.

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## Stable platform for phase-modulation of seed lasers facilitating all-XUV coherent nonlinear time-domain spectroscopy

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Coherent time-resolved spectroscopy is a powerful tool to study ultrafast dynamics in complex systems. Extending this to the XUV spectral region is on the frontier of nonlinear spectroscopy. However, demands on interferometric stability increase when going to short wavelengths and advanced pulse manipulation in the XUV is challenging. In seeded free electron lasers (FEL) the emitted XUV pulses inherit the coherence properties of the seed pulses [1]. This motivates our approach based on performing acousto-optical phase modulation (PM) on the seed laser with subsequent seeding of the FEL and lock-in detection at the harmonics of the seed modulation [2]. In this way demands on interferometric stability are efficiently decoupled from the laser wavelength, and XUV signals are isolated and amplified [3, 4].

We present a compact, stable and transportable platform specifically designed to perform PM on 261nm seed laser pulses. Degrees of freedom for adjustment are reduced to a minimum, in order to gain stability compared to a discrete setup on a breadboard. All optics are tailored to withstand high peak intensities and dispersion is reduced to a minimum. High stability of the platform and the sensitivity of the PM approach was verified observing UV quantum beats (268nm) in a low-density sodium beam ( $1.5 \times 10^8 \text{ cm}^{-3}$ ), detecting photoions with a time-of-flight mass spectrometer at a laser repetition rate of 50Hz. The platform has been implemented in the FERMI FEL seed laser beamline for characterization.

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- [3] Bruder et al., PRA **92**, 053412 (2015)
- [4] Bruder et al., Opt. Lett., OL **43**, 875 (2018)



## Abstracts – Posters

(in alphabetical order)

## Photon antibunching control in a quantum dot and metallic nanoparticle hybrid system

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The interaction of light with metallic nanoparticles (MNPs) supporting plasmonic resonances has attracted a great deal of attention [1]. The presence of the MNP near an emitter (an atom, an atomic ensemble, a molecule, a semiconductor quantum dot,...) changes the environment density of states around the emitter. As a consequence of changes in environment structure, the optical features of the emitter, such as spontaneous decay rate [2] and photon statistics [3], will change. Moreover, the plasmonic structure will impose a strong coupling in non-Markovian regime on the system [4]. In the present contribution, we study the effects of a spherical nano shell on the photon statistics emitted from a semiconductor quantum dot. A schematic of physical system is illustrated in Fig. 1. The quantum dot is supposed as a three-level system in  $\Lambda$  type configuration.

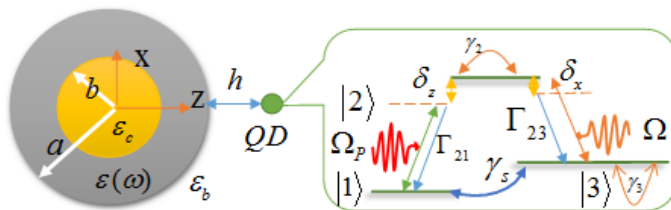
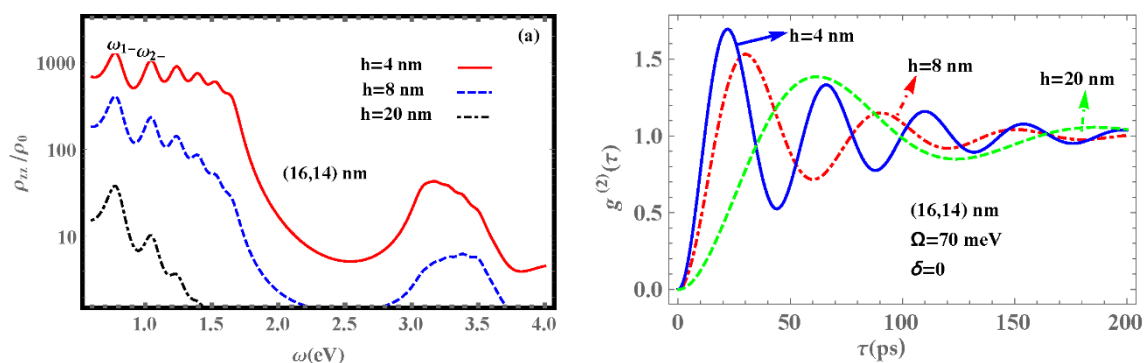


Fig. 1: Schematic illustration of physical system. A three-level quantum dot in vicinity of a metallic spherical nano shell.

The local density of states and the photon statistics of emitted photons from the semiconductor quantum dot are shown in following figures. We take the inner and outer radii of the MNP as 14nm and 16 nm, respectively. The left panel illustrates the local density of states. In this figure the lowest plasmonic resonance is selected as the main mode. The right panel illustrates the photon statistics emitted from the quantum dot. The non-classical nature of emitted photons is an important feature of this system. This figure also exhibits the potential of system as a single photon source.



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## Reaction rates in ultra-cold ${}^6\text{Li}$ dimers

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We present lifetime measurements of deeply bound  ${}^6\text{Li}$  dimers formed through evaporative cooling near a Feshbach resonance, and subsequent transfer via Stimulated Adiabatic Raman Passage (STIRAP). These results comprise the first experimental realization of the formation of these dimers. We have access to several ro-vibrational levels in the  $a(3\Sigma^u)$  manifold, including the lowest lying state in this manifold.

We have performed preliminary lifetime measurements for the  $N = 0$ ,  $v^f = 0, 5, 6, 7, 8, 9$  levels, and are in the process of refining these measurements in order to reliably determine the reaction rate constants for all vibrational levels in the lowest lying manifold. These measurements may help to advance our understanding of ultra-cold chemistry, and the refinement of the experimental techniques required will be important for future work in our laboratory.



## The photon BEC in arbitrary geometries by means of QED: Coupled dissipative dynamics of dye molecules

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Bose-Einstein condensation (BEC) has in the last two decades been observed in cold atomic gases and in solid-state physics. Progress in photonics over the last few years has led to a new challenge in quantum optics and condensed matter: the photon BEC. This has been experimentally observed in a small microcavity filled with a dye medium [1]. Confinement of laser light within such an optical microcavity creates conditions for light to equilibrate as a gas of conserved particles. The cavity mirrors' high reflectivity guarantees that photons live long enough to scatter among the dye molecules, which exchange energy with the photons by repeatedly absorbing and reemitting them. We use the language of macroscopic quantum electrodynamics [2] together with theory of open quantum systems

[3] to describe this phenomenon. We are interested in the realistic description of the cavity geometry, whose frequency-dependent reflection and absorption are fully encoded in the classical Green's function for the electromagnetic Helmholtz equation. This extension of the standard Jaynes-Cummings model to absorbing cavities with realistic geometries opens the door to studying the effects of the coupling of discrete modes in a resonant geometry to the strong body-assisted electromagnetic field of the cavity.

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[3] P. Kirton, J. Keeling, *Phys. Rev. A* 91, 033826 (2015)





## **An investigation on the magnetic properties of Zn<sup>2+</sup> substituted maghemite nanoparticles, prepared by coprecipitation method**

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Iron oxides have a high biocompatibility and are used in biomedicine extensively [1]. In this work single phase maghemite ( $\gamma$ -ferric oxide) and Zn-substituted maghemite ( $\gamma$ -Fe<sub>2</sub>- $\gamma$ Zn<sub>3 $\gamma$</sub> /2O<sub>3</sub>,  $\gamma$ = 0.0, 0.11 and 0.24) nanoparticles were prepared by coprecipitation method at 70 °C. The effects of Zn<sup>2+</sup> substitution on the structural and magnetic properties of the nanoparticles were investigated by X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, magnetometry and magnetic derivative thermogravimetry (DTG/M/) [2]. The results of XRD show that all samples have a single phase spinel structure. FTIR spectra reconfirm formation of maghemite and Zn<sup>2+</sup> substituted maghemite by appearance of the related absorption bands and band shifts because of Zn<sup>2+</sup> substitution [3]. Room temperature magnetization measurements illustrate that all samples are superparamagnets and not saturated at maximum applied magnetic field (9 kOe). Then they extrapolated to determine saturation magnetization. The results show that as Zn<sup>2+</sup> increases, first extrapolated saturation magnetization increases up to 58.15 emu/g for  $\gamma$ =0.11 and then decreases. Also DTG/M/ measurements show that Curie temperature of the samples decreases by increasing Zn<sup>2+</sup> substitution. Such magnetic nanoparticles are usable in magnetic hyperthermia potentially.

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## **Application of X-ray scattering, Geant4 simulation and ATR-FTIR for breast cancer diagnosis**

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Breast cancer is the most common cancer among women around the world and its incident rate is constantly increasing. Early detection of this disease would be helpful to prevent the rapid growth of the cancer cells. Traditional methods such as medical examination/imaging have been used to detect this kind of cancer. Unfortunately, all these methods cannot detect breast cancer in early stages. In this research three different techniques have been used to investigate whether it is possible to track the breast cancer process from early stages. GIXS (Grazing Incidence X-ray Scattering) and ATR-FTIR (Attenuated Total Reflection Fourier Transform Infrared spectroscopy) techniques have been used to collect data from normal and cancerous breast tissues. Moreover, Geant4 simulation toolkit has been used to simulate GIXS data in order to calculate the density of malignancy. Promising results have been found and will be presented. Further research is needed in different countries and different areas.

## Single Shot Electron Imaging of Helium Nanoplasmas

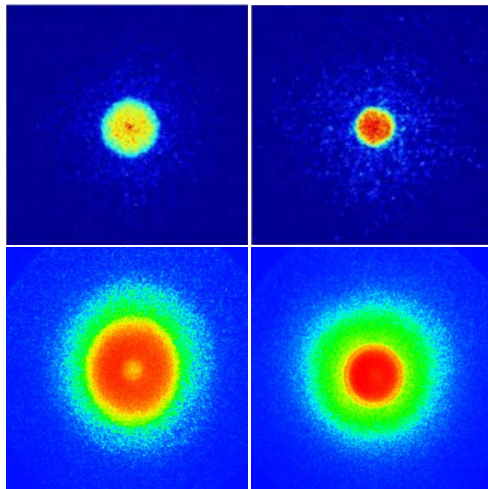
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Strong and short laserfields can turn a helium nanodroplet into a highly charged nanoplasma. The initial ignition just needs a few electrons provided by tunnel ionization of helium or a dopant particle to start an avalanche of ionizations. The cluster is then completely ionized within a few femtoseconds [1]. Repulsion between the ions leads to Coulomb explosion of the cluster and highly energetic ions and electrons are produced. We use the velocity map imaging (VMI) technique to measure the energy and angular distribution of the electrons, and a time-of-flight (TOF) spectrometer to collect the ions. One helium droplet produces enough signal to measure VMI and TOF spectra for individual helium droplets hit by single laser pulses. With pump-probe measurements we investigate the time evolution of the system.



[1] A. Heidenreich et al., New J. Phys.18 (2016) 073046



## The Interaction of Light with Metal-Silver Halide Thin Films

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Metal-silver halide thin films are light-sensitive materials which have a wide application in Optics and Chemistry. Ag-AgCl thin films show multicolour photochromic behaviour when they are irradiated by laser beams with different wavelength. It is possible to write and erase wavelength information on these thin films for several times. When these materials are irradiated by polarized laser beam anisotropy is induced in these films with the thickness less than 100nm. Al-Agl is a different system from Ag-AgCl that could show strong exciton-plasmon coupling in blue region of wavelength.



Notes

Notes



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# IRTG 2079 Annual Convention 2018



23<sup>rd</sup> -27<sup>th</sup> July

Stadthotel Freiburg

Karlstr. 7; 79104 Freiburg

|       | Monday, 23 July 2018                             | Tuesday, 24 July 2018  | Wednesday 25 July 2018 | Thursday 26 July 2018                                     | Friday 27 July 2018                                    |  |
|-------|--|--|------------------------|---|--|--|
| 08:30 |  | PI Meeting<br>Feldberg/Tuniberg                                  | Excursion              |   |  |  |
| 9:00  | Welcome  |  |                        |   |  |  |
| 9:30  | PI lecture<br>Michael Thoss<br>Feldberg/Tuniberg | PI lecture<br>Kirk Madison<br>Feldberg/Tuniberg                  |                        |   | PI lecture<br>Giuseppe Sansone<br>Feldberg/Tuniberg    | PI lecture<br>Roman Krems<br>Feldberg/Tuniberg |
| 10:00 | Matthias<br>Feldberg/Tuniberg                    |  |                        |   | Markus<br>Feldberg/Tuniberg                            | Audrey<br>Feldberg/Tuniberg                    |
| 10:30 | Break<br>Foyer                                   | Break<br>Foyer   |                        |   | Break<br>Foyer   | Break<br>Foyer                                 |
| 11:00 | Fumika<br>Feldberg/Tuniberg                      | Manish<br>Feldberg/Tuniberg                                      |                        |   | Brendan<br>Feldberg/Tuniberg                           | Tobias<br>Feldberg/Tuniberg                    |
| 11:30 | Andreas<br>Feldberg/Tuniberg                     | Pinrui<br>Feldberg/Tuniberg                                      |                        |   | Luke Melo<br>Feldberg/Tuniberg                         | Julian<br>Feldberg/Tuniberg                    |
| 12:00 | Pascal<br>Feldberg/Tuniberg                      | Janine<br>Feldberg/Tuniberg                                      |                        |   | Sebastian<br>Feldberg/Tuniberg                         | Daniel<br>Feldberg/Tuniberg                    |
| 12:30 | Lunch<br>Hotel Restaurant                        | Lunch<br>Hotel Restaurant  |                        |   | Lunch<br>Hotel Restaurant                              | Lunch<br>Hotel Restaurant                      |
| 13:30 | Reyhaneh<br>Feldberg/Tuniberg                    | Jonas<br>Feldberg/Tuniberg                                       |                        |   | Uli<br>Feldberg/Tuniberg                               | Meral<br>Feldberg/Tuniberg                     |
| 14:00 | Kariman<br>Feldberg/Tuniberg                     | Oliver<br>Feldberg/Tuniberg                                      |                        |   | Simon<br>Feldberg/Tuniberg                             | Marcel<br>Feldberg/Tuniberg                    |
| 14:30 | Jordan<br>Feldberg/Tuniberg                      | Aghigh<br>Feldberg/Tuniberg                                      |                        |   | Jun Dai<br>Feldberg/Tuniberg                           | Rodrigo<br>Feldberg/Tuniberg                   |
| 15:00 | Break<br>Foyer<br>PAC 1                          | Break<br>Foyer   |                        |   | Break<br>Foyer   | Break<br>Foyer                                 |
| 16:00 | PAC 2  | PAC 3  |                        |   | PAC 5  | PAC 7  |
|       |  | Lab Tour<br>Issendorff<br>Freiburger Material<br>Forschung (FMF) |                        |   | Lab Tour<br>Schätz<br>Gustav-Mie-Haus                  | Labtour<br>Dulitz<br>Physics High Rise         |
| 17:00 | Soccer Match<br>at the Dreisam                   | PAC 4  |                        |   | PAC 6  | PAC 8  |
|       |  | Lab Tour<br>Stienkemeier<br>Phisics High Rise                    |                        |   | Lab Tour<br>Sansone tbc.<br>Verfügungsgebäude<br>(VF)  |  |
| 18:00 |  | Posterseession<br>Physics High Rise<br>Foyer 1st floor           |                        |   | Posterseession<br>Physics High Rise<br>Foyer 1st floor | PAC 9  |
| 19:00 | BBQ at the Dreisam<br>green area at Sandfangweg  | Dinner<br>/ Pls' Dinner<br>Hotel Restaurant                      |                        | Dinner<br>Hotel Restaurant                                | Dinner<br>Hotel Restaurant                             | Dinner<br>Hotel Restaurant                     |
| 20:00 |  |  |                        | After dinner talk<br>Takamasa Momose<br>Feldberg/Tuniberg |  |  |

UF PI decides where the PAC meeting takes place and inform PhD student and UBC PI.