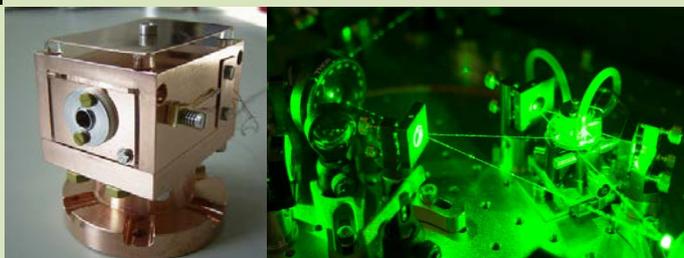


ANNUAL CONVENT 2017
IRTG CoCo

Cold Controlled Ensembles in Physics and Chemistry



BOOK OF ABSTRACTS

3rd CoCo Annual Convent

July 31 – August 4, 2017

University of British Columbia, Vancouver, Canada



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 CONVENT IS AN IMPORTANT PART OF THE STRUCTURED GRADUATE PROGRAM OF THE IRTG 2079. THE RESEARCHERS FROM UBC/VANCOUVER AND ALBERT-LUDWIGS UNIVERSITY 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

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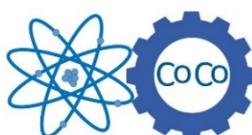
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Financial Support





General Information

Duration

Monday, July 31, 2017, 9:00 a.m. – Friday, August 4, 2017, 4:30 p.m.

Location

The meeting will take place at the:

Michael Smith Laboratories 101
Vancouver Campus
2185 East Mall
Vancouver, BC Canada V6T 1Z4

The poster sessions, lunch and coffee breaks will take place at the Michael Smith Laboratories 102.

Travel Information – Individual Journeys

You can use public transport from the Vancouver International Airport (YVR) to UBC campus. Take the Canada Line from the airport and get off at Broadway City Hall. Switch to the 99 B-Line bus and exit at the terminal stop of the line. You can plan your trip beforehand at: <http://tripplanning.translink.ca/>

Accommodation

Master and PhD students from the University of Freiburg will be accommodated in single rooms at the Pacific Spirit Hostel. Bed linen and towels will be provided.

Pacific Spirit Hostel
Place Vanier Residence
1935 Lower Mall, Vancouver BC

For Post Docs and PIs we reserved single rooms at the Walter Gage Residence. Bed linen and towels will be provided.

Walter Gage Residence
5959 Student Union Boulevard, Vancouver BC

Meals & Drinks

Meals and drinks during the scientific program are included. Breakfast and dinner need to be organized individually. Food is offered inside the AMS Students Nest building and at various coffee bars on campus, or at the University Village/Market place.

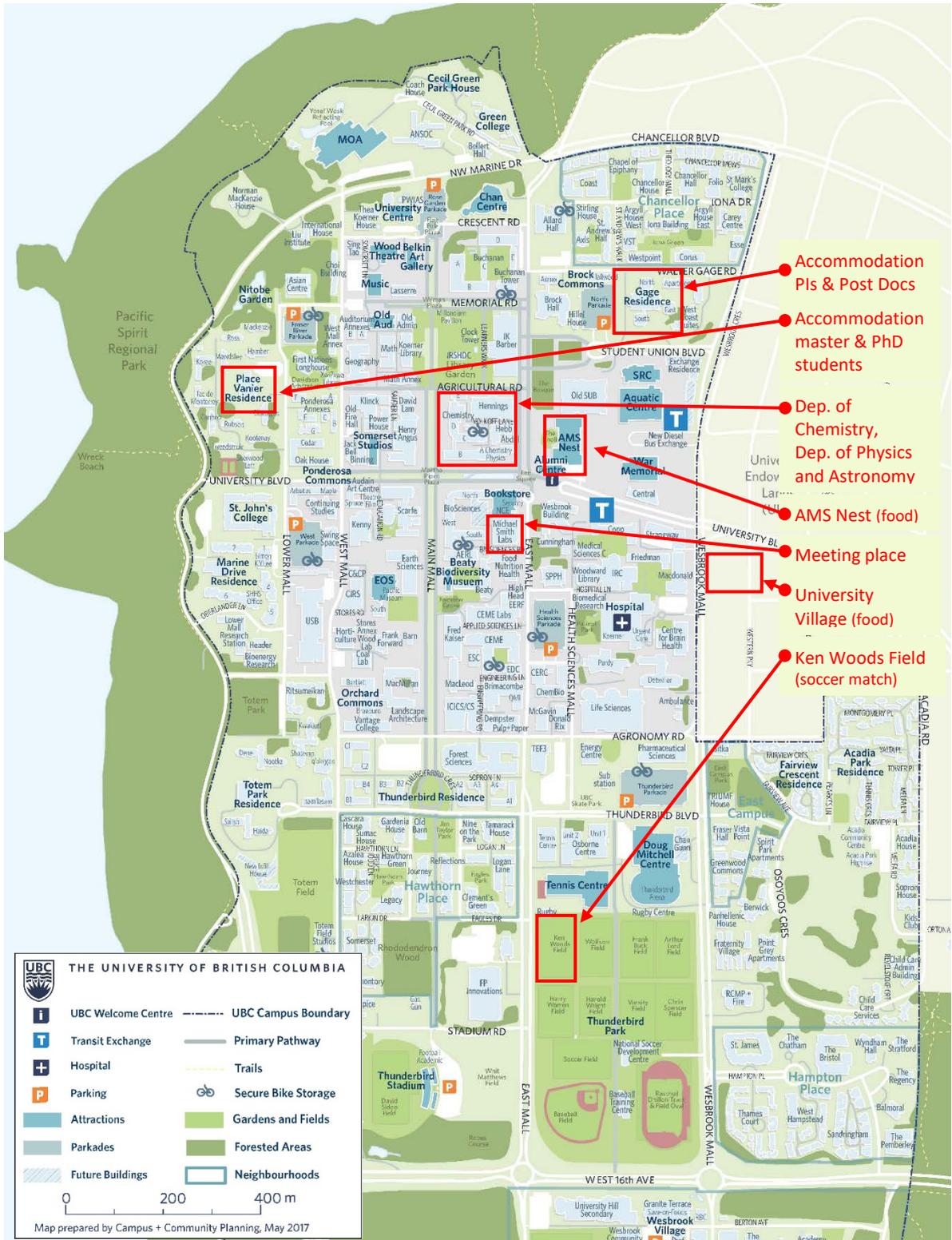
Excursion

A hiking trip is organised on Wednesday, August 2, 2017, please bring proper shoes.

WiFi

Eduroam will be available throughout the campus.

UBC Campus





Scientific Program

Monday, July 31, 2017

9:00 a.m.	Frank Stienkemeier, Takamasa Momose: Opening remarks
9:30 a.m.	Roman Krems: "Applications of machine learning to constructing potential energy surfaces for complex molecules: can machine learning help us to solve the inverse scattering problem?"
10:30 a.m.	Coffee break
11:00 a.m.	Sharareh Izadnia: "Correlated decay mechanisms in weakly bound acene molecules attached to neon clusters"
11:30 a.m.	Aghigh Jalhedoost: "High temperature pulsed valve for organic cluster generation"
12:00 p.m.	Lunch break
2:00 p.m.	Matthias Bohlen: "From rare gas to hydrogen-bonded clusters: Size distributions of supersonic beams from a pulsed valve using the titration technique"
2:30 p.m.	Oliver Stauffert: "Ab-initio electron-phonon coupling in polyacenes"
3:00 p.m.	Jordan Fordyce: "Molecular Superrotors in Helium Nanodroplets"
3:30 p.m.	Coffee break
4:00 p.m.	Markus Debatin: "Setup for experimental studies on Ba ⁺ - Li interactions"
4:30 p.m.	Pascal Weckesser: "Trapping and Controlling Barium Ions for Ultracold Atom-Ion Experiments"
5:00 p.m.	Postersession

Tuesday, August 1, 2017

9:00 a.m.	Tobias Schätz: "Optically Trapping Ions while having a coffee?"
10:00 a.m.	Sebastian Fuchs: "Casimir-Polder Potential and Casimir Force Involving Topological Insulators"
10:30 a.m.	Coffee break
11:00 a.m.	Reyhaneh Ghassemizadeh: "Effects of fractional charges on vibrational shifts of IR and Raman-active modes using Density Functional Theory"
11:30 a.m.	Ulrich Bangert: "Two-dimensional Electronic Spectroscopy of Controlled Isolated Systems"
12:00 p.m.	Lunch break
1:30 p.m.	Postersession
2:30 p.m.	Joshua Cantin:



	"Surface-sensitive molecular interferometry: beyond ^3He spin echo experiments"
3:00 p.m.	Marcel Binz: "Phase-modulated fs spectroscopy on alkali metal-doped helium nanodroplets"
3:30 p.m.	Coffee break
4:00 p.m.	Kariman Elshimi: "Photoelectron spectroscopy of size-selected clusters at free electron lasers"
4:30 p.m.	Andreas Wituschek: "Towards coherent time resolved all-XUV spectroscopy"
5:00 p.m.	PAC meetings intensive discussions
6:30 p.m.	PI Dinner

Wednesday, August 2, 2017

9:00 a.m.	Excursion
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Thursday, August 3, 2017

9:00 a.m.	Stefan Buhmann: "Harnessing the quantum vacuum: from Casimir forces to interatomic Coulomb decay"
10:00 a.m.	Simon Dold: "Optimizing a gas aggregation source for large cluster production"
10:30 a.m.	Coffee break
11:00 a.m.	Jonas Grzesiak: "Reactive Scattering between Metastable Helium and Magneto-Optically Trapped Lithium"
11:30 a.m.	PAC meetings intensive discussions
12:00 p.m.	Lunch break
1:30 p.m.	lab tours individual discussions
3:30 p.m.	Soccer match

Friday, August 4, 2017

9:00 a.m.	PI Meeting
10:00 a.m.	Denis Uhland: "Lithium-6 Triplet Ground State Spectroscopy and STIRAP"
10:30 a.m.	Coffee break
11:00 a.m.	Julian Schmidt: "Optical trapping of ion Coulomb crystals"
11:30 a.m.	PAC meetings intensive discussions
12:00 p.m.	Lunch break
2:00 p.m.	Tobias Brünner:



	"The role of particle (in-) distinguishability for many-particle dynamics in optical lattices"
2:30 p.m.	John Sous: "SSH Bipolarons in Quantum Devices and Materials"
3:00 p.m.	Manish Vashishta: "Microwave trapping of NH ₃ molecules"
3:30 p.m.	Coffee Break
4:00 p.m.	Takamasa Momose, Frank Stienkemeier: Closing remarks



PAC meetings

PAC meetings

PAC Meeting/Discussion on Tuesday, August 1, 2017

- 5:00 p.m. Stauffert, Walter, Krems
- 5:00 p.m. Bohlen, Stienkemeier, Jones
- 5:00 p.m. Weckesser, Schätz, Madison
- 5:45 p.m. Jalehdoost, Issendorff, Jones
- 5:45 p.m. Bangert, Stienkemeier, Momose
- 5:45 p.m. Fuchs, Buhmann, Krems

PAC Meeting/Discussion on Thursday, August 3, 2017

- 11:30 a.m. Elshimi, Issendorff, Jones
- 11:30 a.m. Binz, Stienkemeier, Milner
- 11:30 a.m. Ghassemizadeh, Walter, Momose
- 11:30 a.m. Schmidt, Schätz, Madison

PAC Meeting/Discussion on Friday, August 4, 2017

- 11:30 a.m. Wituschek, Stienkemeier, Jones
- 11:30 a.m. Dold, Issendorff, Grant
- 11:30 a.m. Gresziak, Dulitz, Momose



Abstracts – Talks & Lectures

(in alphabetical order)

Two-dimensional Electronic Spectroscopy of Controlled Isolated Systems

Ulrich Bangert, Lukas Bruder, Marcel Binz, Daniel Uhl, Katharina Schneider, Andreas Wituschek and Frank Stienkemeier.

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

Two dimensional electronic spectroscopy (2DES) is a powerful tool to study coherences and correlations on ultrafast time scales. Until now, 2DES has been limited almost exclusively to condensed phase studies. Our aim is to apply 2DES to controlled isolated systems by using doped helium nanodroplet beams. Helium nanodroplets provide the dopant with a cold environment and minimal perturbation, which are ideal conditions to study the behavior of an individual system in a well-controlled environment.

However, the target density in doped helium droplet beams is several orders of magnitude lower than in bulk condensed phase samples. Furthermore, 2DES depends on the third order response of the sample to the incident light. Together, this leads to particularly small signals. We adapt a phase modulation technique combined with lock-in detection to overcome this issue [1]. This technique has already shown significant sensitivity improvements for coherent pump-probe spectroscopy in helium nanodroplets [2].

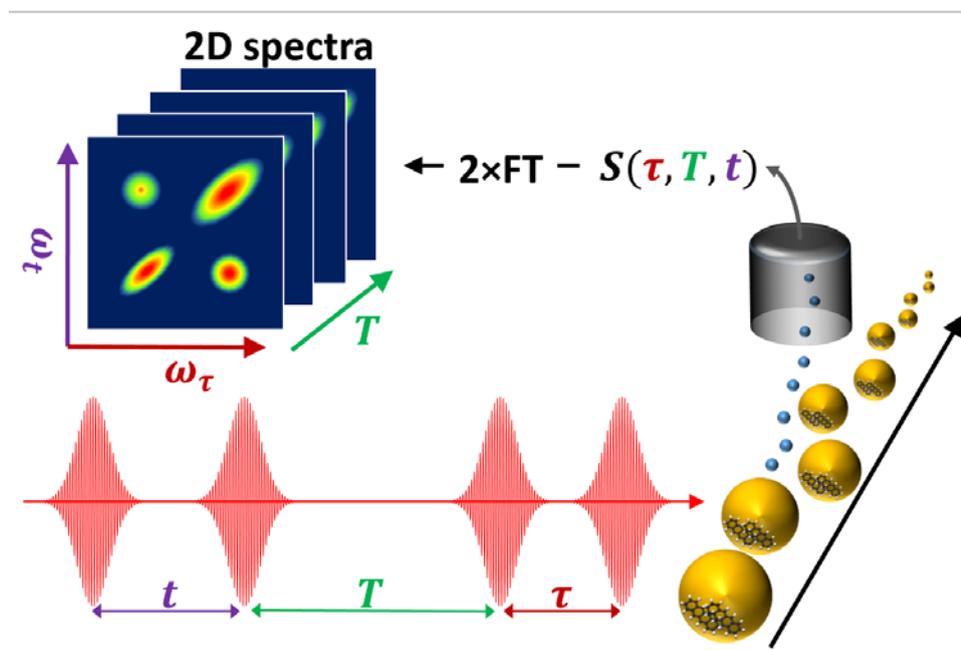


Figure 1: Schematic of the experiment without phase modulation. A train of four fs-pulses is used to excite the dopant within the droplets. The excited state population is then measured by photo ionization or fluorescence. The resulting signal is Fourier transformed with respect to the inter pulse delays τ and t yielding 2D-spectra at different t times T .



One advantage of 2D spectroscopy is that in the 2D spectra homogeneous and inhomogeneous broadening mechanisms are readily disentangled. For this reason, 2D spectroscopy has been used to characterize the dynamics of solvents such as the ultrafast rearrangement dynamics of water [3]. In a similar way, 2DES may be used to get more insights into the helium droplet properties when doped with different species.

We currently do characterization measurements and initial measurements of alkali doped helium nanodroplets.

[1] P. Tekavec, G.A. Lott, and A.H. Marcus, *J. Chem. Phys.* **127**, 214307 (2007)

[2] L. Bruder, M. Binz, and F. Stienkemeier, *Phys. Chem. Chem. Phys.* **17**, 23877 (2015)

[3] M. L. Cowan, B. D. Bruner, N. Huse, J. R. Dwyer, B. Chugh, E. T. J. Nibbering, T. Elsaesser, and R. J. D. Miller, *Nature* **434**, 199 (2005)



Phase-modulated fs spectroscopy on alkali metal-doped helium nanodroplets

Marcel Binz, Katharina Schneider, Ulrich Bangert, Daniel Uhl, Lukas Bruder and Frank 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].

Having shown the applicability of this method for doped He droplet experiments, using a 80 MHz repetition rate Ti:Sa oscillator [2], we are currently building a new setup with a 200 kHz repetition rate noncollinear optical parametric amplifier. This will eliminate some ambiguities observed in the former measurements caused by the high repetition rate of the employed laser system. The planned setup and first experimental results will be shown. Additionally, the implementation of a fast shutter made out of a hard-disk drive into our vacuum setup will be presented. As the opening time and frequency can be readily varied, this kind of shutter is optimally suited to separate different signal contributions e.g. from effusive background and doped droplet signal.

[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).

From rare gas to hydrogen-bonded clusters: Size distributions of supersonic beams from a pulsed valve using the titration technique

Matthias Bohlen, Aaron LaForge, Rupert Michiels, Nicolas Rendler and Frank Stienkemeier
Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Mykola Shcherbinin

Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark

Pulsed valves offer many advantages over continuous beam sources such as higher beam densities and reduced gas load. Recently, we developed a pulsed valve in collaboration with UBC, Vancouver, which produces supersonic gas pulses down to $20\mu\text{s}$ duration at repetition rates up to several hundred Hz. The pulsed-valve driver can be adjusted for optimal voltage amplitude, duration and repetition rate. Moreover we established different versions of the valve to accommodate different needs,



Figure 1: Home-built control unit for adjusting the parameters (pulse length, voltage and repetition rate) of the CRUCS valve.

such as improved heat conductance, or chemical resistance. The overall design and geometry of the valve is retained, making it versatile to produce rare-gas and even hydrogen-bonded clusters. Additionally, cryogenic cooling of the valve can be utilized to produce helium nanodroplets. To estimate the cluster size distribution, we use a titration technique [1], which has accurately determined cluster sizes of continuous supersonic beams. Here, we report on a systematic study of cluster size distributions by varying expansion parameters. The technique has been applied to argon, ammonia, and water clusters, and the results are compared to models of Hagena [2] and Bobbert [3], respectively.



Figure 2: Front and Side View of the CRUCS Valve with Visualisation of size

[1] L. F. Gomez, E. Loginov, R. Sliter, A. F. Vilesov 2011 *J. Chem. Phys.* **135** 154201

[2] O. F. Hagena 1981 *Surface Science* **106** 101-116

[3] C. Bobbert, S. Schütte, C. Steinbach, U. Buck 2002 *Eur. Phys. J. D* **19** 183-192



The role of particle (in-)distinguishability for many-particle dynamics in optical lattices

Tobias Brünner, Gabriel Dufour, Alberto Rodriguez, and Andreas Buchleitner *Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany*

Much attention has been dedicated so far to the dynamical impact of interactions - which often can be associated with the progressive suppression of coherence phenomena. On the other hand, little is known on the fundamental role of the interacting particles* degree of mutual (in-)distinguishability in such experiments, while we have learnt from a new generation of photonic interference experiments and theory that controlling the degree of (in-)distinguishability unveils a panoply of novel many-particle interference phenomena. We import this program into the realm of controlled, interacting many-particle quantum systems, specifically for cold atoms in optical lattices, and identify statistical, experimentally readily accessible quantifiers to infer the particles* degree of distinguishability.



Harnessing the quantum vacuum: from Casimir forces to interatomic Coulomb decay

S. Y. Buhmann

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

The quantum vacuum is one of the most counter-intuitive concepts of quantum electrodynamics. Whereas the classical vacuum refers to a region of space that is devoid of any particles or fields, its quantum counterpart contains fluctuating electromagnetic fields even in the most idealised case. The structure of these virtual photons can be significantly altered by the presence of magnetodielectric bodies or media. I will explain how a realistic notion of the quantum vacuum in the presence of such bodies can be given within the theory of macroscopic quantum electrodynamics [1].

The signature of the quantum vacuum is manifest in the interaction of virtual photons with charged matter. As noted by Casimir in 1948, they give rise to the famous Casimir force between two perfectly conducting plates [2]. I will give an overview over the Casimir effect and its significance in nanotechnology, including the possibility to realise a Casimir-based glue [3] or to tune Casimir forces between topological insulators via applied magnetic fields [4].

A second prominent vacuum effect is the spontaneous decay of excited atoms or molecules. As shown by Purcell, it is also sensitive to the presence of magnetodielectric environments [5]. We have recently considered interatomic Coulomb decay as a process where a highly-excited ion transmits its energy to a nearby neutral atom ionising the latter [6]. Using macroscopic quantum electrodynamics, we show how this process can be enhanced by retardation, intervening media or interfaces.

[1] S. Scheel and S. Y. Buhmann, *Acta Phys. Slovaca* **58** (5), 675 (2008); S. Y. Buhmann *Dispersion Forces I - Macroscopic Quantum Electrodynamics and Ground-State Casimir, Casimir–Polder and van der Waals Forces* (Springer, Heidelberg, 2013).

[2] H. B. G. Casimir, *Proc. K. Ned. Akad. Wet.* **51**, 793 (1948).

[3] J. Klatt, P. Barcellona, R. Bennett, O. S. Bokareva, H. Feth, A. Rasch, P. Reith and S. Y. Buhmann, *Langmuir* **33** (21), 5298 (2017).

[4] S. Fuchs, F. Lindel, M. Antezza, G. Hanson, R. Krems and S. Y. Buhmann, submitted to *Phys. Rev. A* (2017).

[5] E. M. Purcell, *Phys. Rev.* **69**, 674 (1946).

[6] L. S. Cederbaum, J. Zobeley, F. Tarantelli, *Phys. Rev. Lett.* **79** (24), 4478 (1997).



Surface-sensitive molecular interferometry: beyond ^3He spin echo experiments

J. T. Cantin and R. V. Krems

Department of Chemistry, University of British Columbia, Vancouver, B.C., V6T 1Z1, Canada

O. Godsi, T. Maniv, and G. Alexandrowicz

*Schulich Faculty of Chemistry, Technion - Israel Institute of Technology, Technion City, Haifa
32000, Israel*

^3He atoms can be used as surface-sensitive atomic interferometers in ^3He spin echo experiments to measure surface morphology, molecular and atomic surface different dynamics, and surface vibrations. However, using the hyperfine states of molecules gives experiments the potential to be less expensive, be more sensitive, and include angle-dependent interactions. The manifold of hyperfine states of molecules is large in comparison to the two nuclear spin states used in ^3He spin echo experiments and allows for increased precision, while simultaneously complicating experimental interpretation. Here, we present the theoretical formulation required to interpret these experiments. In particular, we show how to determine the effect of magnetic lensing on the molecular hyperfine states and use a modified form of the transfer matrix method to quantum mechanically describe molecular propagation throughout the experiment. We also discuss how to determine the scattering matrix from the experimental observables via machine learning techniques. As an example, we perform numerical calculations using nine hyperfine states of *ortho*-hydrogen and compare the results to experiment.



Setup for experimental studies on $Ba^+ - Li$ interactions

Markus Debatin, Pascal Weckesser, Fabian Thielemann, Yannick Minet, Alexander Lambrecht, Julian Schmidt, Leon Karpa and Tobias Schaetz

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

In the ultracold regime atom-atom interactions are dominated by individual scattering channels, which can be controlled through Feshbach resonances [1]. This ultracold regime has been explored during the past decades using neutral particles. Interactions between neutral and ionic atoms the strong $1/r^4$ interaction give rise to a variety of unexplored physical phenomena which can be investigated using hybrid atom-ion setups [2].

Our approach to combine ultracold neutral and ionic atoms aims at immersing optically trapped Barium ions [3, 4] in an ultracold cloud of optically trapped Lithium. In our novel apparatus a magneto-optical trap of Lithium could be created in the center of an ion trap. Enhanced optical access will allow for simultaneous optical trapping of ions and neutrals. In the talk I will give an update on recent progress in the experiment.

[1] F. Ferlaino et al., *Cold Molecules: Theory, Experiment, Applications (2008)*, Ultracold Feshbach molecules

[2] A. Haerter et al., *Contemporary Physics*, volume 55, issue 1, pages 33-45 (2014).

[3] T. Huber et al., *Nat. Comm.* 5,5587 (2014).

[4] A. Lambrecht et al., arXiv preprint arXiv:1609.06429 (2016).



Optimizing a gas aggregation source for large cluster production

Simon Dold, Samuel Kellerer and Bernd von Issendorff

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

X-Ray diffraction of clusters has been shown to be a viable tool to reconstruct the three dimensional structure of gas phase clusters[1]. Our goal is to utilize this to investigate the ultrafast structural changes that occur in clusters when subject to intense femto-second laser pulses.

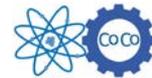
To this end the clusters in the interaction region must be sufficiently large so that their structural changes are of the order of the X-Ray wavelength and scattering cross-sections yield enough scattered photons to infer spacial features of the particle.

The production of clusters > 20nm in [1] is still not well understood and a controlled and stable cluster delivery is a precondition for performing time-resolved measurements.

Optimizing our cluster source for this purpose necessitates detection of large clusters in the lab. Deposition on substrate and subsequent imaging using high resolution microscopy techniques is one way, but lacks an immediate response when altering source parameters.

In addition to microscopy we exploit Mie-scattering as a tool to detect large clusters while operating the cluster source.

[1] Barke et. al The 3D-architecture of individual free silver nanoparticles captured by X-ray scattering



Photoelectron spectroscopy of size-selected clusters at free electron lasers

K. Elshimi, A. Ruf and B. v. Issendorff

Fakultät für Physik/VF, Stefan-Meier-Str. 19, D-79104 Freiburg, Germany

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. It will be combined with an existing high-intensity magnetron cluster source and a low-temperature ion trap for cluster thermalization. The three spectrometers are adapted to both the intense cluster beams as well as to the specific parameters imposed by the 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 ion time-of-flight mass spectrometer supported by measurements on an existing machine at Flash. Preliminary results will be shown in this poster.

[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, Ian MacPhailBartley, and Valery Milner

*Department of Physics and Astronomy, The University of British Columbia, Vancouver BC,
Canada*

An optical centrifuge is used to control the rotation and alignment of molecules embedded in Helium nanodroplets. By combining two circularly polarized chirped laser pulses, a rotating field is created that can spin anisotropically polarizable molecules to extreme rotational frequencies. Doping Helium nanodroplets with these “superrotors” is used for the study of the rotational dynamics due the droplets’ cryogenic, superfluid properties. Using the optical centrifuge, the dopant molecules are set in ultrafast rotation and the femtosecond probe pulse follows to ionize the system. The recorded velocity map ion image is analyzed to determine the rotational state of the molecules. This project is aimed at revealing new information about the dissipation of rotational energy and the interaction of the helium matrix with molecular superrotors.



Casimir-Polder Potential for Laser-Driven Atoms

Sebastian Fuchs, Stefan Yoshi Bahmann

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

Roman Krems

Department of Chemistry, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada

Within the framework of macroscopic QED we study the interaction between an atom driven by a coherent laser field with a surface and compute the Casimir-Polder potential. We use two different ideas to approach this goal. In the case where the atom is not driven resonantly and remains in its initial state, we apply a perturbative approach for the laser-induced dipole moment and the electric field stemming from the atomic polarizability. Beside the ordinary Casimir-Polder potential and the laser potential we find a new nonadditive potential term and show that it is of experimental significance under certain conditions. This method can be contrasted to a resonantly driven atom showing Rabi oscillations between its excited state and the ground state. In a next step we extend this model to a larger number of atoms with the help of Master equations and investigate the collective behavior of an atomic cloud next to a surface by using Dicke states.



Effects of fractional charges on vibrational shifts of IR and Raman-active modes using Density Functional Theory

R. Ghassemizadeh and M. Walter

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

Organic molecules, such as polycyclic carbohydrates, are promising for future use in a new generation of solar cells. To investigate electronic structure and charge transfer characteristics of these molecules, we apply (Time-dependent) Density Functional Theory (TD-DFT).

In this work we focus on interactions between charge carriers and molecular vibrations in different carbon-based molecules with various intramolecular symmetries. Due to addition of fractional charges, our studies indicate, that vibrational frequencies $\omega(q)$ are changing compared to the natural species.

We present the dependency of vibrational shifts of IR- or Raman-active modes on added fractional charges. An outlook about Raman-active vibrational shifts as finger print of charge transfer in donor-acceptor complexes in a common study with experimental collaborators is given.



Reactive Scattering between Metastable Helium and Magneto-Optically Trapped Lithium

J. Grzesiak, S. Hofsäss,, F. Stienkemeier, M. Mudrich, K. Dulitz

Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str.3, 79104 Freiburg i.Br.

The experimental study of Penning ionization reactions, i.e., the reactive scattering of metastable rare gas atoms with neutral species, has recently attracted a lot of attention through the observation of orbiting resonances at low collision energies [1]. We present first results leading to a detailed study of reactive scattering between supersonically expanded metastable helium atoms and ultracold lithium atoms confined in a magneto-optical trap. We also show that our cryogenically cooled source provides intense, velocity-tunable and cold supersonic beams of metastable helium atoms, and we discuss the efficiency of metastable atom production using two conceptually different, homemade discharge units.

References:

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

Correlated decay mechanisms in weakly bound acene molecules attached to neon clusters

Sharareh Izadnia, Frank Stienkemeier

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

Charge/excitation transfer along with the corresponding decay/loss mechanism are fundamental aspects in light harvesting, organic photovoltaics, and optoelectronic devices. Aggregates of organic molecules isolated on neon clusters are probed in order to understand collective processes of electronically excited species. These processes in weakly interacting systems offer a unique means to study energy and charge transfer processes.

Singlet fission (SF) is a particularly unique decay mechanism where an excited-molecule in its S_1 state can transfer energy to a neighbouring S_0 molecule, whereby two species are in the first triplet state. Furthermore, SF can increase the efficiency of organic electronics and photovoltaics, creating multiple charge carriers from one photon [1-3].

Here, we show the experimental observation of fluorescence lifetime reduction of tetracene, pentacene, and anthracene by controlling the number of molecules placed on the surface of neon clusters. These complexes are ideally suited to probe the interaction of molecules as a function of intermolecular distance.

We attribute these effects to singlet fission [4]. Moreover, we observe Dicke superradiance [5] in the same systems, describing an ensemble of excited molecules emitting radiation collectively as coupled-quantum lifetimes and an enhancement in the radiative intensity. Experimental results indicate that triplet-triplet annihilation is another process that can influence the system, depending on the substance and aggregate.

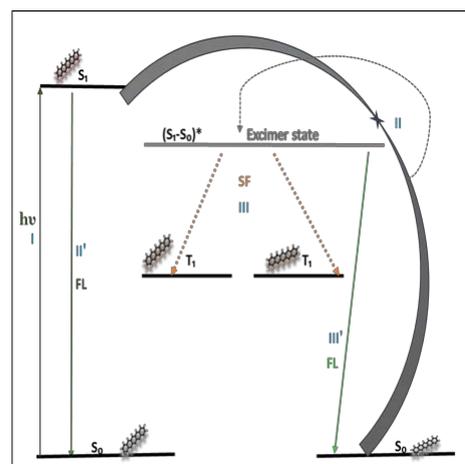


Figure 1. Depiction of singlet fission.

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High temperature pulsed valve for organic cluster generation

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Understanding the electronic properties of organic molecular solids attracted a lot of interest, because of their vast applications in science and technology.¹ The molecular clusters of organic materials can offer an excellent model to study the evolution of electronic properties from single molecule to bulk solid.² Molecular clusters are usually produced by supersonic jet expansion.^{2,3} For reaching to enough cold condition, in order to generate molecular clusters through the weak van der Waals interaction, one needs high temperature and high pressure valves.^{2,4} In this work we present the construction of a pulsed solenoid valve,^{5,6} which can operate at the temperature as high as 600°C. This valve will be used in the future for production of different organic molecular clusters.

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Applications of machine learning to constructing potential energy surfaces for complex molecules: can machine learning help us to solve the inverse scattering problem?

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Constructing accurate potential energy surfaces for polyatomic molecules is a major challenge. For a molecule with a large number of degrees of freedom, the difficulty arises both from the large number of ab initio computations required and from the uncertainty as to where in the configuration space to place the ab initio points in order to obtain the most accurate representation of the surface. I will show that both of these problems can be addressed with a machine learning technique based on Gaussian process regression. I will first show that Gaussian process regression yields a qualitatively good representation of the surface with a very small number of ab initio points (~ 200 for a 6D surface). I will then illustrate the application of Bayesian optimization with Gaussian processes as an efficient method for sampling the configuration space of polyatomic molecules. Bayesian optimization is based on iterative procedure, where, at each iteration, the surface is constructed by Gaussian process regression and a small set of ab initio points is added in the part of space determined by the maximizing the so-called acquisition function. The acquisition function quantifies the improvement of the accuracy of the potential energy fit thus obtained. Time permitting, I will also discuss how Gaussian process regression can be used for obtaining the dynamical observables with error bars reflecting the inherent uncertainty of the ab initio calculations and other applications in molecular physics research.



Optically Trapping Ions while having a coffee?

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Isolating ions and atoms from the environment is essential in experiments on a quantum level. For decades, this has been achieved by trapping ions with radiofrequency (rf) fields and neutral particles with optical fields. We demonstrated the trapping of ions by interaction with light [1,2,3]. We take these results as starting point for finally combining the advantages of optical trapping and ions [4]. In particular, ions provide individual addressability, high fidelities of operations and long-range Coulomb interaction, significantly larger compared to those of atoms and molecules.

We aim to demonstrate the prospects of our approach in the context of interaction and reaction at ultra-low temperatures as a showcase. Following the seminal work of other groups e.g. Vuletic, Koehl and Denschlag) in hybrid traps, we plan to embed optically trapped ions into quantum degenerate gases to reach lowest temperatures, circumventing the currently inevitable excess kinetic energy in hybrid traps, where ions are kept but also driven by rf- fields [5]. It might permit to enter the temperature regime where quantum effects are predicted to dominate, (i) in many-body physics, including the potential formation and dynamics of mesoscopic clusters of atoms of a BEC, binding to the impurity ion, as well as (ii) the subsequent two-particle s-wave collisions, the ultimate limit in ultra-cold chemistry.

I will start with a tutorial introduction on trapping particles.

Subsequently, I will focus on our recent results [6] on optically trapping $^{138}\text{Ba}^+$ in a bi- chromatic far-off-resonant dipole trap sufficiently isolated and providing lifetimes of seconds.

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A. Lambrecht, J. Schmidt, P. Weckesser, M. Debatin, L. Karpa, T. Schaetz, arXiv:1609.06429v2 (2016)

Optical trapping of ion Coulomb crystals

Julian Schmidt, Alexander Lambrecht, Pascal Weckesser, Markus Debatin, Leon Karpa and Tobias Schaetz

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Ion Coulomb crystals are the key to many applications with trapped ions, as the crystal phonons mediate interaction between ions and allow coupling of electronic and motional states on the quantum level [1]. In cold chemistry experiments, Coulomb crystals have allowed to study reaction rates of trapped atomic and molecular ions with neutral particles in a controlled environment [2]. However, rf-micromotion in ion traps poses fundamental limits for applications with higher-dimensional Coulomb crystals and in ultracold chemistry experiments. Optical dipole traps for trapped ions [3, 4, 5] do not exhibit this micromotion, but only trapping of single had been demonstrated thus far.

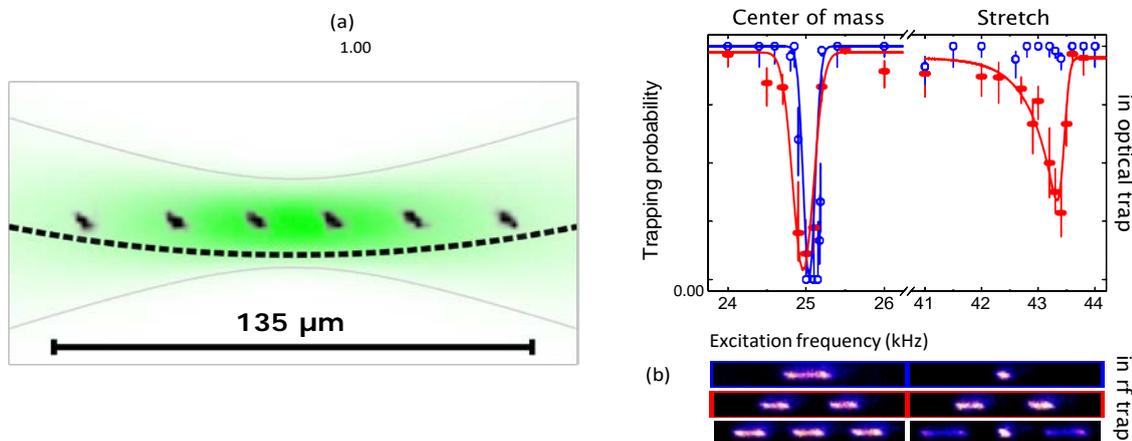


Figure 1: Existence of center-of-mass (COM) and stretch (STR) modes in optically trapped Coulomb crystals

We now demonstrate trapping of ion crystals consisting of up to six Barium ions inside an optical dipole trap aligned along the crystal axis without confinement by radio-frequency (RF) fields. The dependence on the trap parameters, in particular the interplay of beam waist, Rayleigh length, laser power and axial confinement by DC electric fields is investigated. As a proof-of-principle experiment, we detect the center-of-mass and stretch modes for an optically trapped two-ion crystal, see figure 1. In Paul traps, these motional states are routinely exploited to couple the electronic and motional degrees of trapped ions. Finally, we present prospects for optical trapping of higher-dimensional Coulomb crystals in the absence of RF-driven micromotion.

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[5] A. Lambrecht *et al.*, *arxiv:1609.06429* (2016)



SSH Bipolarons in Quantum Devices and Materials

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I will introduce the Peierls/SSH model of particle-phonon coupling. I will then discuss the single particle picture which is described by a polaron theory and mediated interactions and their interplay which lead to the formation of bipolarons.

I will discuss the relevance to experiments on cold atoms and quantum devices and materials.

Ab-initio electron-phonon coupling in polyacenes

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Polycyclic aromatic hydrocarbons (PAHs) absorbed on ultracold neon clusters are studied in the group of Prof. Stienkemeier with the aim to observe singlet fission processes (which are interesting for current research on organic solar cells) under controlled conditions. The Neon cluster is optically transparent in the considered spectral region. However vibrational coupling between the PAHs and the surface takes place. This gives rise to broadening effects through coupling to low frequency Neon phonons as well as completely new features. We describe electronic and vibronic structure of these molecules with density functional theory (DFT). Hereby we analyse optical spectra including their vibrational substructure. Electronic spectra are calculated using time dependent DFT in the linear response formalism. The vibrational lines are described by Franck-Condon overlaps and show excellent agreement with experimental data. Furthermore, the influence of the environment on the spectra is investigated, where we find strong effects from the neon substrate. These effects can be grasped by DFT and for example the prominent emerging butterfly mode in pentacene can be theoretically explained.

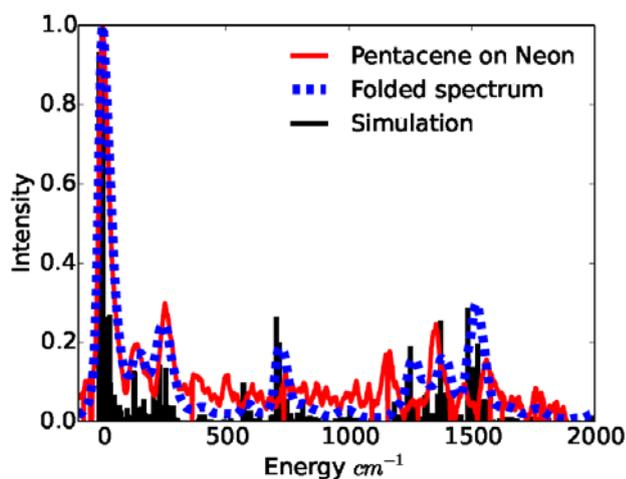


Fig 1. Comparison of the experimental emission spectrum of pentacene on a neon cluster with DFT simulations.



Lithium-6 Triplet Ground State Spectroscopy and STIRAP

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We will present molecular spectroscopy of the excited and ground triplet potentials at high magnetic fields and our efforts toward Stimulated Raman Adiabatic Passage to the lowest lying level in the ground triplet potential.



Microwave trapping of NH₃ molecules

Manish Vashishta

Department of Chemistry, University of British Columbia

Ultra cold molecules offer a rich playground for understanding of new chemistry and physics at low temperature. Existing techniques to produce ultra cold molecules are limited by the type and low phase space density of molecules. Microwave trapping of polar molecules offers a solution to overcome these challenges. In my talk, I will discuss the recent progress made towards the experimental realization of trapping NH₃ molecules using microwaves inside a Fabry-Perot Cavity.

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Trapping and Controlling Barium Ions for Ultracold Atom-Ion Experiments

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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] 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 [8] currently limiting experiments to collision energies on the order of a few mK.

Here we present our novel experimental setup combining Ba^+ ions and Li atoms in an optical dipole trap. On this poster we focus on the Barium segment of the experiment. We demonstrate the Barium laser setup, including a homebuilt frequency doubler, generating laser light at 615 nm. Furthermore we discuss a newly designed ion trap suitable to detect and transfer Ba^+ ions into an optical dipole trap. First trapping attempts of Barium will be presented.

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Towards coherent time resolved all-XUV spectroscopy

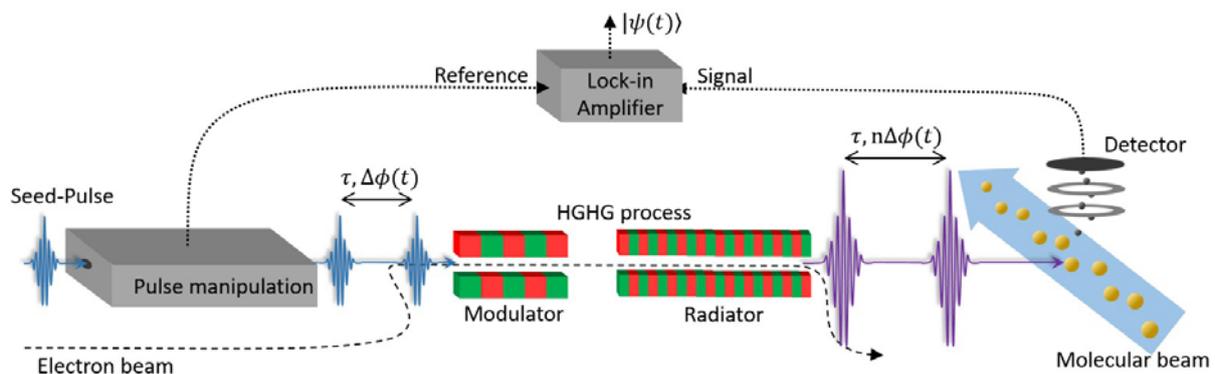
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Coherent time-resolved spectroscopy is a powerful tool to study ultrafast dynamics in complex systems. Extending these techniques to the XUV spectral region would allow studying core excitations, thus providing site-specific information. In order to perform coherent spectroscopy it is necessary to generate multi-pulse sequences and control their phase-relation to a fraction of the wavelength. Several techniques to achieve this have been developed in the IR and VIS regime [1]. However, demands on phase stability increase significantly when going to short wavelengths and advanced pulse manipulation in the XUV is challenging. Recent experiments have shown that in seeded HGHG free electron lasers (FEL) the emitted XUV pulses inherit the coherence properties of the seed pulses [2]. We suggest an approach based on acousto-optical phase modulation on the seed laser with subsequent seeding of the FEL and lock-in detection at the harmonics of the seed modulation. In this way, pulse manipulation can be performed with standard optics. Moreover, demands on phase stability are drastically reduced and signals are efficiently isolated and amplified. We present the first step towards this approach: extending the phase modulation scheme towards UV wavelengths (266nm) and high-intensity femtosecond laser pulses in combination with detection in dilute samples.



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