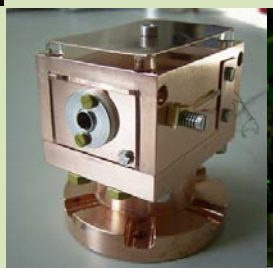
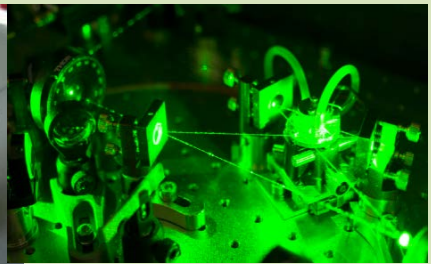
SUMMER SCHOOL 2017

IRTG CoCo

Cold Controlled Ensembles in Physics and Chemistry





BOOK OF ABSTRACTS

2nd CoCo Summer School

ULTRACOLD FEW- AND MANY-BODY SYSTEMS: COLD ON QUANTUM'S TRAIL

August 6 – August 11, 2017

Quest University, Squamish, 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

THE SUCCESSFUL CONCEPT OF OUR LAST YEAR'S SUMMER SCHOOL WILL BE CONTINUED IN THE 2ND IRTG COCO SUMMER SCHOOL "ULTRACOLD FEW- AND MANY-BODY SYSTEMS: COLD ON QUANTUM'S TRAIL". WE AGAIN HAVE BEEN ABLE TO RECRUIT DISTINGUISHED SPEAKERS THAT COVER VARIOUS RESEARCH FIELDS. THE LECTURES WILL COVER SCIENTIFIC QUESTIONS IN THE VICINITY OF THE IRTG RANGING FROM ELECTRONIC EXCITATIONS IN CONDENSED MATTER, OVER COOLED MOLECULAR IONS AND ATOM ION INTERACTIONS, MOLECULES UNDER DEFINED CONDITIONS TO QUANTUM INFORMATION. MAXIMAL CONTROL IS THE CONNECTION BETWEEN THESE TOPICS WHICH IS PROVIDED BY COLD ENVIRONMENTS. THE LECTURES WILL BRING TOGETHER EXPERIMENTAL AND THEORETICAL RESEARCHERS WORKING IN THE FIELD AND ARE DEVOTED TO THE PEOPLE DOING THE REAL WORK: GRADUATE AND DOCTORAL STUDENTS AS WELL AS YOUNG POSTDOCS.

Main Topics

"Photon manipulation and entanglement with cooperative atomic systems" (Theory)

"Hybrid atom-ion trapping" (Experiment)

"Experiments with Large Superfluid Helium Droplets" (Experiment)

"The Casimir-Polder Effect" (Theory)

"Proton diffusion in crystalline silicon: is it classical or quantum-mechanical?" (Theory)

Financial Support

Organisation

IRTG 7079 „Cold Controlled Ensembles in Physics and Chemistry“

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General Information

Duration

Sunday August 6, 2017, 4.00 p.m. – Friday August 11, 2017, 2.00 p.m.

Location

Quest University Canada

3200 University Boulevard, Squamish, B.C. Canada V8B 0N8

www.questu.ca

Travel Information – Shuttles

The closest airport is Vancouver International Airport (YVR). Shuttle busses will operate on Sunday, August 6 at 1:00 p.m. from the UBC in Vancouver to the Quest University in Squamish, and back on Friday, August 11 at 2:00 p.m. and on Saturday, August 12 at 9:00 a.m. to the Vancouver International Airport.

Travel Information – By car

From Vancouver*:* via BC-99 N to Mamquam Road in Squamish

Address: 3200 University Boulevard, Squamish, B.C. Canada V8B 0N8

Accommodation

All participants will be accommodated at the Quest University Canada.

Bed linen and towels will be provided.

Meals & Drinks

Meals and drinks during the scientific program are included in the conference fee.

Excursion

An excursion to D-Wave – The Quantum Computing Company (www.dwavesys.com) is organized on Wednesday, August 9, 2017 afternoon.

WiFi

There is WiFi Access throughout the Quest University campus.

Quest Campus

Scientific Program

Sunday, August 6, 2017

4:00 p.m.	Opening remarks	Michael Walter, Zofia Malachowska
4:30 p.m.	Presentation by participants: 1 slide for 1 min/person	
5:30 p.m.	Poster Session A & Aperitif	Ulrich Bangert, Tobias Brünner, Simon Dold, Erik Frieling, Jonas Grzesiak, Julian Schmidt, Fabian Thielemann, Andreas Wituschek
7:00 p.m.	Dinner	

Monday, August 7, 2017

Till 08:45 a.m.	Breakfast	
09:00 a.m.	"Photon manipulation and entanglement with cooperative atomic systems " (Experiment, Lecture 1)	Susanne Yelin
10:30 a.m.	Coffee break	
11:00 a.m.	Rework Seminar – Lecture 1	Susanne Yelin
12:30 a.m.	Lunch	
2:00 p.m.	Rework Seminar – Lecture 1	Susanne Yelin
3:30 p.m.	Coffee break	
4:00 p.m.	Career event	Roman Krems, Frank Stienkemeier, Michael Walter
5:30 p.m.	Poster Session B & Aperitif	Marcel Binz, Joshua Cantin, Kariman Elshimi, Sebastian Fuchs, Sharareh Izadnia, Brendan Moore, Pinrui Shen, Denis Uhland
7:00 p.m.	Dinner	

Tuesday, August 8, 2017

Till 08:45 a.m.	Breakfast	
09:00 a.m.	“Cooling molecular ions, ultracold atom ion interactions“ (Experiment, Lecture 2)	Eric Hudson
10:30 a.m.	Coffee break	
11:00 a.m.	Rework Seminar – Lecture 2	Eric Hudson
12:30 a.m.	Lunch	
2:00 p.m.	Rework Seminar – Lecture 2	Eric Hudson
3:30 p.m.	Coffee break	
4:00 p.m.	“Experiments with Large Superfluid Helium Droplets” (Experiment, Lecture 3)	Andrey Vilesov

5:30 p.m.	Poster Session C & Aperitif	Matthias Bohlen, Tirthaprasad Chattaraj, Jordan Fordyce, Reyhaneh Ghassemizadeh, Aghigh Jalehdoost, Oliver Stauffert, Manish Vashishta, Pascal Weckesser
7:00 p.m.	Dinner	

Wednesday, August 9, 2017

Till 08:45 a.m	Breakfast	
09:00 a.m.	Rework Seminar – Lecture 3	Andrey Vilesov
10:30 a.m.	Coffee break	
11:00 a.m.	Rework Seminar – Lecture 3	Andrey Vilesov
12:30 p.m.	shuttle bus to D-Wave, lunch packages	
2:00 p.m.	Excursion – D-Wave	
7:00 p.m.	Dinner	

Thursday, August 10, 2017

Till 08:45 a.m	Breakfast	
09:00 a.m.	"The Casimir-Polder Effect" (Theory, Lecture 4)	Daniel Steck
10:30 a.m.	Coffee break	
11:00 a.m.	Rework Seminar – Lecture 4	Daniel Steck
12:30 p.m.	Lunch	
2:00 p.m.	Rework Seminar – Lecture 4	Daniel Steck
3:30 p.m.	Coffee break	
4:00 p.m.	“Proton diffusion in crystalline silicon: is it classical or quantum-mechanical?” (Theory, Lecture 5)	Ralph Gebauer
5:30 p.m.	Sports and drinks	
7:00 p.m.	Dinner	

Friday, August 11, 2017

Till 08:45 a.m	Breakfast	
09:00 a.m.	Rework Seminar – Lecture 5	Ralph Gebauer
10:30 a.m.	Coffee break	
11:00 a.m.	Rework Seminar – Lecture 5	Ralph Gebauer
12:30 p.m.	Closing Remarks & Poster Prize	Frank Stienkemeier
1:30 p.m.	Lunch	
2:00 p.m.	Departure	

Poster Sessions – Participants & Presentations

Poster Session A

Ulrich Bangert, University of Freiburg
Two-dimensional Electronic Spectroscopy of Controlled Isolated Systems

Tobias Brünner, University of Freiburg
The role of particle (in-) distinguishability for many-particle dynamics in optical lattices

Simon Dold, University of Freiburg
Optimizing a gas aggregation source for large cluster production

Erik Frieling, University of British Columbia
Excited state collisions of trapped 87Rb atoms

Jonas Grzesiak, University of Freiburg
Reactive Scattering between Metastable Helium and Magneto-Optically Trapped Lithium

Julian Schmidt, University of Freiburg
Optical trapping of ion Coulomb crystals

Fabian Thielemann, University of Freiburg
Preparing Ultracold Lithium for Atom-Ion Experiments

Andreas Wituschek, University of Freiburg
Towards coherent time resolved all-XUV spectroscopy

Poster Session B

Marcel Binz, University of Freiburg
Phase-modulated fs spectroscopy on alkali metal-doped helium nanodroplet

Joshua Cantin, University of British Columbia
Surface-sensitive molecular interferometry: beyond 3He spin echo experiments

Kariman Elshimi, University of Freiburg
Photoelectron spectroscopy of size-selected clusters at free electron lasers

Sebastian Fuchs, University of Freiburg
Casimir-Polder Potential and Casimir Force Involving Topological Insulators

Sharareh Izadnia, University of Freiburg
Correlated decay mechanisms in weakly bound acene molecules attached to neon clusters

Brendan Moore, University of British Columbia
TBA

Pinrui Shen, University of British Columbia
Primary Pressure Standard with Cold Atoms

Denis Uhland, University of British Columbia
Lithium-6 Triplet Ground State Spectroscopy and STIRAP

Poster Session C

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

Tirthaprasad Chattaraj, University of British Columbia
Quantum walks of interacting particles in low-dimensional lattices

Jordan Fordyce, University of British Columbia
Molecular Superrotors in Helium Nanodroplets

Reyhaneh Ghassemizadeh, University of Freiburg
Effects of fractional charges on vibrational shifts of IR and Raman-active modes using Density Functional Theory

Aghigh Jalhedoost, University of Freiburg
High temperature pusled valve for organic cluster generation

Oliver Stauffert, University of Freiburg
Ab-initio electron-phonon coupling in polyacenes

Manish Vashishta, University of Bristish Columbia
Microwave trapping of NH3 molecules

Pascal Weckesser, University of Freiburg:
Trapping and Controlling Barium Ions for Ultracold Atom-Ion Experiments

Abstracts – Invited Speakers

Photon manipulation and entanglement with cooperative atomic systems

Susanne Yelin

Department of Physics, University of Connecticut, 2152 Hillside Rd, Storrs, CT 06269

E-mail: susanne.yelin@uconn.edu

The goal of these lectures is to understand how cooperative effects, Dicke states, and entanglement are related, and how these effects can be used for quantum information science, or quantum nonlinear optics and topological optical physics. I'll first introduce Dicke states and dipole-dipole interaction caused cooperative effects, and briefly talk about the role of entanglement in this system. At the end, these ideas will be applied to a 2D atomically thin mirrors that allows resonant linear and non-linear photon operations using a clear division between radiant and subradiant modes and how this idea can be used for quantum information science.

Hybrid atom-ion trapping

Eric Hudson

UCLA Department of Physics and Astronomy, University of California, Los Angeles, USA

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Over the last decade, researchers have begun to combine the two “work horses” of AMO physics -- namely, neutral atom traps and ion traps. These, so-called, hybrid traps of neutrals and charged particles are enabling a new era of research in chemistry and physics. There has been much progress in this new field in the last several years and many unanticipated challenges have been overcome. Already, work has uncovered surprising “thermodynamics” in these systems, as well as greatly aided our understanding of charged-neutral collisions and chemistry. While work is continuing on these two fronts, new efforts are starting to explore the quantum limits of these systems with hopes of realizing quantum control of chemistry and new platforms for quantum information processing.

The plan of this lecture is to first present an overview of the field, before delving into the physics behind it. We will review the basics of atom-ion trapping, explore charge-neutral collisions and chemistry, and discuss the “thermodynamics” of the damped-driven system, which is central to the field. Interested students may prepare for the lecture by reading recent review articles [1,2] and the references therein.

[1] O. Dulieu, R. Krems, M. Weidemueller, and S. Willitsch, “Physics and Chemistry of Cold Molecules,” Phys. Chem. Chem. Phys. 13, 18703 (2011).

[2] E.R. Hudson, “Sympathetic cooling of molecular ions with ultracold atoms,” EPJ Techniques and Instrumentation 3, 8 (2016).

Experiments with Large Superfluid Helium Droplets

Andrey Vilesov

Department of Chemistry, University of Southern California, Los Angeles, USA

E-mail: vilesov@usc.edu

Superfluid ^{4}He droplets are versatile media for diverse experiments in physics and chemistry. Due to the very low temperature of helium droplets, ~0.4 K, any embedded particles, which could be clusters of atoms or molecules, are usually in the ground electronic and vibrational state while a few of the lowest rotational states are occupied. In addition to the cold and dormant superfluid environment, the embedded species are uniquely surrounded by helium atoms, almost suited to their sizes and shapes. Furthermore, liquid helium is transparent to electromagnetic radiation from far infrared to vacuum ultraviolet range. All of these properties combine to make helium droplets ideal spectroscopic matrices. Finally, helium droplets are interesting in their own right, as they exemplify an isolated quantum liquid system close to absolute zero temperature. In fact, a droplet as small as ~2 nm in diameter (~60 helium atoms) is already superfluid. Small droplets with a radius from 2 to 5 nanometres and consisting of 10^3 to 10^4 helium atoms, respectively, are well suited for spectroscopic experiments with single molecules and small molecular/atomic clusters. Surface excitations, such as ripplons, represent the most thermodynamically feasible excitations in small droplets; while volume excitations, such as phonons and rotons, remain dormant due to low temperature and finite size effects.

This presentation is focused on the properties of and experiments with large helium droplets with radius ranging from 10 nm to 2 μm and consisting of 10^5 to 10^{12} helium atoms, respectively. Large droplets offer a unique opportunity for forming and studying large clusters ($>10^6$), whose sizes are limited only by the droplet's evaporation enthalpy. In addition to ripplons, volume phonon excitations and global excitations, such as quantum vortices, are also present in large droplets. The presence of quantum vortices as nucleation centers dramatically influences the morphology of the embedded clusters, inducing the formation of filaments.

Here, the thermodynamics and excitations in large droplets will be discussed followed by a primer on the droplets' rate of cooling. Then the production of droplets, and the techniques for characterization of the droplet, such as the flux and the average droplet size, will be discussed. We continue with the discussion of the kinetics involved for the different regimes of cluster aggregation in the droplets, such as that for single- and multiple-center aggregation. This is followed by a short review of spectroscopic measurements done with large droplets and the experiments aimed at cluster deposition and electron microscopy. Finally, a summary of results from recent x-ray coherent diffraction imaging experiments with large helium droplets will be presented. The material will be based on our review article, which will be published soon. [1]

[1] R. M. P. Tanyag, C. F. Jones, C. Bernando, S. M. O. O'Connell, D. Verma and A. F. Vilesov, Experiments with Large Superfluid Helium Nanodroplets. In press: Cold Chemistry: Molecular Scattering and Reactivity Near Absolute Zero; Osterwalder, A., Dulieu, O., Eds.; Royal Society of Chemistry: Cambridge, 2017.

The Casimir-Polder Effect

Daniel Steck

Oregon Center for Optical, Molecular and Quantum Science, University of Oregon Eugene, Oregon, USA

E-mail: dan@steck.us

The Casimir-Polder effect--the force between an atom or molecule and other uncharged bodies--is one of the most interesting manifestations of quantum fluctuations. In this lecture we will review the basics of the CP effect, review some of the experiments that have studied the effect using cold atoms or atomic beams, review the classic calculation, and study some of the pitfalls that arise in such calculations.

Even though the classic calculation of the CP effect dates back to 1048, the development of new, general methods for the computation of Casimir potentials in arbitrary geometries and for arbitrary material properties remains a difficult problem. My recent research focuses on developing the "worldline" method for the numerical computation of CP and Casimir effects. This is a path-integral Monte-Carlo method for computing vacuum- and thermal-state energies of a quantum field. I will review the basics of this method and give an overview on on the generalization of this method to electromagnetism.

Proton diffusion in crystalline silicon: is it classical or quantum-mechanical?

Ralph Gebauer

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These lectures will explore how computer simulations at the atomic scale can be used to understand basic processes in materials science. As a paradigmatic case of study a silicon crystal with implanted protons will be considered. Such systems play an important role in many technological applications. For example in semiconductor devices, hydrogen can be used to passivate defect-related electronic states.

But which sites in the crystalline matrix do the protons prefer to occupy? How easy or difficult is it for them to migrate? Does migration need thermal activation? Or can a proton tunnel quantum-mechanically between equilibrium sites? How strongly is the Si-lattice distorted due to the presence of a proton? Such are just a few questions which arise in this context.

In these lectures, I will give an introduction to how computer simulations can help to find answers. I will explain the basics of density-functional theory and how it can be applied to H-doped silicon.
In the hands-on part of the course, the students will have the occasion to compute a potential energy surface for protons in a Si crystal. Also, the students can develop small codes to solve the Schrödinger equation for a proton in Si, given a computed potential energy surface. In this way, the importance of quantum effects on the diffusion can be estimated.

Abstracts – Poster Session A

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].

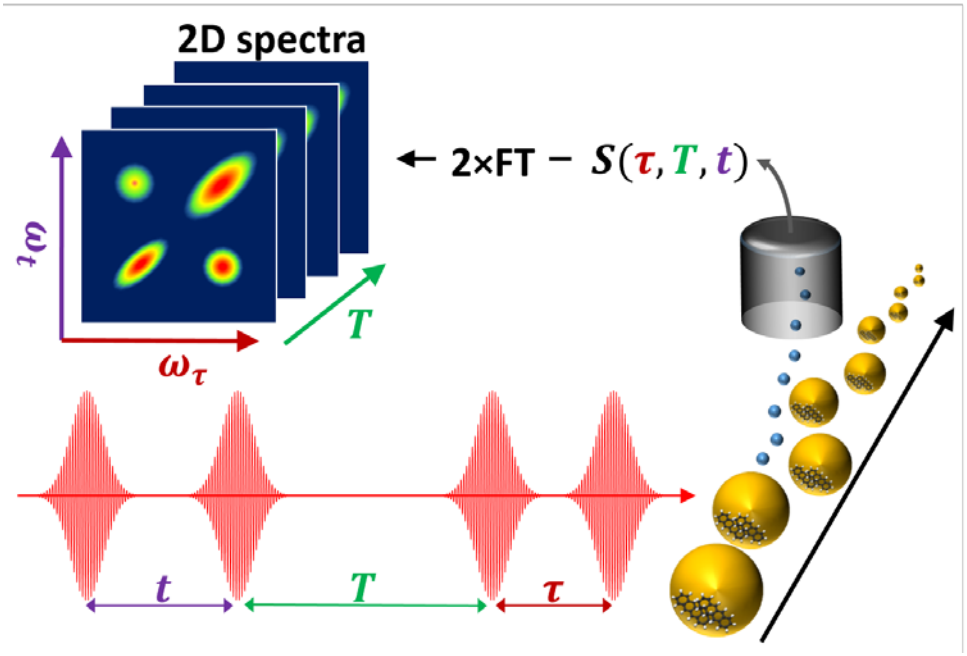

Figure 1: Schematic of the experiment without phase modulation. A train of four fs-pulses is used to excite the dopant within the droplets. The excited state population is then measured by photo ionization or fluorescence. The resulting signal is Fourier transformed with respect to the inter pulse delays 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 disentangeled. 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)

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.

Optimizing a gas aggregation source for large cluster production

Simon Dold, Samual 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

Excited state collisions of trapped 87Rb atoms

Erik Frieling , Yue Shen, Pinrui Shen, Kirk Madison

Department of Physics and Astronomy, University of British Columbia, 6226 Agricultural Road, V6T 1Z1 Freiburg, Germany

James Booth

British Columbia Institute of Technology

We investigate the collision induced loss rate 87Rb atoms from a Magneto-Optical Trap (MOT). By varying the percentage of trapped atoms in the excited state using the in- tensity of the repump laser, we can calculate the velocity averaged collision cross section between excited state and background 87Rb atoms.

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).

Optical trapping of ion Coulomb crystals

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

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

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.

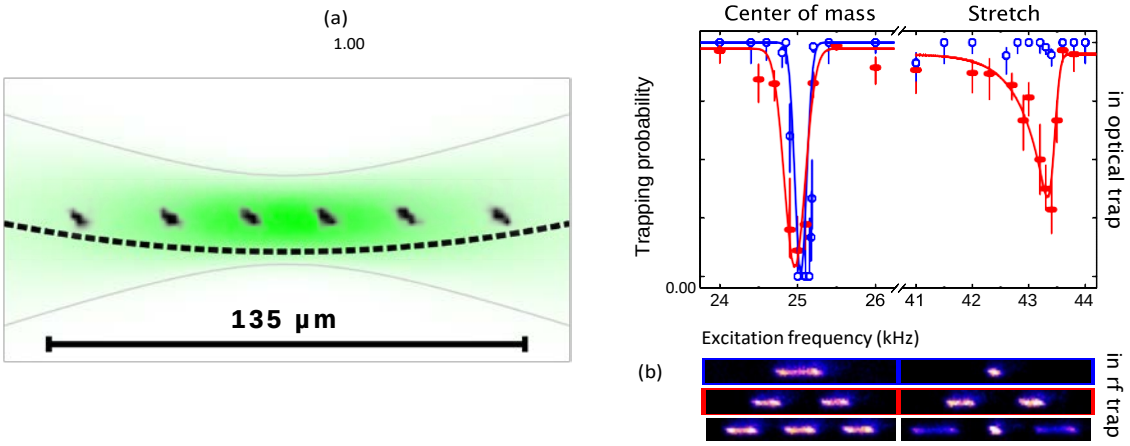

Figure 1: Existence of center-of-mass (COM) and stretch (STR) modes in optically trapped Coulomb crystals

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 fi 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.

References

[1] D.J. Wineland, Rev. Mod. Phys. **85**, 1103 (2013)

[2] R. Thompson, Contemp. Phys.,**1, 56**, 63-79 (2015)

[3] C. Schneider *et al.*, Nat. Phot. **4**, 772775 (2010)

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

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

Preparing Ultracold Lithium for Atom-Ion Experiments

Fabian Thielemann, Pascal Weckesser, Yannick Minet, Alexander Lambrecht, Julian Schmidt, Leon Karpa, Markus Debatin and Tobias Schaetz
Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

The fields of ultracold atoms and trapped ions are important pillars of experimental quantum optics. Recently the expertise of both fields has been combined in hybrid trapping setups to prepare atom-ion mixtures at low temperatures [1]. For these systems interesting new features like Feshbach resonances on the order of tens of Gauss [2] or the formation of mesoscopic, weakly bound molecules [3] have been predicted. As reaching the ultracold regime in hybrid setups is an experimentally challenging task [4,5], these features remain yet to be observed.

In our novel experimental setup we plan to reach the ultracold regime by sympathetically cooling single Barium (Ba^+) ions in a cloud of Lithium (Li) atoms. The atoms and ions will be confined in a combined optical dipole trap to overcome fundamental temperature limits due to micromotion of an ion in a radiofrequency trap [6,7,8].

On this poster we will focus on the Li branch of the setup. We present a modulation transfer spectroscopy laser lock for the Li laser system, a variable pitch Zeeman slower and compact Bitter-design magnetic coils. The current state of our magneto optical trap (MOT) will be put forward.

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

[2] M. Tomza et al., Physical Review A 91.4 (2015): 042706.

[3] R.Cote et al. Phys.Rev.Lett. 89.093001 (2002).

[4] A. Grier et al., Phys. Rev. Lett. 102,223201 (2009).

[5] Härter, A. et al., Applied Physics Letters 102.22 (2013): 221115.

[6] M. Cetina et al., Phys.Rev.Lett. 109,253201 (2012).

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

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

Towards coherent time resolved all-XUV spectroscopy

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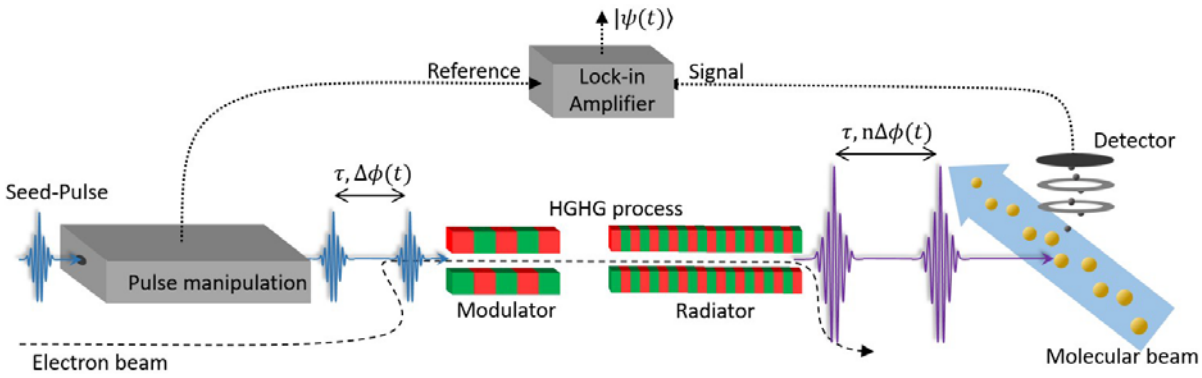
Coherent time-resolved spectroscopy is a powerful tool to study ultrafast dynamics in complex systems. Extending these techniques to the XUV spectral region would allow studying core excitations, thus providing site-specific information. In order to perform coherent spectroscopy it is necessary to generate 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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Abstracts – Poster Session B

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

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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.

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

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^{3}He atoms can be used as surface-sensitive atomic interferometers in ^{3}He 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 ^{3}He 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 hyperfin e 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.

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. 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.

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Casimir-Polder Potential and Casimir Force Involving Topological Insulators

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Due to broken time-reversal symmetry, topological insulators may show very interesting optical properties such as the mixing between perpendicular and parallel polarization. This leads to the possibility of switching between an attractive and a repulsive Casimir-Polder potential between a topological insulator and an atom by applying circularly oscillating dipole moments. An equivalent effect can be observed for Casimir forces involving topological insulators. Motivated by these findings we investigate theoretically the Casimir-Polder potential and the Casimir force for nonreciprocal material and use the results to study two topological insulators: the axion topological insulator and the photonic topological insulator.

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

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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.

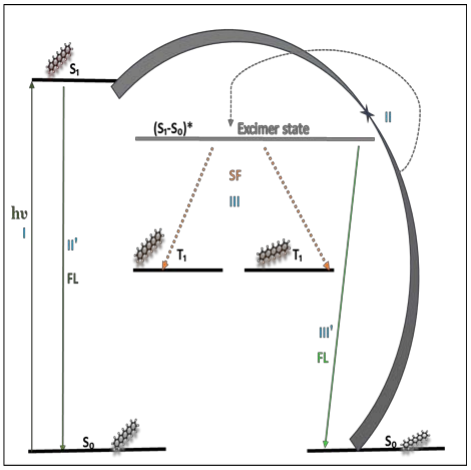

Figure 1. Depiction of singlet fission.

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Primary Pressure Standard with Cold Atoms

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We developed a method of using an ultra-cold ensemble of atoms confined in a trap as an atomic primary pressure standard for the high- and ultra-high vacuum ranges. This primary standard firstly uses a 3D magneto-optical trap (MOT) to trap RUbidium (^{87} Rb) and then transfers them into a quadrupole magnetic trap. The slowly moving, confined "sensor" atoms are sensitive to collisions with background gas particles which can transfer enough momentum to free them from the trap, resulting in loss of the sensor atoms. The measured loss rate is proportional to the density of the background gas particles and to a velocity-averaged collision cross-secction based on fundamental atomic properties [1][2]. The advantages of this cold atom standarad (CAS) are that it is based on immutable atomic properties, can be used to measure the pressure of any species - in contrast with existing pressure standards which only measure either Argon or Nitrogen [3], and it transduces loss rate (timing measurement) into pressure, tying it to one of the base SI units. The CAS is currently being tested against a NIST-calibrated ionization gauge using both Argon and Nitrogen over the pressure range (10^{-6} - 10^{-9}) Torr or (10^{-4} - 10^{-7}) Pa. The gauge factor for Argon is found to be (1.25 $\pm$ 0.02) and the Nitrogen measurements have alllowed the long-range Van der wals coefficient for N_2 - Ar elastic collisions to be determined, C_6=325 $E_h a^6$, which allows us for it to be used as a standard. We also proved the reproducibility of this primary standard. We also studied the Majorana losses in this quadrupole magentic trap and reduced its effect to improve the accuracy of the CAS.

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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.

Abstracts – Poster Session C

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

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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 20μs 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 accomodate 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

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Quantum walks of interacting particles in low-dimensional lattices

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We study the effects of long-range hopping and long-range interparticle interactions on the quantum walk of hard-core bosons in ideal and disordered lattices. We find that the range of hopping has a much more significant effect on the particle correlation dynamics than the range of interactions. While attractively and repulsively interacting pairs with short-range hopping in 1D lattices undergo the same dynamics, long-range hopping introduces asymmetry with respect to the sign of the interaction. We examine the relative role of repulsive and attractive interactions on the dynamics of scattering by isolated impurities and Anderson localization in disordered lattices. We find that weakly repulsive interactions increase the probability of tunneling through isolated impurities and decrease the localization in one- dimensional systems. The results for 1D lattices are obtained by direct diagonalization of the Hamiltonian. For 2D lattices, we employ an approach based on the recursive calculation of the Green's functions for two interacting particles.

Molecular Superrotors in Helium Nanodroplets

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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 supperrotors.

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

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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 w(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.

High temperature pusled 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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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.

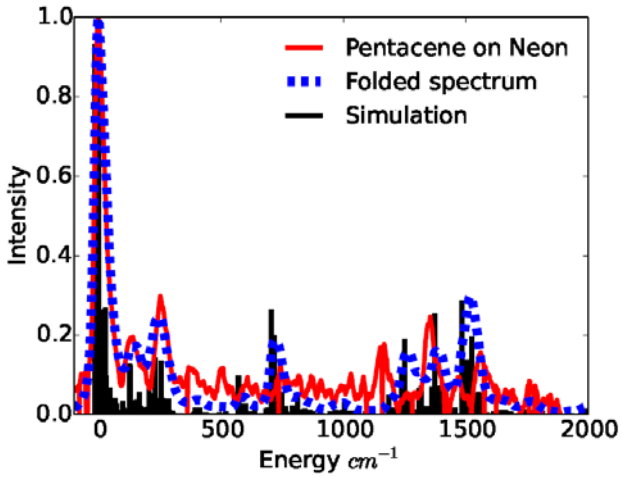

Fig 1. Comparison of the experimental emission spectrum of pentacene on a neon cluster with DFT simulations.

Microwave trapping of NH_3 molecules

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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 615nm. 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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Notes

Program Summer School 2017

ULTRACOLD FEW- AND MANY-BODY SYSTEMS: COLD ON QUANTUM'S TRAIL

	Sunday, August 6	Monday, August 7	Tuesday, August 8	Wednesday, August 9	Thursday, August 10	Friday, August 11
9:00 a.m.	*Arrival*	**Susanne Yelin (Theory): Photon manipulation and entanglement with cooperative atomic systems**	**Eric Hudson (Experiment): Cooling molecular ions, ultracold atom ion interactions**	**Rework seminar - Andrey Vilesov**	**Daniel Steck (Theory): The Casimir-Polder Effect**	**Rework Seminar - Ralph Gebauer**
10:30 a.m.		*Coffee Break*	*Coffee Break*	*Coffee Break*	*Coffee Break*	*Coffee Break*
11:00 a.m.		**Rework Seminar - Susanne Yelin**	**Rework Seminar - Eric Hudson**	**Rework seminar - Andrey Vilesov**	**Rework Seminar - Daniel Steck**	**Rework Seminar - Ralph Gebauer**
12:30 p.m.		*Lunch*	*Lunch*	*bus shuttle to D-Wave Lunch packages*	*Lunch*	Closing remarks and Poster Prize: Frank Stienkemeier
1:30 p.m.						*Lunch*
2:00 p.m.		**Rework Seminar - Susanne Yelin**	**Rework Seminar - Eric Hudson**	D-Wave	**Rework Seminar - Daniel Steck**	*Departure*
3:30 p.m.		*Coffee Break*	*Coffee Break*		*Coffee Break*	
4:00 p.m.	Opening remarks: Michael Walter	**career event**	**Andrey Vilesov (Experiment): Experiments with Large Superfluid Helium Droplets**		**Ralph Gebauer (Theory): Proton diffusion in crystalline silicon: is it classical or quantum-mechanical?**	
4:30 p.m.	Presentation by participants (1 slide for 1 min/person)					
5:30 p.m.	Poster session A and Aperitif	Poster session B and Aperitif	Poster session C and Aperitif		**sports and drinks**	
7:00 p.m.	*Dinner*	*Dinner*	*Dinner*	*Dinner*	*Dinner*	