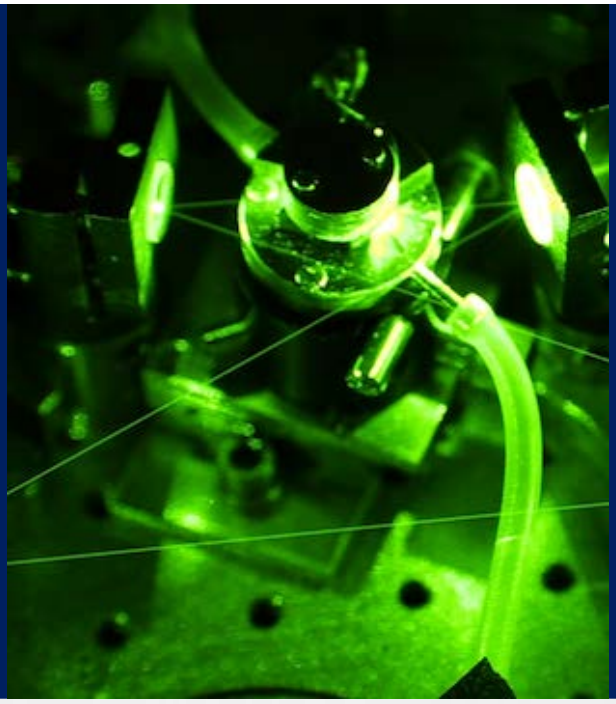

IRTG 2079 CoCo

Cold Controlled Ensembles

in Physics and Chemistry

BOOK OF ABSTRACTS

2nd Annual Convent IRTG 2079

August 1st – August 5th 2016

Caritas Tagungszentrum, Freiburg, Germany

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Impressum

IRTG 2079 / Cold Controlled Ensembles in Physics and Chemistry

Institute for Physics

Albert-Ludwigs-Universität Freiburg

Hermann-Herder-Straße 3

79104 Freiburg

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

THE ANNUAL CONVENT IS AN IMPORTANT PART OF THE STRUCTURED GRADUATE PROGRAM OF THE IRTG 2079. THE RESEARCHES FROM UBC/VANCOUVER AND ALBERT-LUDWIGS UNIVERSITY FREIBURG MEET TO DICUSS THEIR RESEARCH, PLAN FURTHER PROJECTS AND PUBLICATIONS AND STRENGHTEN THE NETWORK BETWEEN THE TWO UNIVERSITIES.

Organisation

IRTG 7079 „Cold Controlled Ensembles in Physics and Chemistry“

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Financial Support

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General Information

Duration

Monday, August 1st, 2016, 9.00 am – Friday, August 5th, 2016, 4.00 pm

Location

Caritas Tagungszentrum

Wintererstr. 17-19

79104 Freiburg

Phone: +49-761 - 200 1801

E-Mail: tagungszentrum@caritas.de

Homepage: http://www.caritas-tagungszentrum.de

Travel Information – Individual Journeys

The Airports which are close to Freiburg are: Frankfurt in Germany, Zurich in Switzerland and Mulhouse/Basel or Strasbourg in France. At all airports there is a train station and a fast connection to Freiburg (ca. 2 hours). From Freiburg train station we would recommend to take a taxi to the Caritas Haus in Wintererstr. 17-19 (about 10 €). You can also take the Tram No. 4 to Tennenbacher Str. From there, it is 1,1 Kilometres to walk. As it is going uphill, we would not recommend to do that with (heavy) luggage.

Hotel

We have reserved mostly single, and a few double rooms. Towels will be provided.

Meals & Drinks

Meals and drinks during the scientific program are included. In the evening, the bar offers drinks, which can be orderd on own costs.

Excursion

A hiking trip through the beautiful landscape of the Black forest is organised on Wednesday (August 3rd, 2016). Additionally there will be a soccer game on Monday evening (August 1st) and a guided city walk on Thursday evening (August, 4th).

W-Lan

There is W-Lan Acess in all public rooms of the center, in the private rooms there might be no stable internet connection.

Scientific Programm

Monday, August 1st, 2016

Till 08:45	*Breakfast*	
09:00	*Introductory remarks*	Frank Stienkemeier
09:30	*Lecture PI 1: Arrested relaxation in an isolated molecular ultracold plasma*	Ed Grant
10:30	*Coffee break*	
11:00	*Doctoral lecture 1: On the bifurcation of a molecular beam ultracold plasma*	Markus Schulz-Weiling
11:30	*Doctoral lecture 2: Counter Rotating Nozzle*	Manish Vashishta
12:00	*Lunch and free time*	
14:00	*Doctoral lecture 3: Enhanced chiral discriminatory van der Waals interactions mediated by chiral surfaces*	Pablo Barcelona
14:30	*Doctoral lecture 4: Singlet fission and repulsive Van der Waals forces*	Oliver Stauffert
15:00	*Doctoral lecture 5: Time-resolved imaging of the dynamics of free metal clusters and nanocrystals*	Simon Dold
15:30	*Coffee Break*	
16:00	*Intensive discussion on favored topics*	
17:00	*Postersession (Posters from the doctoral lectures of Monday and Tuesday)*	
18:00	*Soccer Game*	
20:00	*Dinner*	

Tuesday, August 2nd, 2016

Till 08:45	*Breakfast*	
09:00	*Lecture PI 2: Experimental studies of quantum chaos with laser-kicked molecules*	Valery Milner
10:00	*Doctoral lecture 6: Casimir-Polder Potential Between a Driven Atom and a Surface*	Sebastian Fuchs
10:30	*Coffee break*	
11:00	*Doctoral lecture 7: Quantum Friction and Markovianity*	Juliane Klatt
11:30	*Doctoral lecture 8: Fluorescence lifetime reduction of organic complexes studied by cluster isolation spectroscopy*	Sharareh Izadnia
12:00	*Lunch and free time*	
14:00	*Doctoral lecture 9: Quantum localization of particles with dipolar tunnelling in three-dimensional lattices of finite size*	Joshua Cantin
14:30	*Doctoral lecture 10: TBA*	Alexander Ruf
15:00	*Doctoral lecture 11: Detection of multiple-quantum coherences in dilute samples*	Lukas Bruder
15:30	*Coffee break*	
16:00	*Lab tours*	
17:30	*PAC Meetings/Discussion A*	
20:00	*Dinner in a Biergarten*	

Wednesday, August 3rd, 2016

Till 08:45	*Breakfast*	
09:00	*Hiking trip*	
18:00	*Dinner*	
20:00	*After-Dinner-Lecture: Ultracold Antihydrogen*	Taka Momose

Thursday, August 4th, 2016

Till 08:45	*Breakfast*	
09:00	*Lecture PI 3: Machine learning for quantum molecular dynamics: Gaussian Process models for improved predictions of molecular collision observables*	Roman Krems
10:00	*Doctoral lecture 12: Characterization of pulsed nozzles and thereby produced clusters and Introduction to charge transfer investigations in Pentacene/Perfluoropentacene-molecules, isolated in Helium droplets*	Matthias Bohlen
10:30	*Coffee break*	
11:00	*Challenges and Perspectives of Ultracold Atom-Ion Experiments*	Markus Debatin
11:30	*Doctoral lecture 13: Progress on Optical Trapping of Ba+*	Julian Schmidt
12:00	*Lunch and free time*	
14:00	*Doctoral lecture 14: Towards Ultracold Chemistry - A new experimental setup combining Lithium Atoms with Barium Ions*	Pascal Weckesser
14:30	*Doctoral lecture 15: Study of Electron Transport in Organic Molecules using Constrained Density Functional Theory*	Reyhanneh Ghassemizadeh
15:00	*Doctoral lecture 16: Cold Penning-Reactions using a Li-MOT*	Jonas Grzesiak
15:30	*Coffee Break*	
16:00	*Postersession (Posters from the doctoral lectures of Thursday and Friday)*	
17:00	*PAC Meetings/Discussion B*	
18:00	*Dinner*	
20:00	*Guided City Walk*	

Friday, August 5th, 2016

Till 08:45	*Breakfast*	
09:00	*PI Meeting*	
10:00	*Doctoral lecture 17: Influence of particle distinguishability on interference phenomena in optical lattices*	Tobias Brünner
10:30	*Coffee break*	
11:00	*Doctoral lecture 18: Imaging excited state dynamics of doped helium nanodroplets in real time*	Johannes von Vangerow
11:30	*Intensive discussion on favored topics*	
12:00	*Lunch and free time*	
13:30	*Doctoral lecture 19: TBA*	Gene Polovy
14:00	*Doctoral lecture 20: Lattice models with long-range and number-non-conserving interactions with Zeeman excitations of ultracold magnetic atoms*	Rodrigo Vargas Hernandez
14:30	*Doctoral lecture 21: Mass and Photoelectron Spectroscopy of Organic Molecules*	Aghigh Jalehdoost
15:00	*Doctoral lecture 22: Bipolarons in the Su-Schrieffer-Heeger (SSH) model*	John Sous
15:30	*Coffee Break*	
16:00	*Closing remarks*	Takamasa Momose, Frank Stienkemeier

PAC meetings

PAC Meeting/Discussion A (Tuesday, August 2nd, 17:30)

17:30

- Fuchs, Buhmann, Krems
- Ruf, Stienkemeier, Milner
- Dold, v. Issendorff, Grant

18:15

- Klatt, Buhmann, Krems

PAC Meeting/Discussion B (Thursday, August 4th, 17:00)

17:00

- Ghassemizadeh, Walter, Momose
- Schmidt, Schätz, Madison
- Barcelona, Buhmann; Krems

17:30

- Grzesiak, Mudrich, Momose
- Stauffert, Walter, Krems
- Weckesser, Schätz, Madison

Notes

Abstracts – Talks & Lectures

(in alphabetical order)

Enhanced chiral discriminatory van der Waals interactions mediated by chiral surfaces

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

Hassan Safari
Physics amd Photonics Department, Graduate University of Advanced Technology, P.O. Box 76315-117, Mahan, Kerman Iran

Akbar Salam
Department of Chemistry, Wake Forest University, Winston-Salem, NC 27109, USA

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

We predict a discriminatory interaction between a chiral molecule and a purely electric molecule which is mediated by a chiral body. To achieve this, we generalize the van der Waals interaction potential between two ground-state molecules with electric, magnetic and chiral response to non-trivial environments.
The force is evaluated using second-order perturbation theory with an effective Hamiltonian. Chiral media enhance or reduce the free interaction via many-body interactions. We also suggest a symmetric configuration where the electric and magnetic contributions of the van der Waals interaction are zero, making the chiral component the dominant contribution. The latter is discriminatory with respect to enantiomers of different handedness.

Characterization of pulsed nozzles and thereby produced clusters and Introduction to charge transfer investigations in Pentacene/Perfluoropentacene-molecules, isolated in Helium droplets

Matthias Bohlen, Rupert Michiels, Aaron LaForge, Raphael Katzy, Mykola Shcherbinin, and Frank Stienkemeier
Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Pulsed nozzles in general offer many advantages over continuous beams, such as higher densities and reduced gas load. The home-built nozzle, developed in cooperation with UBC produces gas pulses down to 20 µs duration at several hundred Hz repetition rate. Investigations of power consumption and other characteristics of operation are presented, as well as size determinations by titration for water and heavy water clusters. A comparison with modelling (done by Bobbert et. al.) [1]is also presented.

Furthermore a new project regarding charge transfer investigations in helium droplets, doped with pentacene and perfluoropentacene is introduced. The HENDI method [2] enables us to investigate the spectra of single molecules or complexes in an ultracold (370 mK) and weak interacting environment, in which pentacene and perfluoropentacene can form electron donor/acceptor complexes. Compared to previous measuements of these complexes in solution (performed by Broch et. al.) [3], we hope for a immensely improved spectral resolution by approximately 2 orders of magnitude.

[1] C. Bobbert, S. Schütte, C. Steinbach, and U. Buck, Eur. Phys. J. D, **19**, 183-192 (2002)
[2] J. P. Toennies, A. F. Vilesov, Angew. Chem. Int. Ed., **43**, 2622 – 2648 (2004)
[3] K. Broch, U. Heinemeyer, A. Hinderhofer, F. Anger, R. Scholz, A. Gerlach, and F. Schreiber, Phys. Rev. B **83**, 245307 (2011)

Detection of multiple-quantum coherences in dilute samples

Lukas Bruder

Multiple-quantum coherence (MQC) signals have been used to explore higher-lying molecular states and many-body phenomena in various systems[1-3]. Detecting such higher order effects usually requires particularly sensitive methods. I will present a simple approach based on femtosecond pump-probe spectroscopy combined with quasi-continuous phase modulation which allows efficient isolation of MQC signals [4]. The detection of multiphoton quantum beats in atomic vapors and supersonic doped helium droplet beams will be demonstrated. Furthermore, collective resonances of up to four-body correlations are observed, which is surprising considering the low density in our samples. Phase-sensitive detection reveals distinct phase shifts of these resonances which depend on the hyperfine states contributing to the collective resonances. A theoretical explanation of these findings is currently being worked out. Our approach can readily be extended to higher dimensional spectroscopy. Moreover, it may facilitate coherent time-resolved spectroscopy in the XUV spectral range. A proof-of-principle study for the latter approach will be presented as well.

[1] N. Christensson, F. Milota, A. Nemeth, I. Pugliesi, E. Riedle, J. Sperling, T. Pullerits, H.F. Kauffmann, and J. Hauer, J. Phys. Chem. Lett. 1, 3366 (2010).
[2] X. Dai, M. Richter, H. Li, A.D. Bristow, C. Falvo, S. Mukamel, and S.T. Cundiff, Phys. Rev. Lett. 108, 193201 (2012).
[3] D.B. Turner and K.A. Nelson, Nature 466, 1089 (2010).
[4] L. Bruder, M. Binz, and F. Stienkemeier, Phys. Rev. A 92, 053412 (2015).

Influence of particle distinguishability on interference phenomena in optical lattices

Tobias Bünner, Gabriel Dufour, Alberto Rodriguez and Andreas Buchleitner

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

Cold, interacting atoms in tilted optical lattices exhibit coherent dynamics, for instance Bloch oscillations in position and momentum space. The influence of interactions between the particles was studied and can generally be associated with a suppression of the coherence phenomena. However, the role of the particle-indistinguishability on this dynamics has not been investigated systematically yet. From many-photon interference experiments we know that the degree of distinguishability has a non-trivial influence on the evolution of the underlying many-particle state, and manifests itself in the outcomes of coincidence measurements. In a similar fashion, we want to identify how and where the indistinguishability can be observed in the dynamics of cold, interacting atoms in tilted optical lattices. We compare the outcomes of different observables for two distinguishable versus indistinguishable atom species. In the non-interacting case, we find that one-particle observables are not affected by the distinguishability of the atoms, while two-particle observables let us discern the evolution of distinguishable from indistinguishable particles. In the interacting case, additional frequencies appear in the dynamics of distinguishable atoms.

Title: Quantum localization of particles with dipolar tunnelling in three-dimensional lattices of finite size

J. T. Cantin, T. Xu, and R. V. Krems
Department of Chemistry, University of British Columbia, Vancouver, B.C., V6T 1Z1, Canada

It is generally assumed that quantum particles with dipolar long-range hopping do not undergo Anderson localization in 3D disordered lattices. However, this is valid only for lattices of infinite size. The delocalization of particles with long-range hopping occurs through resonant couplings between sites with the same on-site energy. As the lattice size grows, the energy for each lattice site within a finite volume has a non-zero probability to be equal to the energy of a site outside this volume. The number of such resonances diverges with the system size. If the lattice size is finite, the number of resonances is finite and may not be sufficiently large to cause delocalization. This raises the question: can quantum transport be suppressed by reducing the size of the system? To answer this, we compute the localization-diffusion phase diagram for a quantum particle with dipolar long-range hopping in a finite-size three-dimensional lattice with diagonal and off-diagonal disorder. We characterize the diffusion-localization transition as a function of the system size and the amount of diagonal and off-diagonal disorder. Our calculations show that the diffusion-localization transition could be detected using excitations of polar molecules in an optical lattice as probe particles [1].

[1] Cantin, J. T.; Xu, T.; Krems, R. V., arXiv:1604.01493.

Challenges and Perspectives of Ultracold Atom-Ion Experiments

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

Hybrid ultracold atom-ion experiments allow for the investigation of a variety of novel effects such as ultracold scattering and reactions, cluster formation or polarons [1]. Targetting the s-wave regime as the ultimate goal, a lot of interesting physics can be investigated on the pathway. In the early stages, elastic and inelastic scattering rates as well as possibilities of sympathetic cooling can be examinated. For $Ba^+ + Rb$, light-assisted reactions have already been observed at temperatures of 600 mK [2] and recently 2.2 mK [3]. For even lower collision energies, optical trapping of ions [4] permits to go past the intrinsic micromotion-induced limit to atom-ion sympathetic cooling in paul traps[5, 6]. Already at temperatures two orders of magnitude above the s-wave limit reaction rates are predicted to differ from the approximation assumed in Langevin theory [7]. Finally at ultralow temperatures, cluster formation could be observed [8]. In this talk we give an overview of the expected physics in different regimes and the corresponding experimental techniques. As main examples we will cite combinations of Ba^+Rb, and Ba^+Li which are investigated in our existing and a second yet to be built apparatus.

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

[2] F. H. J. Hall et al., Mol. Phys. 111, 1683-1690 (2013).

[3] A. Krükow et al., arXiv preprint arXiv:1602.01381 (2016).

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

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

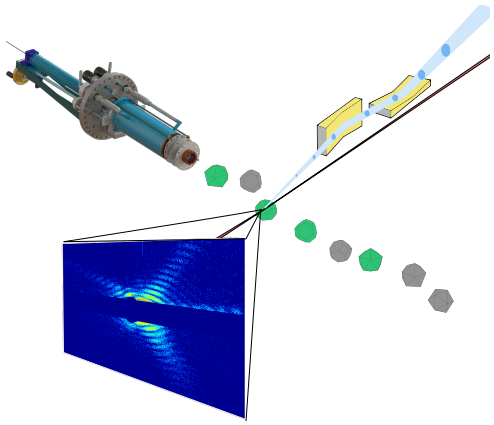
[6] B. Hoeltkemeier et al., Phys. Rev. Lett. 116.23 (2016): 233003.

[7] K. Jachymski et al. Phys. Rev. Lett. 110, 213202 (2013).

[8] R.Coté et al. Phys.Rev.Lett. 89.093001 (2002).

Talk: Time-resolved imaging of the dynamics of free metal clusters and nanocrystals

Bernd von Issendorff and Simon Dold
Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany



I aspire to utilize ultrashort X-Ray pulses as a tool to resolve ultrafast processes in nanoscale systems.

Since the advent of free electron x-ray lasers scattering on single particles in gas phase has come within reach. The shape of large metal clusters seems to be an ideal property for investigation as it is, in contrast to the atomic structure of single molecules, accessible to scattering in single shots with current x-ray light intensities[1]. In such a scheme, novel insights into phase transitions of free metalparticles on the nanoscale are expected to be accessible, as well as heat induced morphological changes, such as vibrations of the particles.

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

References

[1] Ingo Barke, Hannes Hartmann, Daniela Rupp, Leonie Flückiger, Mario Sauppe, Marcus Adolph, Sebastian Schorb, Christoph Bostedt, Rolf Treusch, Christian Peltz, et al. The 3d-architecture of individual free silver nanoparticles captured by x-ray scattering. *Nature communications*, 6, 2015.

[2] H. Haberland, M. Karrais, and M. Mall. A new type of cluster and cluster ion source. *Zeitschrift für Physik D Atoms, Molecules and Clusters*, 20(1):413–415, 1991.

Casimir-Polder Potential Between a Driven Atom and a Surface

Sebastian Fuchs and Stefan Buhmann
Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Within the framework of macroscopic QED we study the interaction of an atom that is driven by a coherent laser field with a surface and compute the respective Casimir-Polder potential. We study this scenario in two different regimes. If the atom is driven off-resonantly and remains in its initial state, we can split the atomic dipole moment into a free contribution associated with spontaneous polarization and an induced part given by a polarizability and the driving field. Consequently, the total Casimir-Polder potential also consists of a standard Casimir-Polder part and a laser-induced potential. We contrast this to resonantly driven atom showing Rabi oscillations between its excited state and the ground state. In a next step we seek to extend this model to a larger number of atoms and investigate the collective behavior using Dicke states.

Study of Electron Transport in Organic Molecules using Constrained Density Functional Theory

Reyhaneh Ghassemizadeh, Michael Walter
Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Photocurrent generation in organic photovoltaics (OPVs) relies on the dissociation of the excitons into free electrons and holes at donor/acceptor heterointerfaces. The low dielectric constant of organic semiconductors leads to strong Coulomb interactions between electron-hole pairs that should in principle oppose the generation of free charges. The exact mechanism by which electrons and holes overcome this Coulomb trapping is still unclear. In our work, we try to better understand theoretically the charge transport mechanisms at the atomic scale. Single donor/acceptor pairs may be trapped in cold hydrogen or raregas matrix, where spectra can be recorded in unprecedented precision. We aim to look precisely into the vibronic transitions important in CT excitons as their fingerprints and hence make use of quantum chemical ab-initio methods such as density functional theory for describing the ground state of the system. However DFT and TDDFT are not capable of describing charged systems. Charge transfer can be model by quantum mechanical approaches using green functions such as GW method which needs lots of computational efforts, or one can still use DFT by adding an external potential to KS equations which forces predefined atoms to carry a specified charge or magnetization, named Constrained DFT[1] which is our tool for this study.

[1] Benjamin Kaduk et al. Chem.Rev. **112**, 321–370 (2012) .

Arrested relaxation in an isolated molecular ultracold plasma

Markus Schulz-Weiling[1], Hossein Sadeghi[2], Mahyad Aghigh[2], James S. Keller[2], and Edward Grant[1,2]
[1]*Department of Physics & Astronomy,* [2]*Department of Chemistry,*
University of British Columbia, Vancouver, BC V6T 1Z3, Canada

While small isolated quantum systems undergo well-defined wave packet dynamics, the observables in very large, locally isolated quantum systems generally relax to states of maximum entropy. Explaining this, the eigenstate thermalization hypothesis (ETH) holds that the unitary dynamics of arbitrary superpositions yield equilibrium expectation values as a time-average [1, 2]. Thus, in this picture – despite the deterministic nature of the Schrödinger equation and the absence of outside perturbations – an arbitrarily prepared isolated quantum system relaxes to a thermal equilibrium that is somehow hardwired in its eigenstates. Indeed, unimolecular rate theory depends on energy randomization, and quantum systems as small as three transmon qubits exhibit ergodic dynamics. [3].

But, theory predicts the existence of certain interacting many-body systems that lack intrinsic decoherence and preserve topological order in highly excited states. These systems exhibit local observables that retain a memory of initial conditions for arbitrarily long times. Such behaviour has important practical and fundamental implications. For this reason, experimental realizations of isolated quantum systems that fail to thermalize have attracted a great deal of interest [4, 5].

Here we describe particular conditions under which an ultracold plasma evolves from a molecular Rydberg gas of nitric oxide, adiabatically sequesters energy in a reservoir of mass transport, and relaxes to form a spatially correlated strongly coupled plasma. Short-time electron spectroscopy provides evidence for complete ionization. The long lifetime of the system, particularly its stability with respect to recombination and neutral dissociation, suggest a robust process of self-organization to reach a state of arrested relaxation, far from thermal equilibrium.

---

[1] Rigol M, Dunjko V, Olshanii M: **Thermalization and its mechanism for generic isolated quantum systems**. *Nature* 2008, **452**(7189):854–858.
[2] Eisert J, Friesdorf M, Gogolin C: **Quantum many-body systems out of equilibrium**. *Nature Physics* 2015, **11**(2):124–130.
[3] Neill C, et al: **Ergodic dynamics and thermalization in an isolated quantum system**. *arXiv:* 2016, **1601.00600v2**.
[4] Kondov SS, McGehee WR, Xu W, DeMarco B: **Disorder-Induced Localization in a Strongly Correlated Atomic Hubbard Gas**. *Phys Rev Lett* 2015, **114**(8):083002.
[5] Schreiber M, Hodgman SS, Bordia P, Lüschen HP, Fischer MH, Vosk R, Altman E, Schneider U, Bloch I: **Observation of many-body localization of interacting fermions in a quasi-random optical lattice.** *Science* 2015, **349**:842–845.

Cold Penning-Reactions using a Li-MOT

J. Grzesiak, F. Stienkemeier, M. Mudrich
Physikalisches Institut, Universität Freiburg,
Hermann-Herder-Str.3, 79104 Freiburg i.Br.

Cold reactive scattering, especially in merged beams, has recently attracted wide attention.[1] Our setup for measuring elastic scattering of cold atoms and molecules originating from a rotating nozzle and atoms trapped in a Li-MOT has been extended for investigating reactive scattering. To this end we use a pulsed supersonic and cryogenic source with different homemade discharge units to provide an intense and cold beam of metastable rare gas atoms. We discuss the optimization of the metastable source as well as first results on cold Penning reactions of the pulsed beam atoms with the ultracold Li-atoms from the MOT.

References:

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

Fluorescence lifetime reduction of organic complexes studied by cluster isolation spectroscopy

Sharareh Izadnia, Frank Stienkemeier
Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

Charge and excitation transfer and corresponding decay and loss mechanism are the key aspects to be understood in connection with the function of light harvesting, organic photovoltaics and optoelectronic devices. In our studies we probe aggregates of organic molecules formed and isolated on rare gas clusters in order to understand collective processes of electronically excited systems.
Singlet fission (SF) was first reported in the 1960s by Singh [1]. In a dense system, the molecule which is excited to its singlet state can partially transfer its energy to a neighboring ground state molecule, and thereby create two molecules excited to a triplet state [2] assuming it is energetically allowed. With this, singlet fission can increase the efficiency of organic electronics and photovoltaic by creating multiple charge carriers from one single photon.
Here, we report the experimental observation of fluorescence lifetime reduction of tetracene, pentacene and anthracene by directly tuning the number of molecules are placed on the surface of neon cluster. Such complexes are ideally suited to probe the role of e.g. the number and the intermolecular distance of interacting molecules. Furthermore, we observe at the same systems Dicke superradiance [3] and triplet annihilation processes, depending on the substance and the aggregate properties. Results are discussed in the context of the spectroscopy of the complexes and decay mechanism of the aggregates.

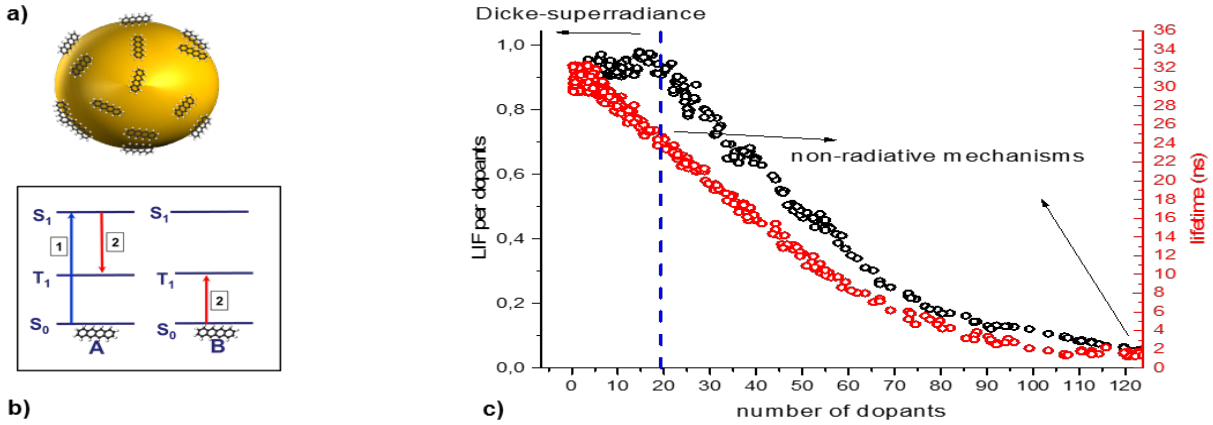


Fig: a) illustration of the doped clusters. b) depicts the process of singlet fission.
c) lifetime reduction in an ensemble of pentacene molecules attached to large neon cluster.

[1] S. Singh, W. J. Jones, W. Siebrand, B. P. Stoicheff, and W. G. Schneider,"Laser generation of excitons and uorescence in anthracene crystals," The Journal of Chemical Physics, vol. 42, no. 1, pp. 330-342, 1965.
[2] M. B. Smith and J. Michl, "Singlet fission" Chem. Rev., vol. 110, no. 11, pp. 6891{6936, 2010.
[3] M. Müller, S. Izadnia, S. M. Vlaming, A. Eisfeld, A. LaForge, and F. Stienkemeier, "Cooperative lifetime reduction of single acene molecules attached to the surface of neon clusters," Phys. Rev. B, vol. 92, p. 121408, Sep 2015.

Mass and Photoelectron Spectroscopy of Organic Molecules

A. Jalehdoost, B. von Issendorff,
Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg, Germany

The mass and Photoelectron spectrum of the molecules of Tetracene[1], Anthracene, Benzanthracene, Perylene, Rubrene and Pentacene were measured. Pt atom was used for doing the calibration. From the results obtained from the photoelectron spectroscopy, the energy levels of the studied organic molecules were predicted. The PE spectrometer was a magnetic bottle one and the mass spectrometer was a time-of-flight spectrometer[2].

[1] M. Mitsui; N. Ando; A. Nakajima, J. Phys. Chem. A, Vol III, No. 39 (2007).
[2] B. M. Svanqvist, PhD Thesis, Albert Ludwig Universität Freiburg (2011).

Title: Quantum Friction and Markovianity

J. Klatt, H.-P. Breuer and S.Y. Buhmann

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Quantum friction is the velocity-dependent force between two polarizable objects in relative motion, resulting from quantum-fluctuation mediated transfer of energy and momentum. Due to its short-ranged nature it has proven difficult to observe.

Theoretical attempts to determine the velocity-dependence of the drag experienced by an atom moving parallel to a surface arrive at contradicting results. Scheel and Buhmann[1] predict a force linear in relative velocity v by employing the quantum regression theorem (QRT). Intravaia[2], however, predicts a v^3 power-law starting from a non-equilibrium fluctuation-dissipation theorem (FDT).

This contradiction is brought along by a difference in the long-time behavior of correlations of the type $\langle \boldsymbol{d}(t)\boldsymbol{d}(t')\rangle$, where $\boldsymbol{d}$ is the atomic dipole operator. The QRT approach assumes Markovianity and thus exponential decay of correlations, whereas the FDT formalism acknowledges a power-law behavior of that decay for very large times, but comes at the cost of being restricted to stationary systems.

We employ the time-convolutionless expansion (TCL) for probing Markovianity and subsequently follow the QRT route in order to study an atom flying towards a surface – an intrinsically non-stationary setup. We derive signatures of the relative motion in the atom's decay rates and level shifts, calculate the friction experienced by the atom and compare both to results obtained from time-dependent perturbation theory.

[1] S. Scheel and S. Y. Buhmann, Phys. Rev. A **80** (2009)

[2] F. Intravaia et al., Phys. Rev. A **89** (2014)

Roman Krems

Machine learning for quantum molecular dynamics: Gaussian Process models for improved predictions of molecular collision observables

Abstract:

I will illustrate that statistical learning techniques based on kriging (Gaussian Process regression) have enormous potential for improving the predictions of classical and/or quantum scattering theory. I will discuss the following applications of Gaussian Process regression: (i) efficient non-parametric fitting of multi-dimensional potential energy surfaces without the need to fit ab initio data with analytical functions; (ii) obtaining scattering observables as functions of individual PES parameters; (iii) using classical trajectories to interpolate quantum results; (iv) extrapolation of scattering observables from one molecule to another; (v) obtaining scattering observables with error bars reflecting the inherent inaccuracy of the underlying potential energy surfaces.

I will argue that the application of Gaussian Process models to quantum scattering calculations may potentially elevate the theoretical predictions to the same level of certainty as the experimental measurements and can be used to identify the role of individual atoms in determining the outcome of collisions of complex molecules.

I will show examples and discuss the applications of Gaussian Process models to improving the predictions of scattering theory relevant for the cold molecules research field.

References

(1) Jie Cui and R. V. Krems, “Gaussian Process Model for Collision Dynamics of Complex Molecules”, Phys. Rev. Lett. 115, 073202 (2015).

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(3) Jie Cui and R. V. Krems, “Efficient non-Parametric Fitting of Potential Energy Surfaces for Polyatomic Molecules with Gaussian Processes”, arXiv: 1509.06473.

Progress on Optical Trapping of Ba^+

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Examining collisions of atoms and ions at extremely low temperature will permit gaining information about the corresponding sympathetic cooling rates and subsequent quantum effects, such as cluster formation of an ion binding atoms within the common $1/r^4$ potential[1]. In the last years several experimental groups investigated cold collisions between atoms and ions, leading to a better understanding of the atom-ion interaction [2-5]. Our approach to reach the regime of ultracold interaction is to precool a Ba^+ ion, trapped in a conventional Radio-Frequency (RF) trap, by Doppler cooling. By transfering the ion into an optical dipole trap[6], followed by sympathetic cooling via an ambient Rb cloud we plan to overcome the current limitations set by heating due to RF micromotion. In other words, since the atoms can also be trapped purely optically one should be able to reach collision energies in the BEC-regime with this method. We present our apparatus and show the latest results on optical trapping of both atoms and ions. While sketching the general experimental techniques we use we focus on the progress we have made in increasing the lifetime of the Ba^+ in the dipole trap.

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[2] A. Härter et al., Contemp. Phys. **55**, 33 (2014)
[3] A.T. Grier et al., Phys. Rev. Lett. **102**, 223201 (2009)
[4] L. Ratschbacher et al., Nature Phys. **8**, 649 (2012)
[5] F. H. J. Hall et al., Mol. Phys. **111**, 1683-1690 (2013)
[6] T. Huber et al., Nat. Comm. **5**, 5587 (2014)

Experimental studies of quantum chaos with laser-kicked molecules

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In 1958, Philip Anderson showed that the translational motion of a quantum particle along a periodic lattice is greatly suppressed by disorder, with the particle's wave function localized in space. Seemingly unrelated "dynamical localization" of angular motion was later found in a very different system - the periodically kicked quantum rotor. In 1982, Shmuel Fishman and collaborators pointed out that the mechanisms behind Anderson and dynamical localizations are very similar. This discovery stimulated an active study of quantum localization, most notably with ultra-cold atoms in optical lattices, yet until now, Anderson localization has never been seen in a system of true quantum rotors.

I will discuss our recent results on the first direct observation of Anderson localization in an ensemble of freely rotating diatomic molecules "kicked" by a periodic sequences of femtosecond pulses [1]. I will present two hallmarks of Anderson localization: the exponential distribution of the molecular angular momentum, and the suppression of the rotational energy growth despite the repetitive kicking. As the localization stems from the destructive interference of quantum pathways, it is susceptible to noise and decoherence. By introducing two types of noise, in timing and amplitude of the periodic kicks, we demonstrate the collapse of the localized state and the recovery of the diffusive growth of energy.

[1] M. Bitter, V. Milner, submitted, arXiv:1603.06918 (2016).

Ultracold Antihydrogen

Takamasa Momose

Antihydrogen atom, composed of an antiproton and positron, is the antimatter counterpart of the simplest atom, hydrogen. One can now create one (or a few) antihydrogen atom(s) at AD (Antiproton Decelerator) hall at CERN, Switzerland. Researchers are studying antihydrogen in order to investigate fundamental symmetries between matter and antimatter, or more specifically, to investigate why there is more matter than antimatter in the universe. There are severals groups who are working on physics of antihydrogen at CERN. Among them, APLHA (Antihydrogen Laser PHysics Apparatus) project was the first who trapped an anthydrogen atom for >1000 seconds in a magnetic trap (Nature Physics, 7, 558 (2011).) They further recorded the first resonant quantum transitions of antihydrogen in microwave region (Nature 483, 439 (2012)). ALPHA is currently trying to detect the 121nm Lyman-Alpha "electronic" transition of antihydrogen, and use that transition to laser cool antihydrogen below 100 mK. Ultracold antihydrogen will provide opportunities for the study of 1s-2s ultra-precision spectroscopy, neutrality of antihydrogen, and interaction with gravity. On-going and planned experiments at ALPHA will be presented.

Optical trapping of Coulomb crystals

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Ion Coulomb crystals are the key to many applications with trapped ions, since the complexity in classically computing quantum systems typically increases exponentially with particle number. Ion Coulomb crystals have therefore been under investigation since they were first observed almost thirty years ago [1,2].
We now demonstrate trapping of one-dimensional ion crystals of up to six Barium ions inside an optical dipole trap [3] aligned along the crystal axis. The Paul trap is used for preparation of the ions and turned off for optical trapping. The dependence on the trap parameters, in particular the interplay of Rayleigh length, laser power and axial confinement by DC electric fields, is investigated. It is shown how optical trapping of the Coulomb crystal can be used to deterministically load N-ion crystals. Finally, we investigate the survival of the crystal structure inside the optical trap by co-trapping (bright) Barium 138 ions with a (dark) isotope of Barium which acts as a marker ion inside the crystal.

[1] D.J. Wineland et al., Phys. Rev. Lett. **59**, 2935-2938 (1987)
[2] H.C. Nägerl et al., Appl. Phys. B **66**, 603–608 (1998)
[3] T. Huber et al., Nat. Comm. **5**, 5587 (2014)

On the bifurcation of a molecular beam ultracold plasma

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Ultracold neutral plasmas (UNPs) present a well-defined framework in which to study many-body Coulomb systems in a regime of strong coupling. The Coulomb correlation parameter, Γ, defines a plasma in terms of the dimensionless ratio of Coulomb energy to thermal energy. Correlation gives rise to exotic dynamics on a vast range of length scales.

Our experiment cools a jet of nitric oxide in a supersonic beam to sub-Kelvin temperatures. Double-resonant laser excitation creates an ellipsoidal Gaussian excitation volume of high Rydberg states ($\rho > 10^{12}$ cm^{-3}). Some of these Rydberg molecules undergo Penning ionizing collisions to form free ions and electrons. A fraction of electrons (<1%) escape, creating a positive trapping potential. The remaining free electrons act as plasma seed and ionize Rydberg molecules by electron impact. The system avalanches to plasma. Electron-Rydberg inelastic collisions deactivate a residual population of Rydberg molecules, heating the electron bath to > 170K [1].

While the concept of plasma avalanche holds for the whole Rydberg ellipsoid, different density regions avalanche on different timescales. Recent work suggests that Rydberg avalanche occurs in the core tens of nanoseconds before the outer wings. The combination of hot electrons and steep density gradients leads to an ambipolar eruption of the core.

This shock transfers a fraction of the energy of expanding ions to molecules in the peripheral Rydberg gas. These wings bifurcate and exhibit arrested relaxation extending for a millisecond or more [2].

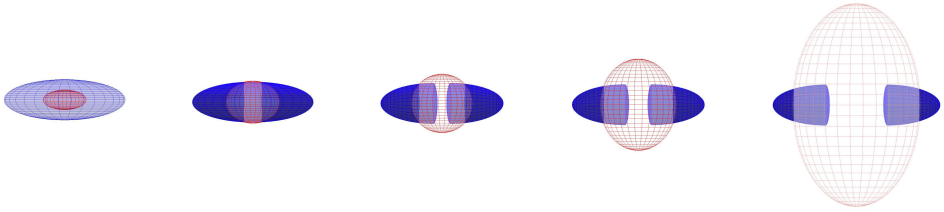

Figure 1: A plasma forms at the core of a Rydberg ellipsoid. It errupts ambipolar and leaves the bifurcated outer wings of the ellipsoid, in a state of arrested relaxation, behind.

[1] N. Saquet et al., J. Phys. B: At. Mol. Opt. Phys. **45** (2012) 175302 (9pp).

[2] M. Schulz-Weiling and E. Grant, J. Phys. B: At. Mol. Opt. Phys. **49** (2016) 064009 (9pp).

Title: Summer school 2016

Bipolarons in the Su-Schrieffer-Heeger (SSH) model

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We explore the interactions of polarons and, in particular, the formation of bi-polarons in systems with particle - phonon couplings described by the Su-Schrieffer-Heeger (SSH) model. In this model, relevant for electrons in conjugates polyenes and excitons in molecular solids and aggregates, the interactions with phonons depend on the kinetic energy of the bare particle. We illustrate the effect of the particle statistics (hardcore bosons vs soft bosons vs fermions) on the binding of polarons and study the two-polaron phase diagram of the SSH model in various interaction regimes.

Singlet fission and repulsive Van der Waals forces

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We describe electronic structures for organic molecules, which are interesting for current research on organic solar cells, with density functional theory (DFT). By doing so, we presents additional insight on the processes called singlet fission, where a single singlet excitation is split among two molecules and dissociates into two triplet excitations.
With DFT it is possible to characterize these triplet states, that are so far only proposed and not yet experimentally shown. Absorption spectra, photo-electron spectra and vibrational fingerprints are obtained. This can allow for experimental setups to show triplet population and proof the occurrence of singlet fission.
A further project is to investigate Van der Waals forces. For simple systems, the Van der Waals interaction is well know and leads to a weak, attractive force. In more complex systems the Van der Waals interaction can play an important role and even change its nature and become repulsive.
The primary characteristics of the Van der Waals potential are given by the London formula $U_{VdW} \sim C_6 / R^6$, where the C_6 coefficients are dictated by the polarisability and the electronic states of the molecule. Hereby the occupied as well as the unoccupied states are involved, due to virtual transitions. These virtual transitions also have a big influence on the sign of the C_6 coefficient. For a ground state molecule only upward transitions to higher energy levels are possible and the C_6 coefficient is always positive. For excited state molecules also downward transitions are possible, the C_6 coefficient can change its sign and the Van der Waals interaction can get repulsive.
Time dependent DFT (TDDFT) [1] and Greens-function methods (GW) [2] give access to these quantities. With this, we aim to obtain a better understanding of Van der Waals forces in general and investigate especially excited states molecules with repulsive Van der Waals forces.

[1] EKU Gross, W Kohn - Adv. Quantum Chem, 1990
[2] F Aryasetiawan and O Gunnarsson, Rep. Prog. Phys. 61 237 , 1998

Lattice models with long-range and number-non-conserving interactions with Zeeman excitations of ultracold magnetic atoms

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We consider Zeeman excitations in an ensemble of highly magnetic atoms (such as Dy) trapped in an optical lattice, with one atom per lattice site, in a limit of few excitations. We show that the Zeeman excitations can be used as probe particles to investigate lattice models with significant and tunable inter-site interactions and particle number-non-conserving terms. In particular, we show that the ratio of the kinetic energy and particle - particle interaction energy in these lattice models can be tuned in a wide range by transferring the atoms to different Zeeman states. We propose to use the resulting controllable models for the study of the effects of direct particle interactions and particle number-non-conserving terms on Anderson localization. Using an example of an optical lattice partially populated with Dy atoms, we show that quantum walk of the Zeeman excitations leads to Anderson localization over experimentally feasible time scales. We also derive the polaron Hamiltonian arising from the coupling of the Zeeman excitations with the translational motion of the atoms in the lattice potential. We show that the mathematical form of the particle - phonon interactions depends on the Zeeman states involved in the excitation, interpolating between the Su-Schrieffer-Heeger and breathing-mode polaron models.

Counter Rotating Nozzle

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CRN deceleration is a mechanical method of producing intense cold, slow beams of atoms and molecules, which utilizes the peripheral velocity of the high-speed rotating nozzle to offset the beam's velocity. There are many advantages of this technique in making cold particles. For example, the velocity of the beam can be easily tuned by changing the rotating speed of the nozzle. Moreover, this method of deceleration can be applied to almost all species of particles especially heavy molecules that are difficult to slow with current state-of-the-art techniques. Latest results will be presented in the talk.
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2.Gupta et al., J. Phys. Chem. A ***1999,*** *103,* 10670-10673
3.Gupta et al., J. Phys. Chem. A ***2001,*** *105, 1626-1637*
4.Strebel et al., Phys. Rev. A **2010,** *81,* 033409
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Imaging excited state dynamics of doped helium nanodroplets in real time

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François Coppens
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This contribution will focus on photo-induced dynamics of rubidium (Rb) atoms attached to the surface of quantumfluid helium nanodroplets. A femtosecond (fs) pump-probe sequence is initiated by resonant excitation to droplet perturbed states correlating to the Rb 6p and 5p atomic orbitals. Subsequently, a fs probe pulse ionizes the Rb atom and velocity map ion and electron images are recorded. Depending on excitation wavelength and pump-probe delay, dynamics involving either desorption or submersion as well as formation of Rb^+He_n $= 1, 2$ complexes are observed. The experimental results will be discussed and compared to simulations based on time dependent density functional theory.

Towards Ultracold Chemistry - A new experimental setup combining Lithium Atoms with Barium Ions

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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, 5]. In order to control the atom-ion interaction 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] 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 [7, 8] currently limiting experiments to collision energies on the order of a few mK.

Recent theories indicate that heavy ions and light atoms - as $^{138}Ba^{+}$ and $^{6,7}Li$ - are advantageous in numerous aspects. For these combinations it might be possible to reach the s-wave regime, despite the heating effect of the Paul trap [7]. Furthermore, using Lithium allows to probe the fermionic (^{6}Li) and bosonic (^{7}Li) nature of the collision partners and might circumvent three-body loss rates observed in recent experiments [9].

In this talk we present our new experimental setup combining Ba^{+} ions and Li atoms in an optical dipole trap. We give details about the new ion trap, our laser system and about challenges we have encountered while planning the new experiment.

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

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

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

[8] B. Hoeltkemeier et al., Phys. Rev. Lett. 116.23 (2016): 233003.

[9] A. Kruekow et al., arXiv preprint arXiv:1602.01381 (2016).

Time-Table Annual Convent 2016

Monday, August 1st	Tuesday, August 2nd	Wedn. Aug. 3rd	Thursday, August 4th	Frieday, August 5th
9:00 F. Stienkemeier: Intr. Remarks **9:30** Ed Grant: PI Lecture 1 **10:30** Coffee break **11:00** M. Schulz-Weiling: Doc. Lecture 1 **11.30** M. Vashishta: Doctoral Lecture 2 **12:00** Lunch and free time **14:00** P. Barcellona: Doctoral Lecture 3 **14:30** O. Stauffert: Doctoral Lecture 4 **15:00** S. Dold: Doctoral Lecture 5 **15:30** Coffee break **16:00** Discussion **17:00** Postersession **18:00** Soccer Game **20:00** Dinner	**9:00** Valery Milner: PI Lecture 2 **10:00** S. Fuchs: Doctoral Lecture 6 **10:30** Coffee break **11:00** J. Klatt: Doctoral Lecture 7 **11.30** S. Izadnia: Doctoral Lecture 8 **12:00** Lunch and free time **14:00** J. Cantin: Doctoral Lecture 9 **14:30** A. Ruf: Doctoral Lecture 10 **15:00** L. Bruder: Doctoral Lecture 11 **15:30** Coffee break **16:00** Lab Tours **17:30** PAC Meetings/Discussion A **20:00** Dinner in a "Biergarten"	**9:00** Hiking trip - Excursion **18:00** Dinner **20:00** After-Dinner-Lecture: Taka Momose	**9:00** Roman Krems: PI Lecture 3 **10:00** M. Bohlen: Doctoral Lecture 12 **10:30** Coffee break **11:00** Markus Debatin **11.30** J. Schmidt: Doctoral Lecture 13 **12:00** Lunch and free time **14:00** P. Weckesser: Doc. Lecture 14 **14:30** R. Ghassemizadeh: D. Lecture 15 **15:00** J. Grzesiak: Doctoral Lecture 16 **15:30** Coffee break **16:00** Postersession **17:00** PAC Meetings/Discussion B **18:00** Dinner **20:00** Freiburger City Walk/Guided Tour	**9:00** PI Meeting **10:00** T. Brünner: Doctoral Lecture 17 **10:30** Coffee break **11:00** J. v. Vangerow: D. Lecture 18 **11:30** Discussion **12:00** Lunch and free time **13:30** Gene Polovy: Doctoral Lecture 19 **14:00** R. Hernandez: Doc. Lecture 20 **14:30** A. Jalehdoost: Doc. Lecture 21 **15:00** John Sous: Doctoral Lecture 22 **15:30** Coffee break **16:00** T. Momose, F. Stienkemeier: Closing remarks