SUMMER SCHOOL 2018

IRTG CoCo

Cold Controlled Ensembles in Physics and Chemistry

BOOK OF ABSTRACTS

3rd CoCo Summer School

Coherent Dynamics of Cold Molecular Ensembles

Theoretical and Experimental Methods

July 29 – August 03, 2018, Brand bei Bludenz, Austria

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 PREVIOUS SUMMER SCHOOLS WILL BE CONTINUED IN THE 3RD IRTG COCO SUMMER SCHOOL “COHERENT DYNAMICS OF COLD MOLECULAR ENSEMBLES THEORETICAL AND EXPERIMENTAL METHODS”. WE AGAIN HAVE BEEN ABLE TO RECRUIT DISTINGUISHED SPEAKERS THAT COVER VARIOUS RESEARCH FIELDS. THE LECTURES WILL COVER SCENTIFIC QUESTIONS FROM THE HEART OF COLD AND CONTROLLED CHEMISTRY AND PHYSICS. THE RANGE FROM FUNDAMENTALS OF NON-ADIABATIC DYNAMICS IN TIME-DEPENDENT DENSITY FUNCTIONAL THEORY, OVER QUASIPARTICLES IN SUPER-FLUID HELIUM, X-RAY FEMTO-CHEMISTRY UP TO THE MICROSCOPY OF QUANTUM-GASES AND ULTRACOLD RYDBERG GASES. THE LECTURES WILL BRING TOGETHER RESEARCHERS WORKING IN THE FIELD AND ARE DEVOTED TO THE PEOPLE DOING THE REAL WORK: GRADUATE AND DOCTORAL STUDENTS AS WELL AS YOUNG POST-DOCS.

Main Topics

“X-ray Femotochemistry and Cluster Physics” (Experiment)

“Angulon Quasiparticles” (Theory)

“Time-Dependent Density Functional Theory and Non-Adiabatic Dynamics” (Theory)

“Microscopy of Quantum Gases” (Experiment)

“Ultracold Rydberg Gases” (Experiment)

Financial Support

LIGHT CONVERSION
TOPAG Lasertechnik
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Organisation

IRTG 7079 „Cold Controlled Ensembles in Physics and Chemistry“

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General Information

Duration

Sunday July 29, 2018, 4.00 p.m. – Friday August 3, 2018, 2.00 p.m.

Location

Hotel Garni Scesaplana
Muhledorfle 158, 6708 Brand (near Bludenz), Austria
https://scesaplana.s-hotels.com/

Travel Information – Shuttles

The closest airport is Zürich International Airport (CH). Shuttle busses will operate on Sunday, July 29 at 12:00 a.m. from the bus parking at Jacob-Burckhardt-Straße, 79104 Freiburg, and back on Friday, August 03 at 2:00 p.m.

Travel Information – By car

A14/E43 to Innsbruck, exit: Brandnertal (58), turn right to Brand /Brandnertal and follow the road for 9 km.

Accommodation

All participants will be accommodated at the Scesaplana Garni Hotel at Brand (Bludenz). Bed linen and towels will be provided. The hotel is equipped with swimming pool and a spa area, which will be available for the participants.

Meals & Drinks

Meals and drinks during the scientific program are included in the conference fee. The lunches will take place in the hotel, one softdrink is included. Dinners will take place in following restaurants:

Sunday, Monday, Wednesday and Thursday – Colrosa Stüble
Tuesday: Alpentenne

2 drinks (softdrink or beer or wine) are included.

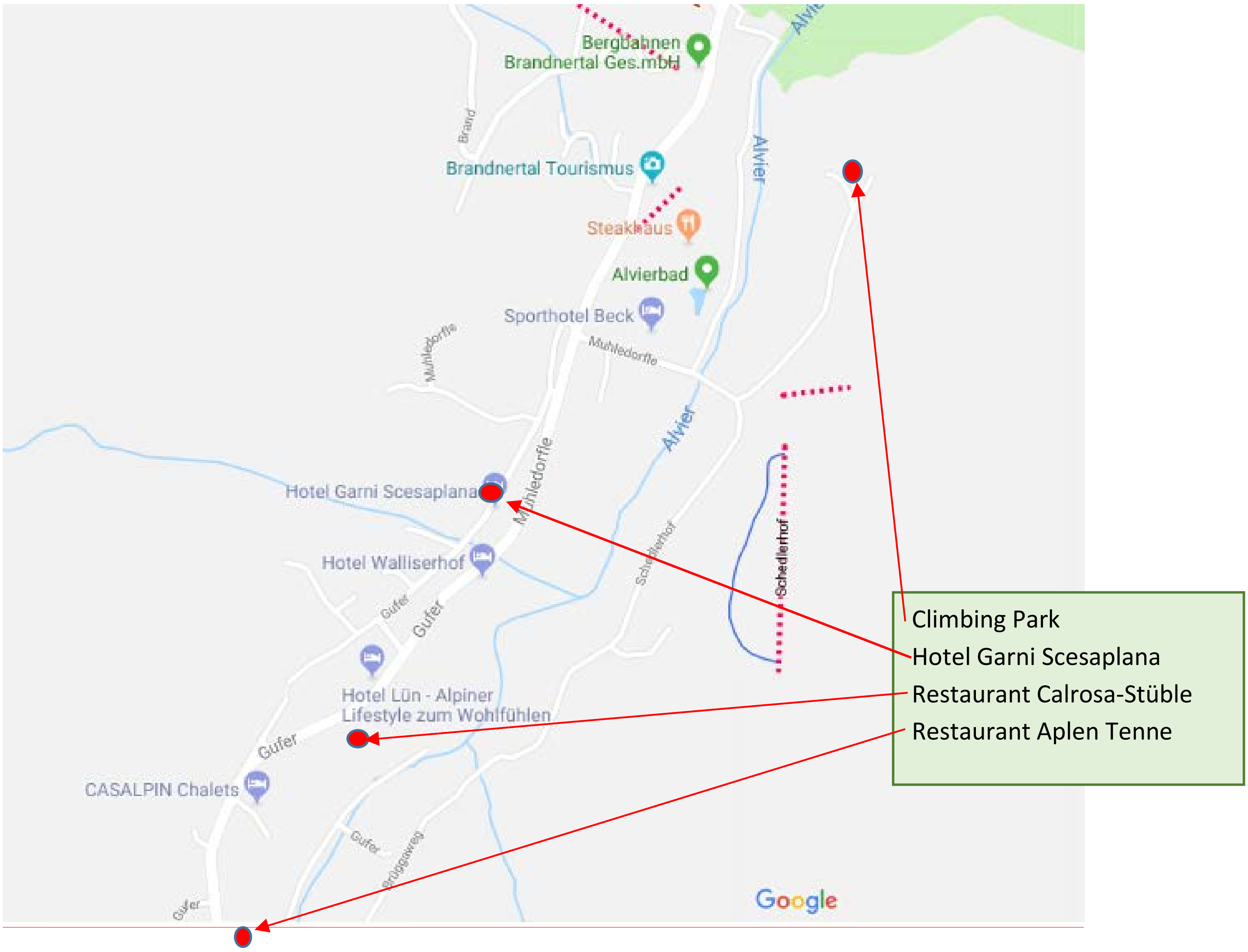
Excursion / Free time activities

An excursion to Lünersee is organized on Wednesday, August 1, 2018 afternoon. On Thursday afternoon, a visit of climbing park in Brand is planned.

WiFi

There is WiFi Access throughout accomodation area.

Brand – Map and Impressions



Scientific Program

Sunday, July 29, 2018

4:00 p.m.	Opening remarks and Introdution of participants	Michael Walter, Zofia Malachowska
5:00 p.m.	Poster Session A	M. Bohlen, J. Fordyce, J. Franz, R. Ghassemizadeh, A. Jalehdoost, I. Lindemann, L. Melo, O. Stauffert, D. Uhl, P. Weckesser
6:30 p.m.	Poster Session B	U. Bangert, V. Behrendt, K. Elshimi, E. Frieling, B. Moore, T. Muthu-Arachchige, A. Scognamiglio, P. Shen, M. Vashishta
8:00 p.m.	Dinner	Restaurant Colrosa Stüble

Monday, July 30, 2018

9:00 a.m.	"X-ray Femtochemistry and Cluster Physics " (Experiment, Lecture 1)	Tim Laarmann
10:30 a.m.	Coffee break	
11:00 a.m.	Rework Session I – Lecture 1	Tim Laarmann
12:30 p.m.	Lunch	
2:45 p.m.	Group Photo	
3:00 p.m.	Rework Session II – Lecture 1	Tim Laarmann
4:30 p.m.	Coffee break	
5:00 p.m.	“Time-Dependent Density Functional Theory and Non- Adiabatic Dynamics” (Experiment, Lecture 2)	Neepa Maitra
8:00 p.m.	Dinner	Restaurant Colrosa Stüble

Tuesday, July 31, 2018

09:00 a.m.	Rework Session I – Lecture 2	Neepa Maitra
10:30 a.m.	Coffee break	
11:00 a.m.	Rework Session-II – Lecture 2	Neepa Maitra
12:30 p.m.	Lunch	
3:00 p.m.	„The angulon quasiparticle: from molecules in superfluids to ultrafast magnetism“ (Experiment Lecture 3)	Mikhail Lemeshko
4:30 p.m.	Coffee break	Restaurant Alpen Tenne

5:00 p.m.	Rework Session I- Lecture 3	Mikhail Lemeshko
6:30 p.m.	Poster Session C	M. Ari, M. Debatin, S. Dold, N. Dozmorov, Y. Gorbachev, J. Schmidt, F. Suzuki, A. Wituschek
8:00 p.m	Dinner	

Wednesday, August 1, 2018

09:00 a.m.	Rework Session II- Lecture 3	Mikhail Lemeshko
10:30 a.m.	Coffee break	
11:00 a.m.	Career Seminar	Christiane Füldner
12:30 p.m.	Lunch	
13:05 p.m.	Excursion - Lünersee	
8:00 p.m.	Dinner	Restaurant Colrosa Stüble

Thursday, August 2, 2018

09:00 a.m.	"Microscopy of Quantum Gases" (Theory, Lecture 4)	Philipp Preiß
10:30 a.m.	Coffee break	
11:00 a.m.	Rework Session I- Lecture 4	Philipp Preiß
12:30 p.m.	Lunch	
1:15 p.m.	Rework Session II – Lecture 4	Philipp Preiß
2:45 p.m.	Coffee break	
3:15 p.m.	„Ultracold Rydberg Gases” (Theory, Lecture 5)	Shannon Whitlock
5:00 p.m.	Excursion – Climbing Park	
8:00 p.m.	Dinner	Restaurant Colrosa Stüble

Friday, August 3, 2018

09:00 a.m.	Rework Session I – Lecture 5	Shannon Whitlock
10:30 a.m.	Coffee break	
11:00 a.m.	Rework Session II- Lecture 5	Shannon Whitlock
12:30 p.m.	Closing Remarks & Poster Award	Frank Stienkemeier
1:00 p.m.	Lunch	
2:00 p.m.	Departure	

Poster Sessions – Participants & Presentations

Poster Session A

Matthias Bohlen, University of Freiburg
Spectroscopy of perylene diimide and oligoacenes on rare gas clusters

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

Janine Franz, University of Freiburg
The Quantum Zeno Effect in the Local Ionisation of a Bose Einstein Condensate

Reyhaneh Ghassemizadeh, University of Freiburg
Ab initio study on Molecular Charge Transport and Conformational Analysis via IR-Raman Spectroscopy

Aghigh Jalehdoost, University of Freiburg
A new source for organic cluster generation

Isabelle Lindemann, University of Freiburg
Towards Ultracold Atom-Ion Interactions-The Lithium Mot

Luke Melo, University of British Columbia
Integration of Confocal Raman and Interferometric Scattering Microscopies for the Analysis of Nanoscale Complex and Biological Specimens

Oliver Stauffert, University of Freiburg
Electron-phonon coupling with density functional theory including environment effects and polaron dynamics

Daniel Uhl, University of Freiburg
Photoelectron two-dimensional coherent spectroscopy

Pascal Weckesser, University of Freiburg
Investigating Ultracold interactions between Barium + Ions and Lithium atoms

Poster Session B

Ulrich Bangert, University of Freiburg
Many-body resonances in dilute gas-phase systems

Vivien Behrendt, University of British Columbia

Optical quenching of metastable helium atoms via the 4^1P state

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

Erik Frieling, University of British Columbia
Reaction rates in ultra-cold Li dimers

Brendon Moore, University of British Columbia
Infrared Spectroscopy of Alanine Water Clusters and Water Aggregation in Solid Parahydrogen

Audrey Scognamiglio, University of Freiburg
Photo-Ionization and electron-impact-ionization-TOF spectrometry for the detection of large organic molecules embedded in cluster beams

Thilina Senaviratne, University of Freiburg
Towards quantum state controlled reactive scattering at milliKelvin temperatues

Pinrui Shen, University of British Columbia
A primary, self-defining UHV Standard Based on Universal van der Waals Scattering

Manish Vashishta, University of British Columbia
Study of collisional processes of magnetically trapped cold methyl radicals

Poster Session C

Meral Ari, University of Freiburg
Computational Screening of Tetra Thiophenyl-substituted Phthalocyanines as Bulk Heterojunction Solar Cell Materials and Comparison with the Phenoxy-substituted Form

Marcel Binz, University of Freiburg
Coherent multidimenstional spectroscopy of dilute gas-phase annosystems

Markus Debatin, University of Freiburg
Cold interactions between Li and Barium

Simon Dold, University of Freiburg
Optimizing a Gas Aggregation Source for Large Cluster Production

Nikolay Dozmorov, Novosibirsk State University
Modelling of the femtosecond dynamics of the photoinduced desolvation of rubidium atoms from helium nanodroplets

Yaroslav Gorbachev, University of Freiburg
The photon BEC in arbitrary geometries by means of QED: Coupled dissipative dynamics of dye molecules

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

Fumika Suzuki, University of Bristish Columbia
Toward the Seperation of Enantiomers by the Casimir- Polder Force

Andreas Wituschek, University of Freiburg:
Stable platform for phase-modulation of seed lasers facilitating all-XUV coherent nonlinear time-domain spectroscopy

Notes

Abstracts – Invited Speakers

Microscopy of Quantum Gases

Philipp Preiss

Physics Institute, Heidelberg University, Heidelberg, Germany

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One of the biggest challenges in physics ist to understand quantum systems of many particles. Such systems cannot be represented efficiently on a classical computer and their emergent properties can often not be calculated from first principles. Modern approaches using ultracold neutral atoms have opened a direct path to tackling this problem experimentally. Building on quantum optics and atomic physics tools, our experiments provide a platform to implement textbook quantum mechanics, but also to create entirely new, synthetic quantum matter.

I will introduce our recent work on realizing strongly interacting fermionic systems in optical tweezers, where pure quantum states of few particles can be realized deterministically. Using a spin-resolved readout scheme, we are able to detect correlations at the level of individual particles. Combining measurements in position and momentum space reveals the presence of correlations in different bases and of entanglement between particles. Applying these techniques to larger systems can shed light on the emergence of magnetic ordering and superfluid pairing.

Some of the fundamental ingredients of our experiments – indistinguishability of particles and quantum correlations – also occur in quantum states of light. In the rework session, I will demonstrate how to access the correlations features of two-photon states experimentally.

The Angulon Quasiparticle: from Molecules in Superfluids to Ultrafast Magnetism

Mikhail Lemeshko

Institute of Science and Technology, Austria

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Recently we have predicted a new quasiparticle - the angulon - which is formed when a quantum impurity (such as an electron, atom, or molecule) exchanges its orbital angular momentum with a many-particle environment (such as lattice phonons or a Fermi sea) [1,2].

Soon thereafter we obtained strong evidence that angulons are formed in experiments on molecules trapped inside superfluid helium nanodroplets [3]. The angulon theory thereby provided a simple explanation for experimental data accumulated during the last two decades. Moreover, casting the many-particle problem in terms of angulons amounts to a drastic simplification and allows to tackle previously intractable problems related to quantum dynamics [4].

In the lectrures, I will introduce the angulon concept and discuss novel physical phenomena [1,5,6] arising from the angular momentum exchange in quantum many-particle systems. I will describe the applications of angulons to modern experiments on quantum impurities and on non-equilibrium magnetism [7].

[1] R. Schmidt, M. Lemeshko, Phys. Rev. Lett. **114**, 203001 (2015)
[2] R. Schmidt, M. Lemeshko, Phys. Rev. X **6**, 011012 (2016)
[3] M. Lemeshko, Phys. Rev. Lett., **118**, 095301 (2017); Viewpoint: Physics **10**, 20 (2017)
[4] B. Shepperson, A. A. Sondergaard, L. Christiansen, J. Kaczmarczyk, R. E. Zillich, M. Lemeshko, H. Stapelfeldt, Phys. Rev. Lett. **118**, 203203 (2017)
[5] E. Yakaboylu, M. Lemeshko, Phys. Rev. Lett. **118**, 085302 (2017)
[6] E. Yakaboylu, A. Deuchert, M. Lemeshko, Phys. Rev. Lett. **119**, 235301 (2017)
[7] J.H. Mentink, M.I. Katsnelson, M. Lemeshko, arXiv:1802.01638 (2018)

Ultracold Rydberg Gases

Shannon Whitlock

IPCMS (UMR 7504) and ISIS (UMR 7006), University of Strasbourg and CNRS, 67000 Strasbourg, France and Physikalisches Institut, Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany

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Over the last decades, versatile model systems for experimentally studying strongly-correlated many-body quantum systems and their dynamics have been realized. In ultracold atomic gases, produced via laser cooling and trapping, the Hamiltonian governing the equilibrium state and the evolution can be known precisely, the relevant system parameters can be precisely tuned, and key observables can be directly accessed. In most experiments however, the atomic interactions which lead to complex behaviour are relatively simple and short ranged (which is an important distinction from e.g. strongly correlated materials). Highly-excited atoms cooled to near absolute zero temperature, called ultracold Rydberg atoms, have very extreme properties which give rise to completely new physical effects. In particular, because of the weak binding of the outer electron to the nucleus, Rydberg atoms react very sensitively to external fields, and experience extremely strong interactions amongst one another, even over macroscopic length scales. In an ensemble of atoms, these interactions prevent more than one Rydberg atom to be excited at a time, leading to the emergence of strong spatial and temporal quantum correlations. By interfacing laser light with Rydberg atoms, we can engineer synthetic systems for studying complex many-body phenomena with total control over the microscopic and macroscopic degrees of freedom. With this it is possible to manipulate the properties of atoms and light at the quantum level and watch a many-body quantum system evolve under the influence of long-range interactions and in a controlled environment. In this lecture I will provide an overview of the physics of ultracold Rydberg gases, focusing on some of the latest results from the field.

Time-Dependent Density Functional Theory and Non-Adiabatic Dynamics

Neepa Maitra

Department of Physics and Astronomy, Hunter College and the Graduate Center of the City University of New York, New York, USA

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When an atom, molecule, or solid is subject to an external field, computational simulations of the time-dependent Schrödinger equation scale exponentially with the system size, making it impossible to solve for more than a few degrees of freedom. Moreover, the wavefunction contains far more information than we usually want. Instead, time-dependent density functional theory is an exact reformulation of the quantum dynamics of many-body systems, that puts the one-body density as the key player. In these lectures and re-work sessions, we will learn the fundamentals behind the theory, the limitations of currently available functional approximations, recent successes and remaining challenges. If time permits, we will also consider the problem of electron-ion coupling beyond the Born-Oppenheimer approximation, and introduce the exact factorization approach to non-adiabatic dynamics.

[1] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).
[2] E. Runge and E. K. U. Gross, Phys. Rev. Lett. **52**, 997 (1984).
[3] E. K. U. Gross and N. T. Maitra, in *Fundamentals of Time-Dependent Density Functional Theory*, edited by M. A. Marques, N. T. Maitra, F. M. Nogueira, E. K. Gross, and A. Rubio (Springer-Verlag, 2012), pp. 53–97.
[4] N. T. Maitra, J. Chem. Phys. **144**, 220901 (2016)
[5] A. Abedi, N. T. Maitra, and E. K. U. Gross, Phys. Rev. Lett. **105**, 123002 (2010).
[6] A. Abedi, N. T. Maitra, and E. K. U. Gross, J. Chem. Phys. **137**, 22A530 (2012).

X-Ray Femtochemistry and Cluster Physics

Tim Laarmann

Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany
The Hamburg Centre for Ultrafast Imaging CUI, Universität Hamburg

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Modern X-ray science exploring the emerging potential at the interface of high-power lasers and accelerator-based photon sources, such as free-electron lasers (FEL), is a great scientific challenge. The objective is to draw a rather complete microscopic picture of dynamical processes in matter, material and life sciences combining expertise in non-linear optics and accelerator-based research. The development of novel photon sources and methodologies strives to image and coherently tailor functionality in nanomaterials on the molecular length scale and ultrafast time scale, respectively. Here, functionality manifests itself in time-dependent changes of electronic structure, bond distances, and bond angles describing the dynamics of complex many-body systems. In typical experiments, the response on external stimuli is observed and manipulated with ultrafast light in a broad spectral range from X-rays, near-infrared to THz accessing inner-shell electrons, as well as low-frequency excitations.

This lecture will survey some of the experimental methods and tools that are particularly effective in this area and discuss possible future trends. For example, an experimental scheme originally invented for time-domain interferometry in the far-infrared spectral range was successfully transferred to FEL science and technology. Two interleaved gratings split the wavefront of an incoming pulse uniformly across the beam profile providing two pulse replicas with variable delay as shown in the figure 1. It enables to record phase-sensitive autocorrelation traces with attosecond precision at a short FEL wavelength.

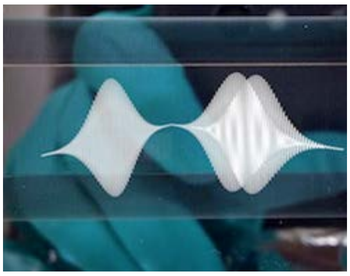

Figure 1: Interferometric autocorrelation with short-wavelength FEL light

[1] S. Usenko, A. Przystawik, M.A. Jakob, L.L. Lazzarino, G. Brenner, S. Toleikis, Ch. Haunhorst, D. Kip, T. Laarmann, Nature Communications **8**, 15626 (2017).

Is doing a postdoc the right thing for you?

Christiane Füldner

Department for Research and Transfer Services, University of Leipzig

E-Mail: christiane.fueldner@zv.uni-leipzig.de

Scientists often do not know enough about their future career options and how they can find appropriate jobs. After having worked hard all their academic lives through school, undergraduate and master studies and having finished their PhDs, they often drift easily into being a postdoc without considering the end of the game. Doing a postdoc appears to be next obvious step. But is it the right one for you? A postdoc is a pivotal career stage for various but not all future careers. It is an academic job and not a continuation of the student status - and it is a period in which you build your CV for prospective careers.

In the workshop we will analyze if doing a postdoc is a possible career step for you and what could be alternative career options. We will be looking at your potential and your skills, as well as where you are and where you want to be. Furthermore, we will discuss how to find a job outside academia.

Abstracts – Poster Session A

Spectroscopy of perylene diimide and oligoacenes on rare gas clusters

Matthias Bohlen, Sharareh Izadnia, Corey A. Rice, Aaron C. LaForge and Frank Stienkemeier

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

Y. Xu and W. Jäger

Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada

The semiconducting character of π-conjugated molecules, such as perylene-derivates or polyacenes are quite promising due to widespread applications of organic electronics. Here we report on spectroscopy of monomers and dimers of perylene diimide (PDI) embedded in helium nanodroplets and adhered to the surface of rare gas clusters. We observed the S1 S0 electronic transition of PDI molecules using laser-induced fluorescence (LIF) as a function of excitation wavelength. The spectrum shows several vibrational transitions as well as dimer contributions, that could be verified by investigations of dependences of the respective features to the PDI partial pressure.[1]

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

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

[2] S. Izadnia, D. Sch¨onleber, A. Eisfeld, A. Ruf, A. C. LaForge, F. Stienkemeier J. Phys. Chem. Let. 8, 2068-2073 (2017).

Molecular superrotors in helium nanodroplets

Jordan Fordyce, Ian MacPhailBartley, and Valery Milner,

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

Frank Stienkemeier

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

An optical centrifuge is used to control the rotation and alignment of molecules embedded in Helium nanodroplets. By combining two chirped, circularly polarized laser pulses, a rotating field is created that can spin anisotropically polarizable molecules to extreme rotational frequencies. Doping Helium nanodroplets with these “superrotors” will be used for the study of new rotational dynamics due the droplets’ cryogenic, superfluid properties. The dopant molecules are set in ultrafast rotation by the optical centrifuge and are subsequently ionized by the femtosecond probe pulse. The recorded velocity map ion image is analyzed to determine the rotational state, or orientation, of the molecules.

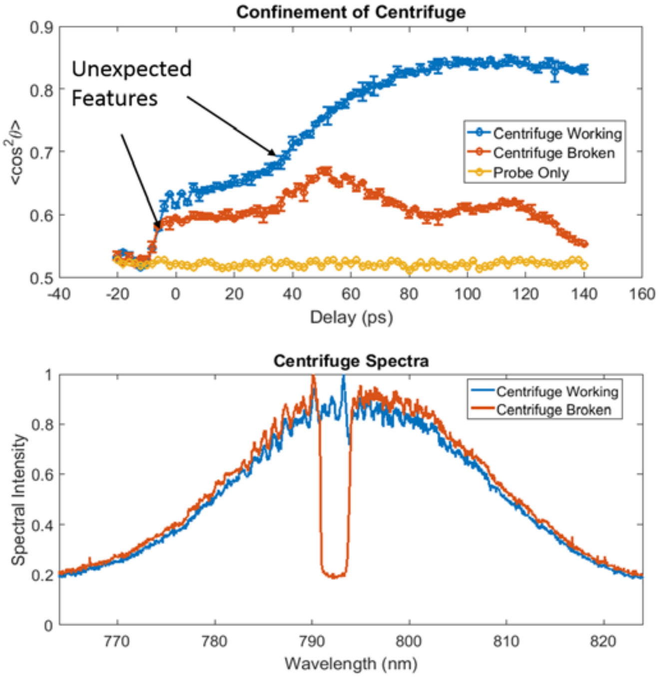

Figure 1: (Top) Effect of confinement from the probe arriving before the centrifuge (negative times) and after the centrifuge (positive times). A value of 1 would be perfectly confined to a line while 0.5 would be an isotropic circle. (Bottom) The corresponding spectra of the centrifuge to the upper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

Because the molecules are anticipated to rotate with a speed well above Landau’s velocity, it is anticipated that the Helium could couple to the rotor, changing it's rotational properties. Therefore, the effect of rotation may only be present during the centrifuge pulse. This requires the onset of rotation and confinement of superrotors in a molecular jet to be well understood. The onset of confinement to the rotational plane from the optical centrifuge, is shown in Figure 1. It was found that the effectiveness of the rotation is very sensitive to the quality of focii overlap which can be difficult due the non-homogeneity after shaping the two pulses. This new understanding of the behaviour of the rotation dynamics will help interpret the effect of the helium matrix with the rotation of molecular superrotors.

The Quantum Zeno Effect in the Local Ionisation of a Bose Einstein Condensate

Janine Franz

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

Juliette Simonet

Center for Optical Quantum Technologies, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

In quantum physics frequent measurement can suppress the dynamics within the measured system. This is called the quantum Zeno effect (QZE). The macroscopic quantum state of a Bose-Einstein condensate (BEC) is one of the few quantum systems allowing the study of the QZE in position measurement. In particular, the local ionisation of the BEC by ultrashort laser pulses is analogous to an irreversible position measurement and can therefore give rise to the QZE. In our theoretical study, we investigate the QZE in a BEC submitted to a local dissipative defect. The behaviour of this open quantum system depends on several parameters: the size of the dissipative defect, effect of inter-atomic interaction, dissipation rate, to name but a few. The quantum Zeno suppression has been quantitatively investigated by numerically solving the time-dependent Gross-Pitaevskii equation, comparing the regimes of continuous local dissipation versus pulsed position measurement. An alternative approach for an ideal BEC in one dimension allows for an intuitive insight into the QZ dynamics.

Ab Initio Study on Molecular Charge Transport and Conformational Analysis via IR-Raman Spectroscopy

Reyhaneh Ghassemizadeh, Michael Walter, Taka Momose

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

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

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

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

A new source for organic cluster generation

Aghigh Jalehdoost and Bernd von Issendorff

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In this project a new source for generation of organic clusters1 is constructed. Since organic clusters are molecular clusters, the supersonic expansion is the preferred method of generation.2 In this method a pulsed valve is used and since the organic material should be evaporated by heating up, the pulsed valve has to work at high temperatures. This new source consists of a pulsed valve with a solenoid as the actuator and all the heated parts are out of metal and it makes possible to increase the temperature to high values like 600ºC. This new design has the advantage of better sealing in compare to the similar designs.3,4 The maximum working temperature for commercially available high temperature pulsed valves is about 300ºC and it is not high enough for the organic materials like Pentacene. So, this new source makes it possible to study the clusters of these organic materials for the first time.

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Towards Ultracold Atom-Ion Interactions - The Lithium Mot

Isabelle Lindemann, Markus Debatin, Pascal Weckesser, Fabian Richter, Fabian Thielemann, Yannick Minet, Julian Schmidt, Leon Karpa, and Tobias Schaetz

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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] and quantum control [3]. To control the atom-ion interaction it is necessary to prepare the mixture at ultracold temperatures. With this new experiment we aim to sympathetically cool the atom-ion mixture into the s-wave regime, where the dynamics can be solely described by a single partial wave.

We present our setup aiming to investigate interactions between laser-cooled neutral Li atoms and Ba+ ions in an optical dipole trap. On this poster we focus on the Li branch of the setup and present the characterization of the Lithium MOT.

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Integration of Confocal Raman and Interferometric Scattering Microscopies for the Analysis of Nanoscale Complex and Biological Specimens

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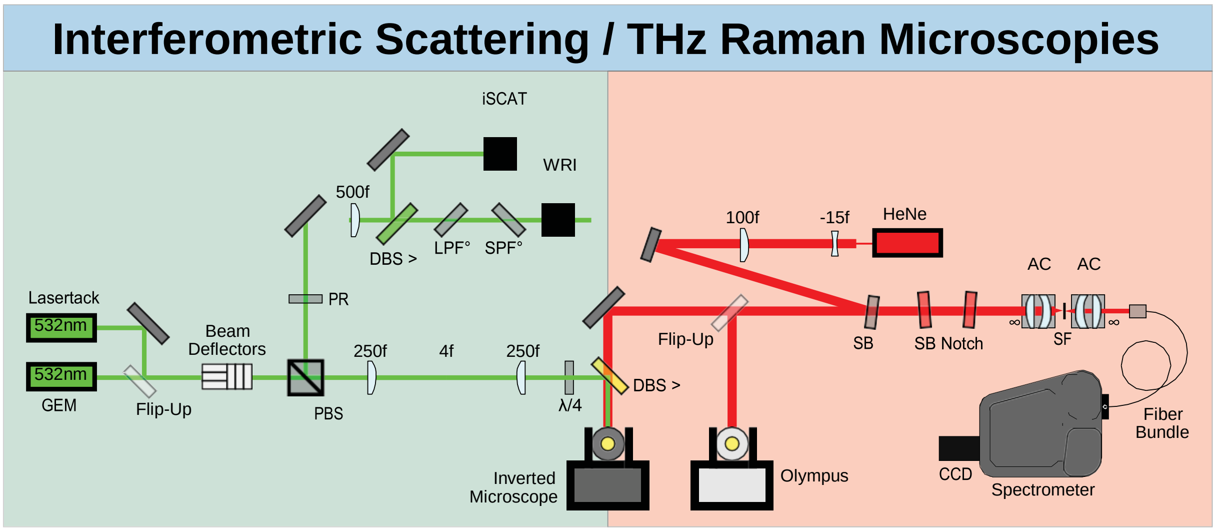

The integration of confocal Raman microscopy with wide-field interferometric scattering (iSCAT)1 microscopy offers a novel advance in the analysis of complex and bio-materials.2 Raman spectroscopy provides information about the chemical morphology of samples; however instruments typically lack the ability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

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

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

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Photoelectron two-dimensional coherent spectroscopy

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

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

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Investigating ultracold interactions between Barium$^+$ ions and Lithium atoms

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The interplay of ultracold atoms and ions has recently gained interest in the atomic com- munity [1], due to its wide applications in quantum chemistry [2, 3] and quantum control [4]. In order to control the atom-ion interaction by means of Feshbach resonances [5] it is necessary to prepare the mixture at ultracold temperatures. At those energies the dynamics of the interaction can be solely described by a single quantum state, known as s-wave scattering. Optical trapping of ions [6, 7, 8] provides a new pathway to achieve ul- tracold atom-ion mixtures in the s-wave regime, as it overcomes the intrinsic micromotion heating effects of a conventional Paul trap [9] currently limiting experiments to collision energies on the order of a few mK.

Here we present our novel experimental setup combining Ba+ ions and Li atoms. So far we have implemented a magento-optical trap (MOT) with 107 Li atoms and a linear Paul trap where we can deterministically load Ba+ individual ions within 1 second. A charac- terization of the MOT and the loading scheme will be presented.

We further show first measurements on the reaction dynamics between individual Ba+ ions with Li atoms. These reactions strongly depend on the initial state of the Ba+ ion, being in agreement with theoretical predictions.

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Abstracts – Poster Session B

Many-body resonances in dilute gas-phase systems

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We investigate the collective behavior of atomic gases at low density and ambient temperature. In this regime, interatomic interactions are small and collective effects are masked by inhomogeneous broadening. Therefore, collective signatures are hard to detect with frequency domain methods. To this end, we have developed a highly efficient timedomain detection method based on a nonlinear femtosecond pump probe excitation scheme [1]. With this method, we detected, for the first time, four-body resonances in a rubidium vapor at densities down to 108 cm$^{-3.}$ Furthermore, we observe phase shifts in the absorption spectrum that are connected to the hyperfine levels of the system. Our findings are surprising considering the weak interparticle interaction present at the studied conditions, which has triggered some interest from theory to explain our results [2,3].

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

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Optical quenching of metastable helium atoms via the 4^1P state

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Our experiments are aimed at studying quantum-state-selected reactive Penning collisions between metastable helium atoms and ultracold lithium atoms. As a first step towards this goal, it is necessary to distinguish between the contributions of the He(2^1S) and the He(2^3S) state to the reaction. In this contribution, we will present a novel scheme for the quenching of the metastable singlet state using optical pumping to the 4^1P state at 397 nm and subsequent decay to the electronic ground state. We will present the experimental setup and preliminary results which illustrate that this scheme offers several experimental advantages compared to previous approaches.

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 analyser, and an ion time-of-flight mass spectrometer. It will be com- bined 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 re- laxation in well-defined nanosystems in quantum-size-regime, while the ion time-of-flight mass spectrometer is used to monitor the cluster size and photo-fragmentation.

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

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Reaction rates in ultra-cold ^{6}Li dimers

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

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

Infrared Spectroscopy of Alanine Water Clusters and Water Aggregation in Solid Parahydrogen

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The formation of gas phase β-alanine zwitterions has been studied using solid *para*-H_2 FT-IR matrix-isolation spectroscopy. β-alanine was co-deposited with mixtures of H2O/ *para*-H_2 to observe the stabilization effect of water molecules on the zwitterion form of β-alanine. Through a comparison with theoretical computations, as well as with crystalline β-alanine FT- IR spectra, the characteristic NH_3 N-H bending vibrational frequency for the zwitterionic form was identified. Analysis of the spectral peak temporal behavior shows that other proposed zwitterion peaks behave similarly to the characteristic NH_3 spectral peak. In agreement with theoretical studies, it has been shown that water can stabilize the zwitterionic form of gas phase amino acids, causing the zwitterion to form preferentially over the neutral form under certain conditions.

The β-alanine zwitterion formation rate may be attributed to aggregation of small water clusters in the solid *para*-H_2 matrix. The aggregation of small water clusters occurs due to diffusion of water molecules in the solid *para*-H_2 matrix. The diffusion of water monomers, as well as dimers, is observed at temperatures as low as 4K. As solid *para*-H_2 is a quantum crystal, the behavior of diffusion in this solid differs from classical solid state diffusion. A comparison between the diffusion of water molecules in the *para*-H_2 matrix and diffusion of impuritons in a quantum crystal is made. As the size of water cluster increases, the aggregation rate displays some similar behavior to the formation rate of β-alanine zwitterions. It is proposed that water clusters of size $n>5$ are responsible for the stabilization of β-alanine in the zwitterionic form in the *para*-H_2 matrix.

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

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

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

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

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Towards quantum state controlled reactive scattering at milli Kelvin temperatures

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Our experiments are aimed at studying reactive collisions at tunable collisional energies in the quantum regime and with full quantum state control of both reaction partners. State-of-the-art experiments have been done in previous years to investigate collisions of ultracold atoms and molecules. However, at ultracold temperatures, scattering processes are dominated by s-wave scattering, so that the reaction rate is temperature dependent. In contrast to that, in the cold temperature regime between 1 mK and 1 K, few partial waves with $l > 0$ influence the scattering process so that the influence of quantum effects in scattering processes, such as barrier tunneling can be observed. In a wider scope, this would not only be beneficial in realizing and challenging existing theoretical models, but also in creating more stable platforms for many-body physics and quantum information via controlling the chemical reaction dynamics. To achieve this, we plan to use an ex-isting setup which consists of a Li MOT as a stationary target and a supersonic beam of metasatble He atoms. At the first stage of my PhD project, I will be implementing a Zeeman slower for metastable He to tune the velocity of the beam, and thus, to control the collision energy.

A Primary, self-defining UHV Standard Based on Universal van der Waals Scattering

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

Study of collisional processes of magnetically trapped cold methyl radicals

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

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

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

Abstracts – Poster Session C

Computational Screening of Tetra Thiophenyl-substituted Phthalocyanines as Bulk Heterojunction Solar Cell Materials and Comparison with the Phenoxy-substituted Form

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

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Coherent multidimensional spectroscopy of dilute gas-phase nanosystems

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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].

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

For this study, we synthesized weakly-bound high-spin Rb_2 and Rb_3 molecules on the surface of the helium nanodroplets as a test bench system. Our method shows an unprecedented sensitivity and resolution which allows us to precisely analyze the photodynamics in Rb_2 attached to the droplet surface and the interaction dynamics of the Rb_3-helium droplet system.

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Cold interactions between Li and Barium

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

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

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Optimizing a Gas Aggregation Source for Large Cluster Production

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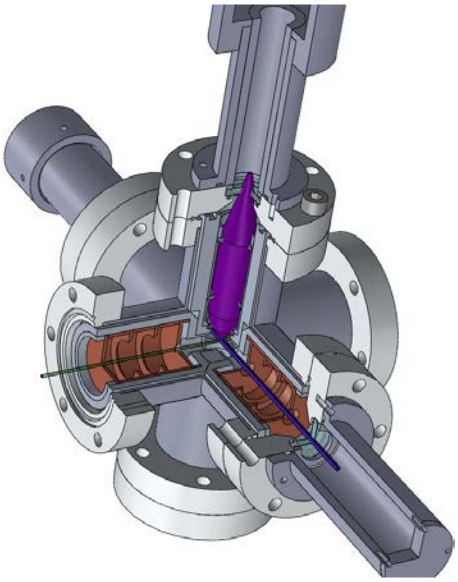

Wide angle X-Ray diffraction has been proven a viable tool to determine the 3D structure of metal clusters[1]. Our goal is to utilize ultrashort X-Ray pulses as a tool to resolve ultrafast processes in nanoscale systems by imaging structure in a time-dependent manner. Diffraction experiments on metal clusters in gas-phase require high intensities of both, clusters and X-ray beam to vanquish low cross-sections for these scattering processes. To overcome this difficulties a carefully taylored source for clusters had to be set up. I will present efforts to characterize the source that have been made to this end, in particular the results of the detection of laserlight scattered off of silver clusters in gas-phase.

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Modelling of the femtosecond dynamics of the photoinduced desolvation of rubidium atoms from helium nanodroplets

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Helium (He) nanodroplets composed of $10^3 – 10^8$ He atoms are widely used as ultracold (0.4K) matrices for the spectroscopy of attached or embedded atomic and molecular species. Recently a progress in the experimental study of the femtosecond dynamics of photoexcited and photoionized rubidium (Rb) atoms attached to helium nanodroplets (HeN) has been achieved with the use of femtosecond pump-probe technique in combination with the velocity map imaging of the photofragments[1]. This approach allowed the authors to investigate the dynamics of solvation and desolvation due to the propagation of wavepackets in the different electronic states of Rb-HeN complex. In a pumping step, Rb-HeN complex was excited by VIS or NIR radiation to a repulsive state. Measured total kinetic energy release of Rb^+ after probe pulse for observed photodissociation channels corresponds to the kinetic energy of the intramolecular motion in the intermediate state at the moment of the electron photodetachment by the probing radiation. The variation of delay time between the pumping and the probing pulses provides information about the propagation of the wavepacket in time.

Previously the simulation of this dynamics has been carried out within classical approach [1]. The authors have simulated classically the system, but it had only the qualitative correspondence with the experimental data. In the current work the desorption model has been modified and the results of the quantum dynamics simulation are presented and compared with experimental results. The suggested approach allows us to get better agreement between the results of simulation and experimental data.

The numerical evolution of wavepackets has been performed with the use of the exponential split operator method [2]. The interaction of wavepackets with the laser field has been considered by perturbation theory. Matlab package Wavepacket [3] and Wolfram Mathematica program have been used in calculations.

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

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Bose-Einstein condensation (BEC) has in the last two decades been observed in cold atomic gases and in solid-state physics. Progress in photonics over the last few years has led to a new challenge in quantum optics and condensed matter: the photon BEC. This has been experimentally observed in a small microcavity filled with a dye medium [1]. Confinement of laser light within such an optical microcavity creates conditions for light to equilibrate as a gas of conserved particles. The cavity mirrors' high reflectivity guarantees that photons live long enough to scatter among the dye molecules, which exchange energy with the photons by repeatedly absorbing and reemitting them. We use the language of macroscopic quantum electrodynamics [2] together with theory of open quantum systems [3] to describe this phenomenon. We are interested in the realistic description of the cavity geometry, whose frequency- dependent reflection and absorption are fully encoded in the classical Green's function for the electromagnetic Helmholtz equation. This extension of the standard Jaynes-Cummings model to absorbing cavities with realistic geometries opens the door to studying the effects of the coupling of discrete modes in a resonant geometry to the strong body-assisted electromagnetic field of the cavity.

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Optical trapping of ion Coulomb crystals

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

We now demonstrate trapping of ion crystals [4] consisting of up to six Barium ions in an optical dipole trap aligned with the crystal axis and without confinement by radio-frequency (RF) fields. The dependence on the trap parameters, in particular the interplay of beam waist, laser power and axial confinement by DC electric fields, is investigated. As a proof-of- principle experiment, we detect the center-of-mass and stretch modes for an optically trapped two-ion crystal. Finally, we present prospects for optical trapping of higher-dimensional Coulomb crystals.

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[4]J. Schmidt et al., Phys. Rev. X 8, 021028 (2018)

Toward the Separation of Enantiomers by the Casimir-Polder Force

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

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

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

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

We present a compact, stable and transportable platform specifically designed to perform PM on 261nm seed laser pulses. Degrees of freedom for adjustment are reduced to a minimum, in order to gain stability compared to a discrete setup on a breadboard. All optics are tailored to withstand high peak intensities and dispersion is reduced to a minimum. High stability of the platform and the sensitivity of the PM approach was verified observing UV quantum beats (268nm) in a low-density sodium beam (1.5x10^{8} cm^{3}), detecting photoions with a time-of- flight mass spectrometer at a laser repetition rate of 50Hz. The platform has been implemented in the FERMI FEL seed laser beamline for characterization.

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Notes

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3rd IRTG CoCo Summer School
Coherent Dynamics of Cold Molecular Ensembles
Theoretical and Experimental Methods
29th July - 3rd August, Brand, Austria

Hotel Garni Scesaplana

Mühledörfle 158 A-6708 Brand / Bludenz, Austria

	Sunday 29th July 2018	Monday 30th July 2018	Tuesday 31st July 2018	Wednesday 1st August 2018	Thursday 2nd August 2018	Friday 3rd August 2018
09:00		**Tim Laarmann** Deutsches Elektronen-Synchrotron X-ray Femtochemistry and Cluster Physics	**Neepa Maitra** Hunter College CUNY USA Rework Session I	**Mikhail Lemeshko** Institute of Science and Technology Austria Rework Session II	**Philipp Preiß** University of Heidelberg Microscopy of Quantum Gases	**Shannon Whitlock** University of Strasbourg Rework Session I
10:30		Break	Break	Break	Break	Break
11:00		**Tim Laarmann** Deutsches Elektronen-Synchrotron Rework Session I	**Neepa Maitra** Hunter College CUNY USA Rework Session II	**Carrere Seminar** **Christiane Füldner** University of Leipzig	**Philipp Preiß** University of Heidelberg Rework Session I	**Shannon Whitlock** University of Strasbourg Rework Session II
12:30		Lunch	Lunch	Lunch	Lunch	Closing session Poster Award
				Bus departure 13:05 Excursion Lünersee	**Philipp Preiß** University of Heidelberg Rework Session II	Lunch
		Group Photo				
15:00	Arrival	**Tim Laarmann** Deutsches Elektronen-Synchrotron Rework Session II	**Mikhail Lemeshko** Institute of Science and Technology Austria Angulon Quasiparticles		Break	Departure
					Shannon Whitlock University of Strasbourg Ultracold Rydberg Gases	
16:00	Welcome + introdution of participants					
16:30		Break	Break			
17:00	Poster session A	**Neepa Maitra** Hunter College CUNY USA Time-dependent Density Funcitonal Theory and non-adiabatic dynamics	**Mikhail Lemeshko** Institute of Science and Technology Austria Rework Session I		Climbing Park	
18:30	Poster session B		Poster session C			
20:00	Dinner	Dinner	Dinner	Dinner	Dinner	

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