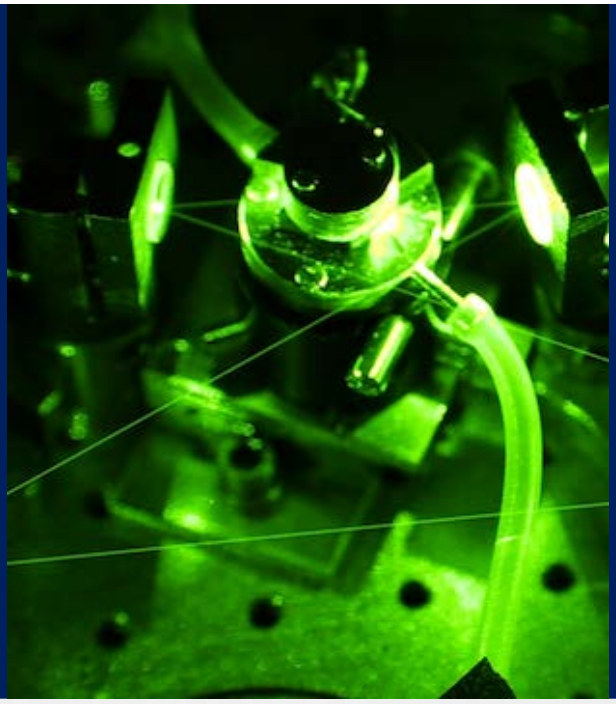

IRTG 2079 CoCo

Cold Controlled Ensembles

in Physics and Chemistry

BOOK OF ABSTRACTS

1st CoCo Summer School

ULTRACOLD FEW- AND MANY-BODY SYSTEMS: QUANTUM MECHANICS MADE CRYSTAL CLEAR

July 24th - July 29th 2016

Centre de Mittelwihr, France

Spectra-Physics. A Newport Company

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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 TOPICS OF THE 1ST CoCo SUMMER SCHOOL INVOLVE SCIENTIFIC QUESTIONS AT THE HEART OF THE IRTG: COLD COLLISIONS AND INTERACTIONS INVOLVING MAXIMAL QUANTUM EFFECTS NOT REACHABLE AT AMBIENT CONDITIONS. THE SUBJECTS RANGE FROM EXPERIMENTAL INVESTIGATIONS OF ULTRACOLD GASES, OVER QUANTUM ROTORS TO THE THEORETICAL DESCRIPTION OF ULTRAFAST LASER INTERACTIONS. THE SCHOOL WILL ADDRESS THESE TOPICS BY PRESENTING BASIC KNOWLEDGE, DEVELOPMENTS AND CURRENT TRENDS VIA A SERIES OF LECTURES AND TUTORIALS PRESENTED BY INTERNATIONALLY LEADING INVESTIGATORS.

Main Topics

Theory: "Light and matter waves propagation in artificial atomic crystals: periodic and disordered configurations“

Theory: "Quantal toolkit for few-body and many-body theory“

Theory: "Coherent Ultrafast Multidimensional Spectroscopy of Molecular Processes with Optical, X-ray, and Quantum Light“

Experiment: "Cold collisions, quantum rotors"

Experiment: "Ultracold polar molecules"

Experiment: "Collison and reaction dynamics of cold molecular few-body systems“

Experiment: "Organic Photovoltaics: energy conversion with molecules“

Financial Support

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IRTG 7079 „Cold Controlled Ensembles in Physics and Chemistry“

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General Information

Duration

Sunday July 24th, 2016, 5.30 pm – Friday July 29th, 2016, 2.00 pm

Location

Centre de Mittelwihr

16 rue du Bouxhof

68630 Mittelwihr, France

www.mittelwihr.com

Travel Information - Shuttles

Shuttles busses will operate on Sunday, July 24th, 3.30 pm, from the Konzerthaus in Freiburg (very close to the train station) to the “Centre de Mittelwihr”, and back on Friday, July 29th, 2:00 pm. The journey lasts about an hour.

Travel Information – Individual Journeys

The Airports which are close to Mittelwihr 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 or Colmar (ca. 2 hours). From Colmar train station there is a regular bus to Mittelwihr (Bus N°106 “Colmar – Route des Vins – Ribeauvillé”). Get off at “Mittelwihr Mairie”. From there to Centre Mittelwihr it is 500 meters walking distance. As busses do not operate very often, (http://www.cg68.fr/horaires-des-bus/horaires-des-bus.html) we would recommend a taxi or we can organize a pick-up.

Travel Information – By car

From Freiburg: via B31 and A5 to Breisach, D415 to Colmar, A35 direction Nancy/Strasbourg/Colmar-Nord - Exit 23 (Bennwihr, Houssen), then take D83 and D4 (direction Kaysersberg) to Mittelwihr

From Strasbourg: RN83 – Exit Ostheim - direction Beblenheim, Riquewihr

From Mulhouse: A35 - Exit Bennwihr, Kaysersberg

General Information

Hotel

For PhD and master students as well as postdocs we have reserved double rooms, for speakers private rooms. Towels will be provided.

Centre de Mittelwihr

16 Rue du Bouxhof

68630 Mittelwihr, France

E-Mail: info@mittelwihr.com

Phone: +33 (0)3 89 47 93 09

Meals & Drinks

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

Excursion

A canoe trip through the beautiful landscape of Alsace is organised on wednesday afternoon (July 27th, 2016).

W-Lan

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

Scientific Programm

Sunday, July, 24th 2016

Till 17:30	*Arrival*	
17:30	*Opening remarks*	Michael Walter & Anne Hillenbach
18:00	*Presentation by Participants:* *1 Slide / 1 Person / 1 Minute!*	
19:00	*Poster Session 1 & Aperitif*	
20:00	*Dinner*	

Monday, July 24th 2016

Till 08:45	*Breakfast*	
09:00	*"Light and matter waves propagation in artificial atomic crystals: periodic and disordered configurations" (Theory, Lecture 1)*	Mauro Antezza
10:30	*Coffee break*	
11:00	*Reworking Session of Lecture 1*	Mauro Antezza
12:30	*Lunch*	
14:00	*Reworking Session of Lecture 1*	Mauro Antezza
15:30	*Coffee break*	
16:00	*"Cold collisions, quantum rotors" (Experiment, Lecture 2)*	Ed Narevicius
17:30	*Coffee break*	
18:00	*Applied Science Lecture:* *"Organic Photovoltaics: energy conversion with molecules"*	Elizabeth von Hauff
19:00	*Poster Session 2 & Aperitif*	
20:00	*Dinner*	

Tuesday, July 24th 2016

Till 08:45	*Breakfast*	
09:00	*Reworking Session of Lecture 2*	Ed Narevicius
10:30	*Coffee break*	
11:00	*Reworking Session of Lecture 2*	Ed Narevicius
12:30	*Lunch*	
14:00	*Coherent Ultrafast Multidimensional Spectroscopy of Molecular Processes with Optical, X-ray, and Quantum Light (Theory, Lecture 3)*	Shaul Mukamel
15:30	*Coffee break*	
16:00	*Reworking Session of Lecture 3*	Shaul Mukamel
17:30	*Coffee break*	
18:00	*Reworking Session of Lecture 3*	Shaul Mukamel
19:30	*Poster Session 3 & Aperitif*	
20:00	*Dinner*	

Wednesday, July 24th 2016

Till 08:45	*Breakfast*	
09:00	"Ultracold polar molecules" *(Experiment, Lecture 4)*	Silke Ospelkaus
10:30	*Coffee break*	
11:00	*Reworking Session of Lecture 4*	Silke Ospelkaus
12:30	*Lunch*	
13:30	*Reworking Session of Lecture 4*	Silke Ospelkaus
15:00	*Excursion – canoe trip*	
20:00	*Dinner*	

Thursday, July 24th 2016

Till 08:45	*Breakfast*	
09:00	*"Collison and reaction dynamics of cold molecular few-body systems" (Experiment, Lecture 5)*	Roland Wester
10:30	*Coffee break*	
11:00	*Reworking Session of Lecture 5*	Roland Wester
12:30	*Lunch*	
14:00	*Reworking Session of Lecture 5*	Roland Wester
15:30	*Coffee break*	
16:00	*"Quantal toolkit for few-body and many-body theory" (Theory, Lecture 6)*	Chris Greene
17:30	*Coffee break*	
18:00	*Career seminar*	Frank Krüger
19:00	*Dinner*	
20:00	*Winetasting*	

Friday, July 24th 2016

Till 08:45	*Breakfast*	
09:00	*Reworking Session of Lecture 6*	Chris Greene
10:30	*Coffee break*	
11:00	*Reworking Session of Lecture 6*	Chris Greene
12:30	*Closing Remarks & Poster Prize*	
13:00	*Lunch*	
14:00	*Departure*	

Postersessions

Postersession 1 - Participants & Presentations

Barcellona, Pablo (University of Freiburg):
Enhanced chiral discriminatory van der Waals interactions mediated by chiral surfaces

Bogomolov, Alexandr (Voevodsky Institute of Chemical Kinetics and Combustion):
The formation of chemically bound argon via photoexcitation of Ar-I2 van der Waals complex

Dare, Kahan & Polovy, Gene (University of British Columbia): TBA

Dold, Simon (University of Freiburg):
Time-resolved imaging of the dynamics of free metal clusters and nanocrystals

Fuchs, Sebastian (University of Freiburg):
From Casimir-Polder Force to Dicke Physics: Interaction between Atoms and a Topological Insulator

Stauffert, Oliver (University of Freiburg):
Singlet fission and repulsive Van der Waals forces

Vargas Hernandez, Rodrigo A. (University of British Columbia):
Lattice models with long-range and number-non-conserving interactions with Zeeman excitations of ultracold magnetic atoms

von Vangerov, Johannes (University of Freiburg): Imaging excited state dynamics of doped helium nanodroplets in real time

Xu, Dongyang (Oxford University): Design and experimental test of compact and robust magneto-optical trap (MOT) source

Postersession 2 - Participants & Presentations

Bibelnik, Natan (Weizmann Institute of Science):
Probing neutral-molecular ion potential via penning ionization

Cantin, Joshua T. (University of British Columbia):
Quantum localization of particles with dipolar tunnelling in three-dimensional lattices of finite size

Damjanovic, Tomislav (University of Basel):
Traveling wave Zeeman deceleration of molecules

Dozmorov, Nikolay (Novosibirsk State University):
Modelling of the Femtosecond Intramolecular Dynamics in the High-Lying Electronic States of Molecular Iodine

Fey, Christian (University of Hamburg):
Stretching and bending dynamics in triatomic ultralong-range Rydberg molecules

Ghassemizadeh, Reyhaneh (University of Freiburg):
Study of Electron Transport in Organic Molecules using Constrained Density Functional Theory

Grzesiak, Jonas (University of Freiburg):
Cold Penning-Reactions using a Li-MOT

Höveler, Katharina (ETH Zurich):
Experimental studies of the ion-molecule reactions $H_2^+ + H_2$ and $H_2^+ + D_2$ at low collision energies with a merged beam apparatus

Izadnia, Sharareh (University of Freiburg):
Superradiance, singlet fission and triplet annihilation processes of organic molecules attached to neon clusters

Jachymski, Krzysztof (University of Stuttgart):
Three-body interactions of slow light Rydberg polaritons

Jalehdoost, Aghigh (University of Freiburg):
Mass and Photoelectron Spectroscopy of Organic Molecules

Koval, Evgeny (JINR University Centre):
Resonant States of Two-dimensional (2D) Hydrogen in Magnetic Field

Koval, Oksana (JINR University Centre):
The Stark Effect in Two-dimensional Hydrogen

Vashishta, Manish (University of British Columbia):
MW trap for polar molecule

von Planta, Claudio (University of Basel):
Cold ion-molecule collisions in a cryogenic hybrid trap

Postersession 3 - Participants & Presentations

Bohlen, Matthias (University of Freiburg):
Highly flexible supersonic expansion valve for the production of various Clusters/Nanodroplets and different doping perspectives

Bruder, Lukas (University of Freiburg):
Detection of multiple-quantum coherences in dilute samples

Klatt, Juliane (University of Freiburg):
Quantum Friction and Markovianity

Ostmann, Paula (TU Dresden):
Single particle dynamics in an ultracold environment: From superfluidity to finite site reheating

Rivlin, Tom (University College London):
High accuracy simulations of Ultracold atom-atom scattering using R-matrix methodology

Ruf, Alexander (University of Freiburg):
TBA

Schmidt, Julian (University of Freiburg):
Long-lived all-optical ion trapping

Shee, Avijit (University of Lille, 1):
Analytic Gradient at the 4-component Relativistic Coupled Cluster Level with Inclusion of Spin-Orbit Coupling

Wasak, Tomasz (University of Warsaw):
Description of ultracold collision between dipole and ion

Notes

Abstracts – Invited Talks

Light and matter waves propagation in artificial atomic crystals: periodic and disordered configurations

Mauro Antezza

University of Montpellier, France

In these lectures we present some results concerning the theoretical study of light waves [1-3] and of atomic matter waves [4-6] propagating in artificial atomic crystals realized by atoms trapped at the notes of an optical lattice and forming 2D or 3D (Bravais or non-Bravais) crystals. The case of not perfectly filled lattices will be also considered to study of the absence of transport due to the occurrence of the Anderson localization in disordered systems.

[1] Fano-Hopfield model and photonic band gaps for an arbitrary atomic lattice
Mauro Antezza, Yvan Castin
Phys. Rev. A 80, 013816 (2009)

[2] Spectrum of light in a quantum fluctuating periodic structure
Mauro Antezza, Yvan Castin
Phys. Rev. Lett. 103, 123903 (2009)

[3] Photonic band gap in an imperfect atomic diamond lattice: penetration depth and effects of finite size and vacancies
Mauro Antezza, Yvan Castin
Phys. Rev. A 88, 033844 (2013)

[4] Quantitative study of two- and three-dimensional strong localization of matter waves by atomic scatterers
Mauro Antezza, Yvan Castin, David A. W. Hutchinson
Phys. Rev. A 82, 043602 (2010)

[5] Matter waves in atomic artificial graphene
Nicola Bartolo, and Mauro Antezza
Europhys. Lett. 107, 30006 (2014)

[6] Matter waves in two-dimensional arbitrary atomic crystals
Nicola Bartolo, and Mauro Antezza
Phys. Rev. A 90, 033617 (2014)

Quantal toolkit for few-body and many-body theory

Chris H. Greene

Department of Physics and Astronomy, Purdue University, USA

The theoretical description of very low energy systems is controlled by quantum mechanics at very long de Broglie wavelengths. Some simplifying aspects in this limit allow for the use of specialized methods and approximations that are especially designed for this long-wavelength physical regime. These include techniques such as the zero-range Fermi pseudopotential, effective range theory, multichannel quantum defect theory, and the adiabatic/nonadiabatic methods such as Landau-Zener theory. Using a theoretical toolkit based on these ideas, we can understand remarkably detailed and complicated quantal behavior of systems such as two-body Fano-Feshbach resonances, atomic and molecular Rydberg spectroscopy, the universal Efimov effect for three neutral particles, and the large scale behavior of degenerate quantum gases. This lecture will survey the theoretical tools that are particularly effective in this area for understanding some of the most interesting and rich phenomena.

Coherent Ultrafast Multidimensional Spectroscopy of Molecular Processes With Optical, X-ray, and Quantum Light

Shaul Mukamel

Department of Chemistry, Department of Physics & Astronomy ,University of California, Irvine, California 92697-2025, USA.

E-mail: smukamel@uci.edu

Multidimensional spectroscopy uses sequences of optical pulses to study dynamical processes in complex molecules through correlation plots involving several time delay periods. Recent extensions of these techniques to the x-ray regime as well as by utilizing the quantum nature of light will be discussed. Applications to excitons in aggregates and to trapped ions will be presented.

Strong coupling of molecules to the vacuum field of micro cavities can modify the potential energy surfaces thereby manipulating the photophysical and photochemical reaction pathways. The ultrafast dynamics of molecules confined in optical micro cavities is investigated. The photonic vacuum state of a localized cavity mode can be strongly mixed with the molecular degrees of freedom to create hybrid field-matter states known as polaritons. Simulations of the avoided crossing of sodium iodide in a cavity which incorporate the quantized cavity field into the nuclear wave packet dynamics will be presented. Numerical results show how the branching ratio between the covalent and ionic dissociation channels can be strongly manipulated by the optical cavity.

Many important photophysical and photochemical molecular processes take place via conical intersections (COIS) where nuclear and electronic degrees of freedom become strongly coupled and the adiabatic Born Oppenheimer approximation beaks down. A new technique, TRUE-CARS, Transient Redistribution of Ultrafast Electronic Coherences in Attosecond Raman Signals, is proposed that can detect the passage through a COIS. Short X-ray pulses can directly detect the passage through a CoIn with the adequate temporal and spectral sensitivity. The technique is based on a coherent Raman process that employs a composite femtosecond/attosecond X-ray pulse to directly detect the electronic coherences (rather than populations) that are generated as the system passes through the CoIn.

Signals that utilize the quantum nature of the optical field by varying parameters of the photon wavefunction rather than classical field delays and frequencies will be presented. Entangled photons provide novel nonlinear spectroscopic probes of excitation-energy-transfer and charge-separation processes in chromophore aggregates. The unusual spectral and temporal characteristics of entangled photon pairs combined with interferometric detection make it possible to manipulate and control two photon absorption and Raman signals and extract information not available with classical light.

1. "Optical Multidimensional Coherent Spectroscopy", S. Cundiff and S. Mukamel. Physics Today , 66 , 44-49 (July 2013)
2. "Cavity femtochemistry; Manipulating nonadiabatic dynamics at avoided crossings", Markus Kowalewski, Kochise Bennett, and Shaul Mukamel. J. Phys. Chem. Lett ,2016, 7, 2050-2054

3. "Suppression of Population transport and Control of Exciton Distributions by Entangled Photons ", F. Schlawin, K.E. Dorfman, B.P. Fingerhut, and S. Mukamel. Nature Communications, 4:1782:DOI:10.1038/ncomms2802 (2013).
4. "Nonlinear optical signals and spectroscopy with quantum light", Konstantin E. Dorfman, Frank Schlawin, and Shaul Mukamel. Reviews of Modern Physics (In Press, 2016) arXiv:1605.06746v1
5. "Nonlinear Spectroscopy of Trapped Ions", F. Schlawin, M. Gessner, S. Mukamel and A. Buchleitner. Phys Rev A, 90, 023603 (2014)
6. "Nonlinear Spectroscopy of Controllable Many-Body Quantum Systems", M. Gessner, F. Schlawin, H. Haffner, S. Mukamel and A. Buchleitner. NJP, **16,** 092001 (2014)
7. "Catching Conical Intersections in the Act; Monitoring Transient Electronic Coherences by Attosecond Stimulated X-ray Raman Signals", Markus Kowalewski , Kochise Bennett, Konstantin Dorfman, and Shaul Mukamel. Phys. Rev. Lett. 115, 193003 (2015).
8. "Monitoring nonadiabatic electron-nuclear dynamics in molecules by attosecond streaking of photoelectrons", Markus Kowalewski, Kochise Bennett, Jeremy Rouxel, and Shaul Mukamel.PRL (In Press, 2016)

Cold collisions, quantum rotors

Ed Narevicius

Weizmann Institute of Science, Israel

Ultracold atomic and molecular gases

Silke Ospelkaus

University of Hannover, Germany

Within this lecture, I will give an overview on recent experiments with ultracold polar molecules. The study of ultracold molecules promises important prospects such as quantum control of chemical reactions, novel methods for quantum information processing and the preparation and study of novel dipolar quantum states of matter.

Within the first lecture, I will give an overview on experimental techniques for the preparation of cold and ultracold molecular samples. In the second lecture, I will then review experiments on quantum state and interaction controlled chemical reactions in the limit of zero temperature making use of ultracold polar molecular samples.
We will accompany the lecture by a "journal club".

Organic Photovoltaics: energy conversion with molecules

Elizabeth von Hauff

Department of Physics & Astronomy, Vrije Universiteit Amsterdam, The Netherlands

Record power conversion efficiencies of organic solar cells have now exceeded 10 % [1] which has long been considered a benchmark for market entry for low cost emerging photovoltaic technologies. Current research is focussed on further improving solar cell performance. Advances in this field require interdisciplinary approaches, as well as cooperation between fundamental and applied research.

The photovoltaic conversion process consists of 4 basic steps: light absorption, charge separation, charge transport and charge collection. The efficiency of each of these steps determines the overall power conversion efficiency of the device. Organic photovoltaics is based on a molecular donor-acceptor system for generation of photocurrent (**Figure 1**). The extended bulk heterojunction formed between the donor and acceptor molecules in thin film facilitates efficient charge separation, while forming closed pathways to the electrodes for the transport of photocurrent.

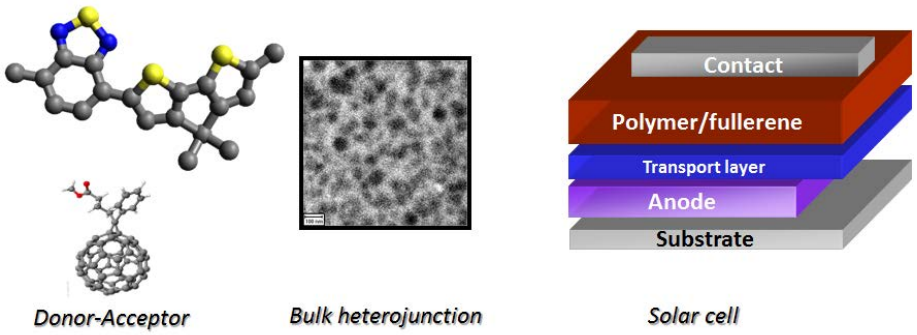

Figure 1:Molecular Donor-Acceptor system, electron microscopy image of the bulk heterojunction thin film active layer and the organic solar cell architecture.

The underlying physical mechanisms of energy conversion steps in organic photovoltaics, particularly charge separation and charge transport, are still not well-understood. In this lecture I will review the basic principles of organic photovoltaics, and discuss how the molecular environment influences carrier separation and recombination [2,3]. Additionally I will talk about current models and open questions about carrier transport in these systems.

References:

[1] M. A. Green, K. Emery, Y. Hishikawa, W. Warta, E. D. Dunlop, *Prog. Photovoltaics Res. Appl.* **2016**, *24*, 3.

[2] M. Hallermann, I. Kriegel, E. Da Como, J. M. Berger, E. Von Hauff, J. Feldmann, *Adv. Funct. Mater.* **2009**, *19*, 3662.

[3] S. Gélinas, A. Rao, A. Kumar, S. L. Smith, A. W. Chin, J. Clark, T. S. van der Poll, G. C. Bazan, R. H. Friend, *Science* **2014**, *343*, 512.

Collison and reaction dynamics of cold molecular few-body systems

Roland Wester

Institute for Ion Physics and Applied Physics, University of Innsbruck, Austria

In this lecture I will discuss the dynamics of inelastic and reactive collisions of polyatomic molecules and molecular ions. At first, the different long-range interactions and their influence on semi-classical and quantum mechanical scattering cross sections will be discussed. Then schemes to describe the short-range interaction will be treated depending on the type and the strength of this interaction. Finally, an experimental methods to study such dynamics will be presented.

Abstracts – Postersession 1

Enhanced chiral discriminatory van der Waals interactions mediated by chiral surfaces

P. Barcellona
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Department of Chemistry, Wake Forest University, Winston-Salem, NC 27198, USA

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Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität Freiburg, Albertstr. 19, 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.

The formation of chemically bound argon via photoexcitation of Ar-I_2 van der Waals complex

A. S. Bogomolov
Institute of Chemical Kinetics and Combustion, Institutskaya Str. 3, Novosibirsk, Russia

G. A. Bogdanchikov and Baklanov
Institute of Chemical Kinetics and Combustion, Institutskaya Str. 3, Novosibirsk, Russia
Novosibirsk State University, Pirogova Str. 2, Novosibirsk, Russia

S.A. Kochubei
Institute of Semiconductor Physics, ac. Lavrent'yev Ave., 13, Novosibirsk, Russia

Van der Waals complex Ar-I_2 is a benchmarking model for a study of the influence of weakly bound environment on molecular photochemistry and photophysics. Previous studies with this complex were focused mainly on the processes with I_2 molecule excited in the lowest excited electronic states. In the current work mechanism of photodissociation of Ar-I_2 complex has been studied with excitation of high-lying Rydberg states (E≈9.2 eV) of I_2 molecule via two-photon ($h\nu$≈4.6 eV) process. Photodissociation of free I_2 with this level of excitation has been studied earlier with the use of velocity map imaging technique [1]. Channels of dissociation of this highly excited I_2 via ion-pair state giving rise to pair I^++I^- as well as via lower lying Rydberg states giving rise to all energetically accessible Rydberg states of I atom have been detected. In the present work influence of Ar on these processes in van der Waals complex Ar-I_2 has been investigated. Complex Ar-I_2 has been generated in supersonic molecular beam. Besides channels observed earlier for free I_2 the new complex-specific channels have been detected which give rise to Ar^+ and ArI^+ ions. The four-photon ionization of Ar (IP=15.7 eV) is negligible in our nanosecond experiments. Image of velocity map of Ar^+ ions shown in Figure 1 indicates formation of molecular precursor containing chemically bound Ar. Mechanism of photodissociation of highly excited complex Ar-I_2 is suggested.

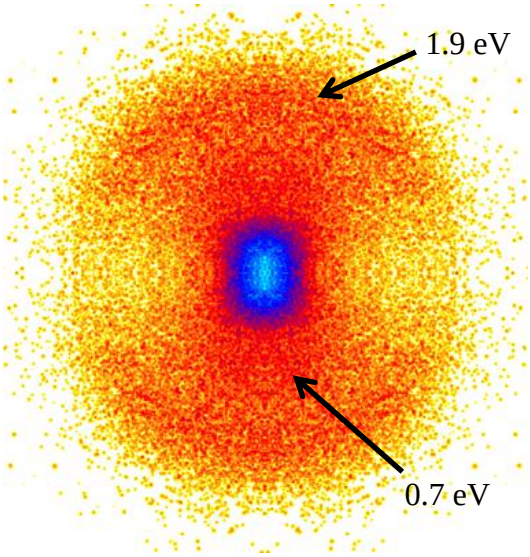


Figure 1. Velocity map image of Ar^+ ions.

This work has been supported by Russian Foundation for Basic Research (grants 16-33-00303 and 16-53-12025).

[1] A.S. Bogomolov, B. Gruener, S.A. Kochubei, M. Mudrich, A.V. Baklanov, *J. Chem. Phys.* **140**, 124311 (2014).

Tunable dual Ti:Sapphire laser system

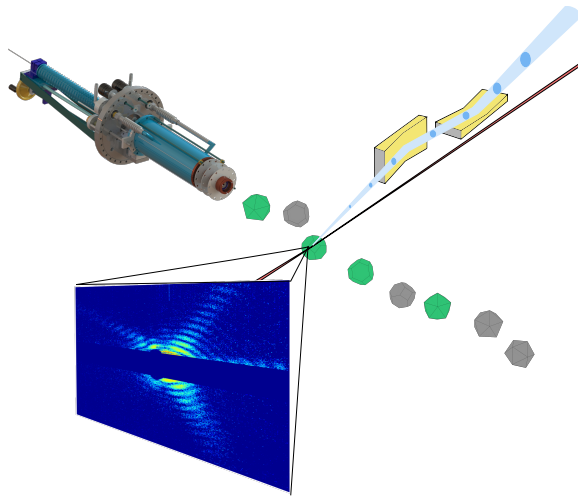
Gene Polovy, Kahan Dare, William Gunton, Kirk W. Madison
Department of Physics, University of British Columbia, 6224 Agricultural Road, Vancouver, BC, Canada

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

We present a tunable dual Ti:Sapphire laser system with a sub-Hertz two-photon linewidth. Both lasers are phase locked to the same fiber-based frequency comb. To achieve a sub-Hertz linewidth we first pre-stabilize the Ti:Sapphire lasers by stabilizing the cavity lengths with piezo-electric elements. This provides a 150 kHz two-photon linewidth. A portion of the pre-stabilized light from each Ti:Sapphire laser is then passed through two acousto-optic modulators (AOMs) driven by ultra-low phase noise voltage controlled oscillators (VCOs). These AOMs provide fast control over the optical frequency and phase of the pre-stabilized light. This light is then compared with the frequency comb and feedback signals are derived and used to make fast corrections to the pre-stabilized light yielding a two-photon linewidth below 1 Hz. By sending a replica of the frequency correction signal from the optical phase-locked-loops to an independent copy of the system, we are also able simultaneously apply intensity modulation to both lasers without compromising the 2-photon linewidths.

Poster: 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].

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 present the current progress of an improved variant of a gas-aggregation source of Haberland sputter source type[2].

References

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From Casimir-Polder Force to Dicke Physics: Interaction between Atoms and a Topological Insulator

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We apply the theory of macroscopic quantum electrodynamics in dispersing and absorbing media to study the Casimir-Polder force between an atom and a topological insulator [1]. The electromagnetic response of a topological insulator surface leads to a mixing of electric and magnetic fields, breaking the time-reversal symmetry [2, 3]. The coupling of these fields to an atom causes shifts of the atom's eigenenergies and modified decay rates near the surface of the topological insulator.
Energy shifts and modified decay rates cannot only be triggered by the presence of a material, but can be caused by other atoms in close proximity as well. The collective dynamics of atoms (Dicke Physics) leads to a superradiant burst [4]. Combining macroscopic QED and Dicke physics opens the door to the investigation of cooperative atom-surface interactions.

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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, which is a phenomenon that occurs in this field of work. In the process of singlet fission, a single singlet excitation is split among two molecules and dissociates into two triplet excitations.
In the experiment only the singlet excitation and an additional, non radiating decay can be observed. With DFT it is possible to estimate the possibility of triplet fission on an energetic basis. Also the triplet states are feasible and characterizations of this triplet states are executed. By doing so, possibilities are given to experimentally 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.

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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.

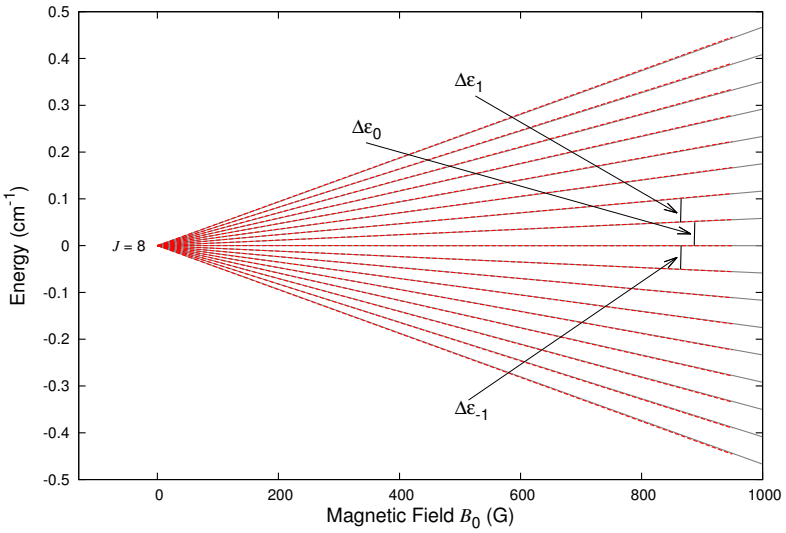

Figure 1: Zeeman levels of a Dy(^5I) atom in the lowest-energy spin-orbit state characterized by $J = 8$. The solid lines – Zeeman levels in a magnetic field $\mathbf{B} = B_0\hat{z}$; the dashed lines – Zeeman levels in a magnetic field $\mathbf{B} = B_0\,(0.1\hat{x} + \hat{z})$.

Imaging excited state dynamics of doped helium nanodroplets in real time

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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.

Design and experimental test of compact and robust magneto-optical trap (MOT) source

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The MOT is the first step of many ultracold atom experiments for its collecting and cooling atoms under room temperature to lower than 1 mK. Those atoms can be further cooled to BEC with evaporative cooling techniques. To achieve cold atoms with long lifetimes, the common practice taken is to collect atoms in a high vacuum chamber and transport them to an ultra-high vacuum (UHV) chamber. A 'MOT source' is a MOT in a chamber that produces a flux of atoms that can be directed to a neighbouring chamber. We are proposing and testing a brand new design of MOT source so that the MOT source can be compact and robust, which also enable us to control the flux of the MOT source.

Abstracts – Postersession 2

Probing neutral-molecular ion potential via penning ionization

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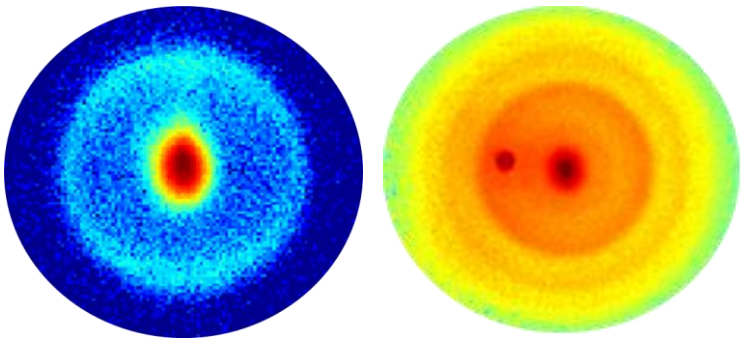
Low energy collisions are dominated by quantum phenomena such as resonances which may change the dynamics dramatically. The sensitivity of quantum effects to the potential details can be exploited to probe the potential with high accuracy. This has been shown in the neutral-neutral case where cold scattering has been recently achieved using our merged beams setup. Colliding ions and neutrals at low energies is challenging experimentally, and several promising techniques utilizing trapped ions are widespread.

Here we introduce our new experimental approach for studying ion-neutral interactions via penning ionization. Since penning ionization occurs at relatively large distance, the dynamics of the outgoing channel is determined by the ionic potential. At low collision energy in the entrance channel only a few partial waves participate, making quantum effects easier to resolve. We use Velocity Map Imaging (VMI) to probe the ionic products' velocity distribution. At low collision energies in some species we witness discrete spaced rings that correspond to velocities that are much higher than the electron recoil and are independent of the initial collision energy. In He(3S)-Ar penning ionization the appearance of such rings might be explained as Feshbach resonances due to the existence of excited spin-orbit states. In penning ionization of He(3S)-H_2 we witness similar discrete bands in the kinetic energy spectrum of H_2^+. We speculate according to the energies of the rings that they originate from resonances with higher vibrational excited states of H_2^+. An isotope effect with different ring energies is observed in reactions with HD and D_2. Our technique is general for every metastable noble gas and neutral molecule. We believe it will open a new way of examining cold ion-neutral interactions.



Ar^+ (left) and H_2^+ (right) hitting the VMI phosphorus plate.
Both ions are products of He(3S) + neutral penning ionization.

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

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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.

Traveling wave Zeeman deceleration of molecules

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In recent years, significant efforts have been invested to develop methods for the production of samples of atoms and molecules at cold ($< 1K$) and ultra-cold temperatures ($< 1mK$). Due to the lack of closed cycling transitions suitable for laser cooling of molecules, different methods have been developed to cool molecules based on the interactions with electric, magnetic and radiation fields. Two methods have been proven to be especially effective in achieving cold samples of atoms and molecules starting from a supersonic beam, namely Stark deceleration and Zeeman deceleration [3]. The developments in achieving samples of molecules at very low temperatures have been motivated by the prospect of studying atomic collisions and chemical reaction with controllable collision energies, performing high resolution spectroscopy and precision measurements for fundamental physics, quantum information processing and quantum simulation [1]. Methods based on deceleration of supersonic molecular beams are particularly well suited for collision experiments since final longitudinal velocity of the sample can be tuned over a wide range with narrow velocity spread in all three directions.

The Zeeman deceleration method relies on the state-dependent interaction of neutral paramagnetic atoms or molecules with a time-dependent inhomogeneous magnetic field. For this reason the Zeeman deceleration technique is especially effective for open-shell systems such as molecular radicals or metastable atoms and molecules.

1 Traveling wave magnetic trap

The decelerator under construction in our laboratory is based on a helical wire geometry as an extension of the setup of Trimeche et al [2]. It produces a traveling wave of magnetic field with tunable longitudinal velocity. Atoms and molecules possessing magnetic dipole moment in so-called low-field-seeking (LFS) states are trapped around the node of the propagating magnetic wave provided that the initial longitudinal velocity of the traveling trap matches the velocity of the molecular beam package. In addition, three-dimensional confinement is achieved by rotating the trap transversely. The time-varying inhomogeneous magnetic fields are produced by coils in a helical wire geometry, as shown in figure 1. They consist of 16 wires of right-handed orientation which produces static magnetic field $\mathbf{B}_i^{Right}$ $(i = 0, ..., 15)$ and 16 wires of left-hand orientation which produces static magnetic field $\mathbf{B}_i^{Left}$ $(i = 0, ..., 15)$ for an applied constant current through the wires. By introducing explicit time dependence of the current, one readily obtains a moving 1D trap along beam direction as show in fig 2. The requirement of a sinusoidal time dependence of the current involves two independently controllable parameters ϕ_z and ϕ_θ, such that the total magnetic field produced by the helix geometry at a given time reads:

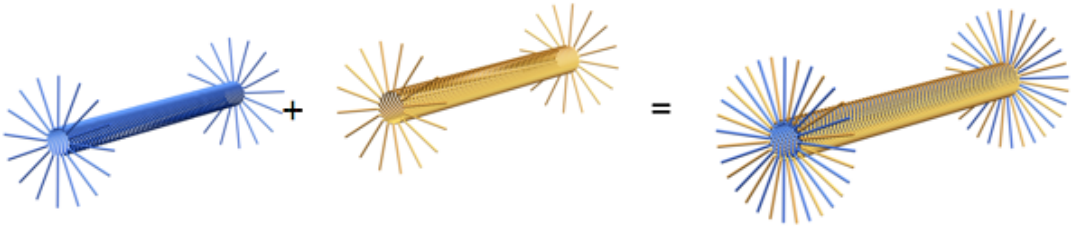

Figure 1: Helical wire geometry consists of 16 wires of right-handed orientation and 16 wires of left-handed orientation.

$$\mathbf{B}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{t})_{total}^{Right} = \sum_{i=0}^{15} cos(i\pi/8 + \phi_z(t) + \phi_\theta(t))\mathbf{B}(\mathbf{x},\mathbf{y},\mathbf{z})_i^{Right}$$

,

$$\mathbf{B}(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{t})_{total}^{Left} = \sum_{i=0}^{15} cos(i\pi/8 + \phi_z(t) - \phi_\theta(t))\mathbf{B}(\mathbf{x},\mathbf{y},\mathbf{z})_i^{Left}$$

.

Initially, the longitudinal velocity of the moving trap matches the beam velocity. The longitudinal velocity of the trap is then linearly reduced, corresponding to a constant deceleration of the magnetic trap in the laboratory frame, such that molecules that are initially trapped in the traveling trap will be decelerated. In conventional Zeeman decelerators the transverse focusing force is usually small and thus transverse motion of molecules significantly reduces phase-space acceptance of the decelerator [4]. Our traveling trap has good confinement over all transverse directions as shown in figure 3 and figure 4, while having the longitudinal and transverse motion of molecules inside the trap decoupled from each other.

Moreover using a non-cylindrical symmetry allows us to produce a local minimum of the magnetic field strength on the molecular beam axis with a tunable non-zero offset field, thereby efficiently preventing Majorana (spin flip) transitions in the moving trap.

2 Driving electronics

Traveling wave Zeeman deceleration of paramagnetic atoms and molecules requires time-dependent gradients in magnetic fields on the order of one Tesla over distances of a few millimeters. For this purpose, a high-power arbitrary waveform current generator was developed at the laboratoire Aime Cotton in Orsay, France. The generator produces bipolar currents of more than 300 A amplitude, with frequencies ranging from DC to 40 kHz. The generator is based on a full H-bridge with parallelized IGBT switches controlled by microchips to deliver arbitrary waveform bipolar currents.

3 Outlook

OH radicals in $X^2\Pi_{3/2}$ state will be the first candidate molecule suitable for Zeeman deceleration in our experiment and we already have developed methods of production of

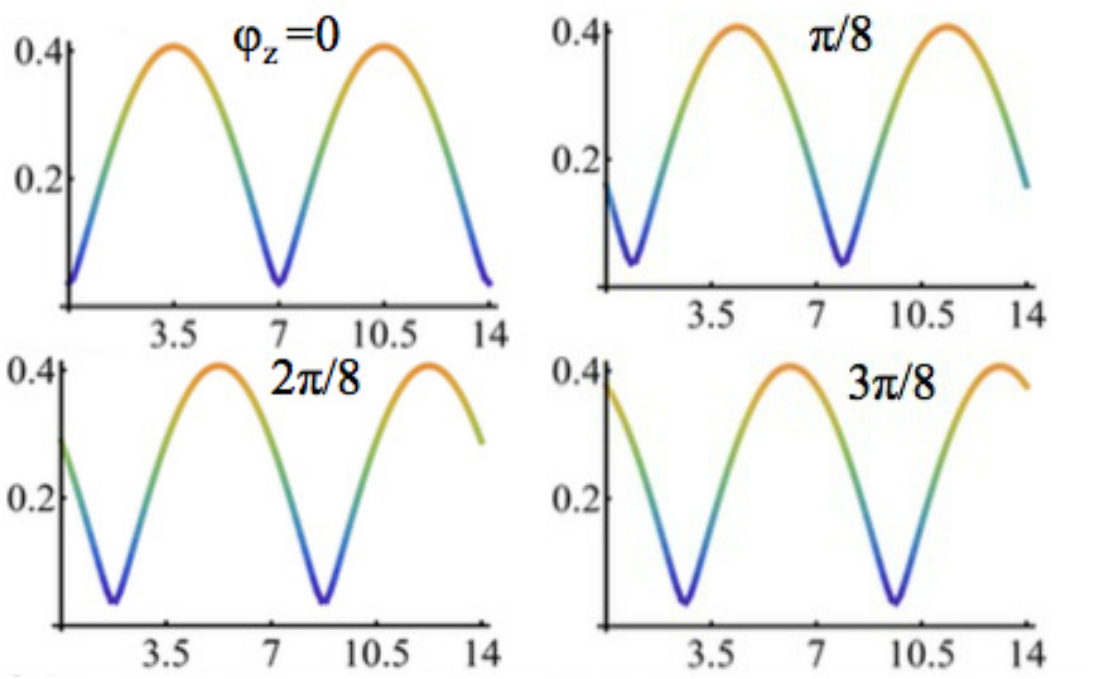

Figure 2: Magnetic field profile for different values of time dependent parameter ϕ_z. Minimum of the magnetic field propagates in positive z direction with increasing parameter ϕ_z.

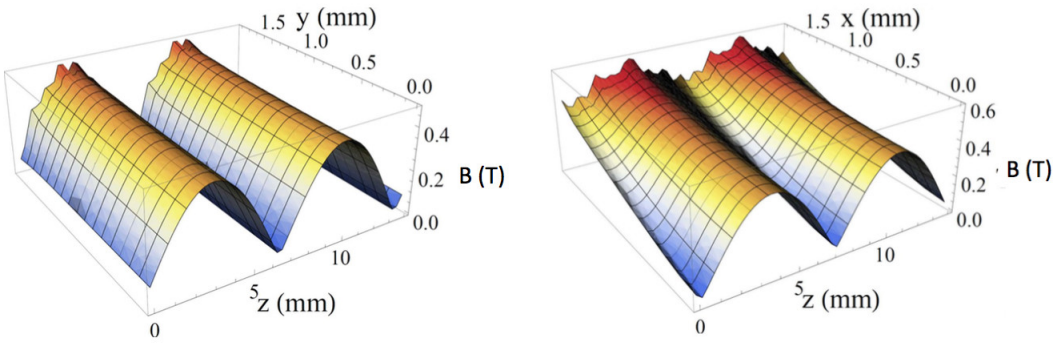

Figure 3: Magnetic field strength profiles for $\phi_\theta = 0$

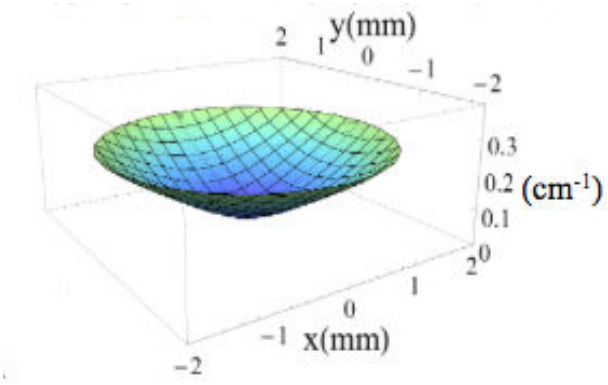

Figure 4: Time-averaged transverse magnetic potential experienced by OH molecules

OH molecular beam source in a specific quantum state, with characterized beam parameters. Our goal is to produce molecular beams with high particle density at any desired longitudinal velocity below initial velocity of the beam for scattering, spectroscopic and coherent experiments. In future, many molecular species could be addressed with a Zeeman decelerator, such as H_2 in $c^3\Pi_u$ state, O_2, NO, NH, CrH and so on. Based on the real trap nature of the decelerator, and effective suppressing of the Majorana transitions, this Zeeman decelerator will avoid losses of molecules at all velocities and will be ideally suited for coupling with a static trap.

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Modelling of the Femtosecond Intramolecular Dynamics in the High-Lying Electronic States of Molecular Iodine

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Molecular iodine I_2 is a benchmarking molecule for the studies of the photophysics of molecular Rydberg and ion-pair (IP) states. Recently a progress in the experimental study of intramolecular dynamics in high-lying electronic states of I_2 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 propagation of wavepackets in the excited Rydberg and the ion-pair states of I_2. In a pumping step, I_2 molecules were excited by UV radiation in a two-photon process in the Rydberg states. Probing radiation provided electron photodetachment from the wavepacket in the excited state giving rise to a pair $I + I^+$. Measured Total Kinetic Energy Release (TKER) for observed photodissociation channels corresponds to the kinetic energy of intramolecular motion in the excited 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.

The important role of the ion-pair states in the predissociation dynamics of excited I_2 has been established. The interpretation of experimentally measured data has been provided with the use of the results of intramolecular dynamics simulation in the IP states within classical approach. In the current work the results of the dynamics simulation within the classical and quantum approaches are presented and compared. Within the classical approach the Newton laws of motion were used for the calculation of reduced mass motion in the ion-pair states. Within the quantum approach the exponential split operator method [2] has been used for a numerical solution of time dependent Schrödinger equation for wavepackets. Wolfram Mathematica program has been used to perform all calculations. The comparison of the experimental data with the results of the modelling allows us to make conclusions on the features of the intramolecular dynamics in the excited states of I_2.

Financial support for this work by the Deutsche Forschungsgemeinschaft (Grant Nos. MU 2347/9-2 and IRTG 2079) and by the Russian Foundation for Basic Research (Grant Nos. 16-53-12025 and 15-03-03204) is gratefully acknowledged.

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Stretching and bending dynamics in triatomic ultralong-range Rydberg molecules

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Diatomic ultralong-range Rydberg molecules (ULRM) consist of a Rydberg atom whose valence electron binds a polarizable ground state atom by low-energy scattering [1, 2]. The underlying binding mechanism and the resulting physical properties differ from those of typical covalent molecules. For instance ULRM possess oscillatory potential surfaces (PES) supporting several equilibrium configurations with huge bond lengths of thousands of Bohr radii a_0.

An interesting generalization are polyatomic ULRM consisting of not only one but several ground state atoms. Here we will present our recent theoretical studies on triatomic ULRM (cf. Fig. 1) in electronic low angular momentum states [3]. A typical

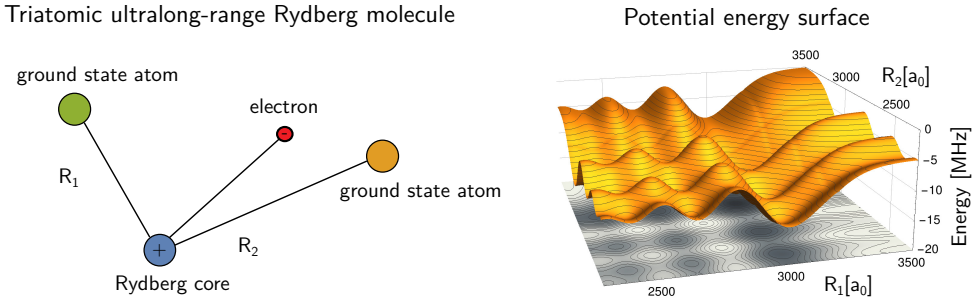

Figure 1: Sketch (l.h.s.) and PES (r.h.s.) of a triatomic ULRM in an electronic $l = 0$ state.

resulting PES is depicted in Fig. 1. Calculating these surfaces for polyatomic ULRM is computationally demanding and we demonstrate how the finite basis set representation of the unperturbed Rydberg electron Green's function can be employed to reduce numerical efforts. The remaining vibrational problem is solved by separating the vibrational bending and stretching dynamics adiabatically. This procedure yields information on the radial and angular arrangement of the nuclei and indicates that angular dependent kinetic couplings between radial vibrations induce a linear structure in the triatomic ULRM.

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

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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 in heterocyclic benzene molecules 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. Using time-dependent DFT might indicates changes in electronic distribution of molecular excited states, however for a precise study of energetics a powerful theory is needed to be able to describe electrons not only in their excited states but also in continuum. To accomplish our aim we consider Constrained DFT[1] to discover the CT states in n-benzene rings molecules.

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Cold Penning-Reactions using a Li-MOT

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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.

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Experimental studies of the ion-molecule reactions $H_2^+ + H_2$ and $H_2^+ + D_2$ at low collision energies with a merged beam apparatus

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Experimental studies of ion-molecule reactions at very low temperatures are essential for the understanding of the chemical processes in interstellar clouds. The temperatures in these clouds range from 10 K to 50 K, corresponding to energies below 5 meV. So far, such low collision energies for ion-molecule reactions could not be obtained in the laboratory because of the inevitable heating of ions by space-charge effects and stray electric fields. These effects can be avoided by studying reactions involving molecules in nonpenetrating high-n, high-l Rydberg states instead of electrically charged ions. As demonstrated experimentally, the high-n Rydberg electron does not influence the ion-molecule reaction occuring within its extended orbit [1], but effectively shields the reaction against external fields.

We have implemented this approach in a merged beam experiment. Two neutral-gas beams are generated by pulsed supersonic expansion. The two beams initially propagate in directions seperated by an angle of 10°. Merging of the two beams is archieved by photoexcitation of the molecules of one beam to high-n Rydberg-Stark states followed by trapping and deflection in the inhomogeneous field of a curved chip-based surface decelerator [2]. Reactions between the positively charged ion cores of the Rydberg molecules in the deflected beam and the neutral molecules in the other beam take place in an about 3 cm-long flight region. Ionic reaction products are detected in a time-of-flight mass spectrometer. The average collision energy can be controlled by de- or ac-celeration of the Rydberg molecules or by changing the temperature of the pulsed valve used to generate the neutral-reactant beam. High energy resolution is achieved by exploiting the spatial dispersion of velocity components in the neutral-reactant beam resulting from the very short opening times of a home-built valve as was already sucessfully exploited in neutral-neutral reactions [3].

The performance of this approach to study ion molecule reactions is demonstrated using the exothermic barrierless reaction $H_2^+(v^+ = 0, N^+ = 0) + H_2(v = 0, N = 0, 1) \rightarrow H_3^+ + H$. This reaction is the initial step of the reaction cycles forming many molecules in the interstellar medium [4]. Collision energies as low as $E/k_\mathrm{b} = 100\,\mathrm{mK}$ could be reached. In this range, the observed reaction cross sections hardly deviate from classical Langevin capture model cross sections, in accord with theoretical predictions [5], [6]. The reaction $H_2^+ + D_2$ provides the possibility to distinguish between charge transfer, D atom transfer, and H^+ ion transfer, and first results in this reaction system will be presented.

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Superradiance, singlet fission and triplet annihilation processes of organic molecules attached to neon clusters

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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.
The collective emission of coherent light is a fundamental process in quantum mechanics. The resulting radiation leads to effects such as lasing, self-amplified spontaneous emission in free electron lasers, and super fluorescence or superradiance. One particular fascinating manifestation of superradiance is the process of spontaneous coherent emission of light by an ensemble of identical excited atoms which was initially predicted by Dicke [1] and later experimentally confirmed [2]. Superradiance has been observed almost universally in weakly interacting systems such as hot dense gases [2], films [3] and Bose-Einstein-Condensates [4]. Here, we report the experimental observation of fluorescence lifetime reduction of tetracene, pentacene and anthracene by directly tuning the number of cooperating molecules confined 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 singlet fission 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.

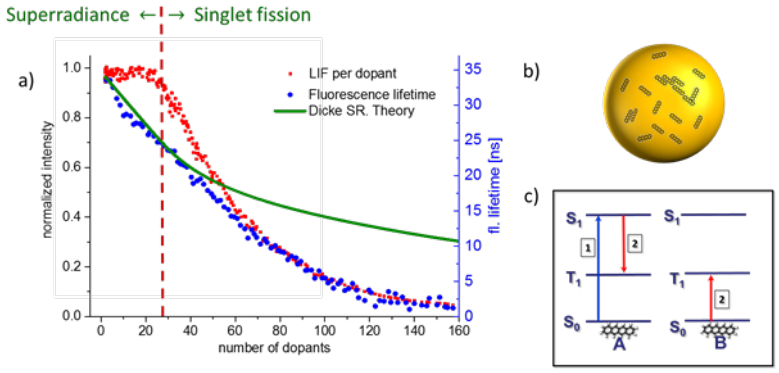

Fig: a) lifetime reduction in an ensemble of pentacene molecules attached to large neon cluster. b) illustration of the doped clusters. c) depicts the process of singlet fission.

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Three-body interactions of slow light Rydberg polaritons

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Rydberg polaritons have recently emerged as a new promising platform for studying quantum nonlinear optics and strongly correlated few-body physics[1,2]. Photons in an atomic medium can be tuned near the conditions of electromagnetically induced transparency with a large contribution of the Rydberg state. Effective interactions between polaritons arise then from strong interactions between Rydberg states. We show that in systems consisting of more than two photons, effective many-body interactions appear in addition to two-body ones[3]. We focus on three-body systems in one-dimensional geometry and analyze how the three-body bound state is modified by these interactions and how the correlation functions of outgoing photons can be used to detect them.

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Mass and Photoelectron Spectroscopy of Organic Molecules

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The mass and photoelectron spectrum of the molecules of Tetracene and Pentacene [1] were measured. Pt atom was used for doing the PES calibration. From the results obtained from the photoelectron spectroscopy, the energy levels of the studied organic molecules can be predicted. The PE spectrometer was a magnetic bottle one [2] and the mass spectrometer was a time-of-flight spectrometer [3].

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Two-dimensional (2D) Hydrogen in a Tilted Magnetic Field

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The numerical algorithm for investigation of the energy spectrum and corresponding wave functions of a two-body system with the anisotropic interaction potential is developed.

We study the model of 2D hydrogen atom in the arbitrarily oriented magnetic field. We have obtained good agreement of the numerical results of the energy spectrum, dipole moments and mean radius with known analytical ones for the 2D hydrogen model [1]. We reproduce the results for the 2D hydrogen in the magnetic field applied perpendicular to the plane of the motion, which were obtained recently by A. Soylu et.al. [1] and by A.V. Turbiner et.al. [2]. In contrast to variational methods used in [2] the convergence of our computational scheme is the same for the magnetic field of an arbitrary strength, which allowed refining results of work [2] for strong fields.

To the authors' knowledge the 2D hydrogen atom in the magnetic field $\vec{B} = \gamma\cos(\alpha)\vec{i} + \gamma\sin(\alpha)\vec{k}$, tilted to the plane of motion, has not been studied yet. The calculated ground state energy dependence on the magnetic field tilt angle α and field strength $\gamma = \left|\vec{B}\right|$, presented in Fig. 1, demonstrates the possibility to control the energy levels by the orientation of the magnetic field.

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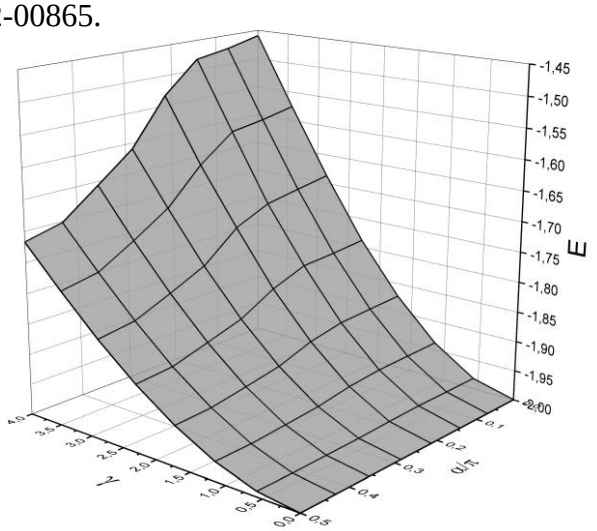

Fig. 1 The 2D hydrogen ground state energy as a function of the magnetic field tilt angle α and the magnetic field strength γ. All quantities are in atomic units.

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Stark Effect in Two-dimensional Hydrogen: a numerical approach

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A computational scheme for the study of the two-dimensional (2D) hydrogen in the AC and DC electric field of an arbitrary strength: resonant state position and width determination – is presented.

The Crank–Nicolson scheme and the split-operator method modification, described in [1,2], converting the 2D time-dependent Schrödinger equation into an iterative process, were applied for the time evolution operator integration. On each iteration, following the method suggested in [3], the 2D partial-differential equation is expanded to the system of differential-difference equations, which is solved with the high-order seven-point finite difference approximation and matrix modification of the sweep method. Due to the anisotropy of the electron-field interaction, the conventional methods of the wave function expansion on the basis set of functions are not efficient.

We have obtained good agreement of the numerical results of the energy spectrum, dipole moments and mean radius with known analytical ones for the 2D hydrogen model [4]. The perfect agreement with the perturbation theory ground state energy shift for the weak DC electric field [4,5] is demonstrated.

The advantages of the scheme are discussed. The diagonal structure of the potential matrix releases from the calculation of potential matrix elements saving computational efforts. The more efficient split-operator technique employment instead of the Crank–Nicolson method greatly reduces the computational time from hours to minutes at the same accuracy of the results.

This work was supported by the Russian Foundation for Basic Research, Grant No. 16-32-00865.

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MW trap for polar molecules: Summer school 2016

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We are interested in the development of a Microwave trap for polar molecules. In contrast to static magnetic or electric field traps, MW trap can trap high field seeking ground rotational states. These are completely immune to inelastic collisions with ultra-cold atoms. Successful development of this technique would lead to more efficient sympathetic cooling of molecules to reach micro-Kelvin regime. A superconducting fabry-perot cavity whose quality factor exceeds 10^6 would be used as a trap. Trap depth of ~500 mK can be generated for NH_3 molecules with such a set up. Conventional decelerators such as Stark or Zeeman can be used to load molecules inside the trap.

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Cold ion-molecule collisions in a cryogenic hybrid trap

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In recent years, collisions of cold atoms with atomic and molecular ions have been studied intensively. The development of "hybrid traps" which allow for the simultaneous trapping of cold neutral atoms and ions have paved the way for gaining insights into the nature of ion-atom collisional processes at very low temperatures [1].

We are currently developing a cryogenic trap for the simultaneous confinement of cold neutral molecules and cold molecular ions. Translationally cold neutral molecules are produced by Stark deceleration and loaded into a magnetic trap [2]. The magnetic trap's center can be mechanically displaced and superimposed with the center of an RF ion trap. The interaction of room temperature black body radiation (BBR) results in rotational excitation of the OH leading to trap loss after few seconds. To alleviate this effect, the hybrid trap is cooled down to 7 K to be shielded from room temperature BBR, which is increases the lifetime of the trapped molecules by several orders of magnitude, commensurate with the trap lifetime of the ions.

This new setup will allow for the first time studies of ion-molecule collisions in the millikelvin regime. We will present a detailed characterization of the experiment and first results on cold ion-molecule collisions.

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Abstracts – Postersession 3

Highly flexible supersonic expansion valve for the production of various Clusters/Nanodroplets and different doping perspectives

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Due to its superfluidity, subkelvin temperature, and extremely weak interaction, helium nanodroplets are a unique type of cluster ideal for embedding a wide variety of atoms, molecules, and clusters. In particular, pulsed nozzles offer many advantages over continuous beams such as higher droplet densities and reduced gas load. We use a home-built (in cooperation with CRUCS Center at UBC, Vancouver) pulsed nozzle, that produces gas pulses down to 20 µs duration at repetition rates up to several hundred Hz. Investigations of power consumption and other properties are presented. A rich variety of applications, that include also production of Water- and Heavy-Water-Clusters, is discussed as well as the characterization of the influence of multiple source parameters on the cluster size distribution.

Additionally, we have recently introduced a new method for doping clusters by laser ablation [1]. Overall, laser ablation allows one to dope droplets with new material such as for high refractory metals [2], carbon nanotubes [3] or large biomolecules that easily fragment with other techniques. Here, we present the results from characterization of the laser ablation setup. In particular, it was shown that pulsed nozzle produce beams of both doped and seeded laser ablated material.

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Detection of multiple-quantum coherences in dilute samples

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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.

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Title: Quantum Friction and Markovianity

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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.

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Single particle dynamics in an ultracold environment: From superfluidity to finite site reheating

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We study the quantum dynamics of a single trapped ion which is in contact with a Bose-Einstein condensate. The ultracold environment acts as a refrigerator, and thus, the influence on the motion of the ion is dissipative. For a theoretical description of the damped quantum dynamics, simple phenomenological master equation approaches are widely used. But instead of calculating the particle dynamics itself, our focus lies on a more detailed description of the environment and the particle-environment interaction. Rather than using a simple damping rate, we aim to describe the effective dynamics of the damped particle using the full bath correlation function. In this way we gain a more thorough theoretical understanding of properties of quantum matter, such as superfluidity, when acting as an environment.
We find that we can divide the dynamical effect of the BEC on the ion into two parts: The initial energy loss and the return of energy to the ion dynamics.
By considering just the initial decay we effectively study an ion coupled to an infinitely large environment and are able to identify a Landau Criterion for a quantum particle in a harmonic trap. On the other hand we see that the finite size of the condensate causes a return of energy, which results in a periodically reheating of the ion. Interestingly the system can be tuned such that this effect can lead to an additional cooling mechanism.

High accuracy simulations of Ultracold atom-atom scattering using R-matrix methodology: Summer school 2016

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New developments in experimental methods have allowed for the routine production of ultracold (sub-Kelvin) atoms and molecules. This has facilitated the study of chemical reactions involving only a small number of partial waves, allowing for unprecedented control over diatomic systems and ultracold chemical reactions. A new computational formalism based on the R-matrix method is presented to simulate atom-atom scattering in this energy regime[1]. The formalism is particularly appropriate for slow collisions occurring on potential energy surfaces with deep wells. Our method utilises software built for high-accuracy diatomic spectra to provide molecular eigenenergies and wavefunctions of the bound system at short internuclear distances (known as the inner region), all independent of scattering energy. The scattering energy is then introduced at the construction and propagation of the R-matrix, meaning a large number of scattering energies can be assessed rapidly with one inner region molecular calculation. This is useful for constructing high-resolution plots of eigenphases and cross-sections as a function of scattering energy, allowing for better analysis of resonance behaviour, which can be useful for controlling ultracold reactions. Our intention is to extend this methodology to atom-diatom scattering and other polyatomic reactions.

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TBA

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Long-lived all-optical ion trapping

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We have demonstrated optical trapping of Barium ions without residual RF-confinement for durations of up to 3s. These results were obtained using a far-detuned single-beam 1064nm optical trap focused to a beam waist of 5m. Compared to our results obtained with Magnesium ions in a near-resonance trap [1] and, more recently, Barium ions in a far-detuned 532nm trap [2], we achieve an improvement in the lifetime of three orders of magnitude.

Since the trapping probability approaches unity for trapping durations of 100ms, our results establish optical ion trapping as a robust tool for the manipulation of cold trapped ions. In atom-ion interaction experiments [3], for example, sympathetic cooling within milliseconds should allow for investigating ultracold interaction and chemistry without micromotion-induced heating effects [4]. We will discuss other possible heating mechanisms for the ion, such as electric-field noise on the DC electrodes or laser beam intensity and pointing fluctuations.

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Analytic Gradient at the 4-component Relativistic Coupled Cluster Level with Inclusion of Spin-Orbit Coupling

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I will present a formulation and implementation of the calculation of (orbital-unrelaxed) expectation values at the 4-component relativistic coupled cluster (CC) level with spin-orbit coupling included from the start. The Lagrangian-based analytical energy derivative technique constitutes the basic theoretical framework of this work. The key algorithms for single reference relativistic coupled cluster have been implemented by allowing for general tensor contractions of up to rank-2 tensors in which the Direct Product Decomposition scheme is employed to benefit from double group symmetry. As a sample application we study the electric field gradient at the bismuth nucleus in the BiX (X=N, P) series of molecules, where the effect of spin-orbit coupling is substantial. Our results clearly indicate that the current reference value for the nuclear quadrupole moment of ^{209}Bi needs revision. We also have applied our method to the calculation of the parity violating energy shift of chiral molecules. The latter property is strictly zero in the absence of spin-orbit coupling.

Description of ultracold collision between dipole and ion

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The generation of hybrid quantum systems of ultracold atomic gases combined with ions opened the possibilities to study new quantum effects. The ability to control the state of ions in traps together with the vast manipulation of trapped atomic clouds put these systems in a special position of studying quantum matter.

The next level of complexity is reached in the systems composed of ultracold samples of polar molecules combined with trapped ions. The recent progress in trapping ultracold molecules paves the way toward the generation of these controlled hybrid systems.

In our work, we focused on the description of the collision process between an ion and a dipole. The long range part of the anisotropic interaction between the particles is given by

$$V(r) = -\frac{qd\cos\theta}{4\pi\epsilon_0 r^2}, \tag{1}$$

where q is the charge of the ion, and d is the electric dipole moment. As the potential falls off with the second power of the distance, which is the same as for the case of the centrifugal barrier, the concept of partial waves looses its usefulness. Therefore, we introduced modified spherical harmonics, which replace the standard spherical harmonics, and that take the angular anisotropy into account. They are given by the eigenproblem of the operator:

$$\hat{U} = \hat{l}^2 - \alpha\cos\theta, \tag{2}$$

where $\hat{l}^2$ is the square of the angular momentum operator, and $\alpha = 2mqd/(4\pi\epsilon_0\hbar^2)$. We solved that problem using numerical calculations. We showed that the low lying eigenvaues can be interpreted in terms of a 2d quantum harmonic oscillator. The large eigenvalues can be obtained with help of the quasi-classical approximation effectively. Also, we shown that the eigenvalues can be interpreted in terms of the solution of 1d Schrödinger equation in an effective potential.

We reformulated the scattering theory in terms of the modified spherical harmonics. We calculated scattering amplitude, elastic cross section and reactive rate constant. As an application, we used the Quantum Defect Theory to describe a highly reactive collision of ion and dipole in the long range potential V. We calculated the reactive rate constant, and shown that it given by the following universal formula:

$$K^{\mathrm{re}} = \frac{\hbar}{mk}F(\alpha), \tag{3}$$

where the collision energy is $\hbar^2k^2/2m$, and F is a function that for large α is given by $\pi\alpha/4$.

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.
Here we present our new experimental setup combining Ba^+ ions and Li atoms in an optical dipole trap. We discuss the advantages of this novel atom-ion combination as well as possible experiments like atom-ion Feshbach resonances. We give details about the planned experimental setup including the new ion trap.

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Notes

Sunday, July 24th	Monday, July 25th	Tuesday, July 26th	Wednesday July 27th	Thursday, July 28th	Friday, July 29th
17.30 Opening remarks **18:00** Presentation by participants: 1 Slide / 1 person/ 1 Minute **19:00** Poster Session & Aperitif **20:00** Dinner	**9:00** Mauro Antezza, Lecture 1 **10:30** Coffee break **11:00** Reworking Session 1a **12.30** Lunch **14:00** Reworking Session 1b **15:30** Coffee break **16:00** E. Narevicius, Lecture 2 **17:30** Coffee break **18:00** Elizabeth von Hauff, Applied Science Lecture **19:00** Poster Session & Aperitif **20:00** Dinner	**9:00** Reworking Session 2a **10:30** Coffee break **11:00** Reworking Session 2b **12.30** Lunch **14:00** Shaul Mukamel, Lecture 3 **15:30** Coffee break **16:00** Reworking Session 3a **17:30** Coffee break **18:00** Reworking Session 3b **19:30** Poster Session & Aperitif **20:00** Dinner	**9:00** Silke Ospelkaus, Lecture 4 **10:30** Coffee break **11:00** Reworking Session 4a **12.30** Lunch **13:30** Reworking Session 4b **15:00** Excursion - Canoe trip **20:00** Dinner	**9:00** Roland Wester, Lecture 5 **10:30** Coffee break **11:00** Reworking Session 5a **12.30** Lunch **14:00** Reworking Session 5b **15:30** Coffee break **16:00** Chris Greene, Lecture 6 **17:30** Coffee break **18:00** Frank Krüger, Career Seminar **19:00** Dinner **20:00** Winetasting	**9:00** Reworking Session 6a **10:30** Coffee break **11:00** Reworking Session 6b **12:30** Closing Remarks & Poster Prize **13.00** Lunch **14:00** Departure