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08-10 June 2022, Warsaw, Poland

Ion–Atom 2022
Program and abstracts

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Excellence Initiative – Research University (2020-2026)

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Center for Integrated Quantum Science and Technology

European Cooperation in Science and Technology (COST)

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Michał Tomza, University of Warsaw, Poland

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Invited Speakers

Georg Bruun, Aarhus University, Denmark

Robin Côté, University of Massachusetts Boston, USA

Johannes Deiglmayr, Univeristy of Leipzig, Germany

Michael Drewsen, Aarhus University, Denmark

Olivier Dulieu, University of Paris-Sud, France

Rene Gerritsma, University of Amsterdam, The Netherlands

Rosario Gonzalez-Ferez, University of Granada, Spain

Eric Hudson, University of California LA, USA

Krzysztof Jachymski, University of Warsaw, Poland

Paul Julienne, Joint Quantum Institute, NIST and the University of Maryland, USA

Heather Lewandowski, JILA, University of Colorado Boulder, USA

Roee Ozeri, Weizmann Institute of Science, Israel

Tilman Pfau, University of Stuttgart, Germany

Sadiq Rangwala, Raman Institute, India

Peter Schmelcher, University of Hamburg, Germany

Thomas Walker, University of Freiburg, Germany

Roland Wester, University of Innsbruck, Austria

Stefan Willitsch, University of Basel, Switzerland

Hot-Topic Speakers

Jacek Gębala, University of Warsaw, Poland

Tobias Grass, ICFO, Spain

Shinsuke Haze, University of Ulm, Germany

Leon Karpa, Leibniz University Hannover, Germany

Florian Meinert, University of Stuttgart, Germany

Marjan Mirahmadi, Fritz Haber Institute of the Max Planck Society, Germany

Lorenzo Oghittu, Hamburg University, Germany

Fabio Revuelta, Universidad Politécnica de Madrid, Spain

Carlo Sias, LENS, University of Florence, Italy

Andriana Tsikritea, University of Liverpool, UK

Agata Wojciechowska, University of Warsaw, Poland

Valentina Zhelyazkova, ETH Zurich, Switzerland

08 June 2022 - Wednesday

Session A1

Chaired by Michał Tomza from University of Warsaw, Poland

08:30	**Registration**	
09:00	**Welcome**	
09:15	**Stefan Willitsch**	Hybrid experiments with complex molecules and ions
09:45	**Olivier Dulieu**	Competing non-radiative inelastic processes in hybrid Li-Ba^+ experiment
10:15	**Shinshuke Haze**	Towards creation of charged-Rydberg molecules in an atom-ion hybrid trap
10:30	**Coffee break**	

Session A2

Chaired by Michael Drewsen from Aarhus University, Denmark

11:00	**Rene Gerritsma**	Observation of collisions between Feshbach dimers and trapped ions
11:30	**Thomas Walker**	Observation of Feshbach resonances between a single barium ion and an ultracold lithium gas
12:00	**Agata Wojciechowska**	Large spin-orbit coupling as a source of Feshbach resonances in ultracold ion-atom mixtures
12:15	**Carlo Sias**	A new ion trap for atom-ion experiments
12:30	**Lunch break**	

Session A3

Chaired by Stefan Willitsch from University of Basel, Switzerland

14:00	**Heather Lewandowski**	Chemical reactions between cold, trapped ions and neutral molecules
14:30	**Roland Wester**	Interactions of trapped negative ions with ultracold atoms
15:00	**Valentina Zhelyazkova**	Ion-molecule reactions near 0 K: the Lambda - doubling-mediated enhancement of the He^+ + NO reaction rate coefficient
15:15	**Andriana Tsikritea**	Charge transfer reactions between rare gas ions and polar molecules

Session A4

Chaired by Roland Wester from University of Innsbruck, Austria

16:00	**Eric Hudson**	Quantum chemistry to quantum logic with molecular ions
16:30	**Poster session**	
18:15	**Workshop Garden Pub**	**For details please refer to page 27**

09 June 2022 - Thursday

Session B1

Chaired by Rene Gerritsma from University of Amsterdam, The Netherlands

09:00	**Georg Bruun**	Ions in atomic Fermi gases and Bose-Einstein condensates
09:30	**Michael Drewsen**	Towards experimental ultracold ion-atoms investigations in Aarhus
10:00	**Leon Karpa**	Ultracold Ion-Neutral Experiments in Composite Optical Traps
10:15	**Lorenzo Oghittu**	Quantum-limited thermometry of a Fermi gas with a charged spin particle
10:30	**Coffee break**	

Session B2

Chaired by Rosario González Férez from University of Granada, Spain

11:00	**Florian Meinert**	Quantum simulations with circular Rydberg atoms
11:15	**Johannes Deiglmayr**	Cold ion-molecule chemistry within the orbit of a Rydberg electron
11:45	**Tilman Pfau**	Observation of a molecular bond between ions and Rydberg atoms
12:15	**Group photo**	
12:30	**Lunch break**	

Session B3

Chaired by Olivier Dulieu from Paris-Sud University, France

14:00	**Roee Ozeri**	Quantum logic detection of single atom-ion collisions and the observation of trap-assisted formation of atom-ion bound states
14:30	**Discussion panel on future of ion-atom; COST meeting - WG4**	
16:00	**Old Town Sightseeing**	**For details please refer to page 27**
19:30	**Conference dinner**	**For details please refer to page 27**

10 June 2022 - Friday

Session C1

Chaired by Heather Lewandowski from JILA, University of Colorado Boulder, USA

09:00	**Peter Schmelcher**	Dynamics and Bound State Formation of Charged Impurities in Ultracold Bosonic Gases
09:30	**Krzysztof Jachymski**	Prospects for quantum many-body physics studies utilizing cold ion-atom systems
10:00	**Tobias Graß**	Three-body Interactions in Ion Chains
10:15	**Fabio Revuelta**	Numerical treatment of an atom-ion pair in spatially displaced traps
10:30	**Coffee break**	

Session C2

Chaired by Roee Ozeri from Weizmann Institute of Science, Israel

11:00	**Rosario González Férez**	Polyatomic ultralong range Rydberg molecules
11:30	**Sadiq Rangwala**	Collisions, exchange symmetry, and diffusion in ultra-cold ion-atom systems
12:00	**Marjan Mirahmadi**	The Role of Long-range Pairwise Interactions in Ion-atom-atom Three-body Recombination
12:15	**Jacek Gębala**	Universality in three-body collisions in ultracold hybrid ion-atom systems
12:30	**Lunch break**	

Session C3

Chaired by Johannes Hecker Denschlag from Ulm University, Germany

14:00	**Paul Julienne**	Molecular product distributions from three-body recombination of ultracold atoms
14:30	**Robin Côté**	Signature of the s-wave scattering due to locking and unlocking of phase shifts in resonant-exchange processes

Poster Session – list of accepted contributions

P1	**Maks Walewski**	Quantum interference effects in cold Rb–Sr^+ collisions high above the ultracold regime
P2	**Jacek Dobrzyniecki**	Quantum simulation of the central spin model with a Rydberg atom and polar molecules in optical tweezers
P3	**Hela Ladjimi**	Interactions of alkaline-earth ions in ground and excited states with H_2 and CO molecules: implications for collision induced decoherence and losses
P4	**João P. Mendonça**	Quantum simulation with ultracold atoms in a topological Rydberg lattice
P5	**Ubaldo Cavazos Olivas**	Compound atomic systems: ionic Bose polaron dynamics
P6	**Marcin Gronowski**	Ultracold interactions of alkali-metal and alkaline-earth-metal ions with spin-polarized metastable helium atoms
P7	**Piotr Kulik**	Feshbach resonances in ultracold atom--ion collisions
P8	**Antonio Negretti**	Dynamics of a trapped ion in a quantum gas: effects of particle statistics
P9	**Fernanda B. V. Martins**	Cold ion chemistry between the He^+ ion and small molecules with a quadrupole moment
P10	**Hamid Berriche**	Electronic structure and prospects for the formation of ionic-molecular alkali-metal-barium: $BaAlk^+$ (Alk=Li, Na, K, Rb, Cs and Fr)
P11	**Markus Deiß**	Using a hybrid atom-ion setup as a flexible platform for cold chemistry experiments
P12	**Adam Linek**	Distortion of the mercury 1S0-3P0 clock line in two-species atomic clock
P13	**Jan Franz**	Generation of symmetry adapted spherical harmonics for molecular collision processes
P14	**Piotr Gniewek**	Interactions of alkaline earth metal ions with diatomic molecules
P15	**Štěpán Roučka**	Isotope exchange equilibrium in the $OH^- + HD <-> OD^- + H_2$ reaction at low temperatures
P16	**Daniel Bosworth**	State transfer protocols using a dragged impurity
P17	**Mateusz Bocheński**	Compact laser system for experiments with isotopic mixtures of ultracold potassium
P18	**Jakub Dobosz**	Towards Non-destructive Heterodyne Atom Number Measurement In An Ultracold Cesium And Potassium Mixture
P19	**Koray Dinçer**	Observations of missing lowest levels of the 0-g purely-long-range state of Cs_2

Ion-Atom 2022 – Talk Abstracts

Hybrid experiments with complex molecules and ions

Stefan Willitsch
Presented by Stefan Willitsch (Department of Chemistry, University of Basel, Switzerland)

Hybrid experiments combining trapped ions with neutrals have recently found widespread applications in both physics and chemistry. One of the frontiers of the field is the advancement to ever more complex, in particular molecular, systems. In the presentation, we will highlight recent experiments combining cold trapped molecular ions with neutral molecules which address questions ranging from fundamental collision physics to the dynamics and mechanisms of complex polyatomic chemical reactions. We will also discuss recent developments in molecular-ion quantum technologies and their applications in molecular and chemical physics.

Competing non-radiative inelastic processes in hybrid Li-Ba^+ experiment

Xiaodong Xing, Ting Xie, Eliane Luc, Nadia Bouloufa-Maafa, Olivier Dulieu
Presented by Olivier Dulieu (Paris-Sud University, France)

We present a theoretical investigation of the collision of a single excited ion $^{138}Ba^+$ ($^2D_{\frac{3}{2},\frac{5}{2}}$) immersed in an ultracold ^6Li gas. We have developed several theoretical models of increasing complexity to determine the governing interactions: the radial coupling, the spin-orbit coupling and rotational coupling. The fine structure quenching, parity-dependent non-radiative charge exchange and non-radiative quenching processes are identified. The results are compared to those of the experiment performed in the group of T. Schätz in Freiburg. The agreement with the experimental results demonstrates the crucial importance of the rotational coupling induced by the initial high angular momentum of the ion.

Towards creation of charged-Rydberg molecules in an atom-ion hybrid trap

Shinsuke Haze, Markus Deiss, Dominik Dorer, Johannes Hecker Denschlag
Presented by Shinsuke Haze (Institute for Quantum Matter, Ulm University, Germany)

The recent development of cold atom-ion hybrid system is providing a versatile platform to study cold chemistry and molecular physics with an unprecedented degree of control and accuracy. In this talk, we discuss our exploration of forming Rydberg molecules whose binding mechanism is based on Rydberg atom-ion interaction. In particular, we present the property of the Rydberg molecular ions as well as calculated potential energy curves. We also show our experimental approach to realize such molecules via photoassociation spectroscopy in our atom-ion hybrid apparatus.

Observation of collisions between Feshbach dimers and trapped ions

Rene Gerritsma
Presented by Rene Gerritsma (University of Amsterdam, The Netherlands)

I will discuss recent experiments in which we observed collisions between trapped Yb^+ ions and and Li_2 Feshbach dimers. Our results open up the possibility to study trapped ions in a bath of fermions in the BEC to BCS crossover regime and to explore quantum effects in atom-ion systems. I will also discuss strategies and prospects for reaching deeper into the quantum regime in rf traps.

Observation of Feshbach resonances between a single barium ion and an ultracold lithium gas

Thomas Walker
Presented by Thomas Walker (University of Freiburg, Germany)

Feshbach resonances have been a tool for controlling interactions between neutral atoms for several decades, but rf-induced heating in rf traps has kept them out of reach in hybrid atom-ion experiments [1]. Recently, however, the ultracold regime has been reached in hybrid systems [2]. In this talk, we report on the observation of magnetic Feshbach resonances between a $^{138}Ba^{+}$ ion and an ultracold cloud of ^{6}Li in the few-partial-wave regime [3]. By tuning the ambient magnetic field, we demonstrate enhancement both of sympathetic cooling through elastic two-body collisions and of three-body recombination. The combination of of $^{138}Ba^{+}$ and ^{6}Li is chemically stable over 1000s of collisions when both are prepared in their electronic ground states [4]. This, coupled with the large mass imbalance and control over stray fields down to 3mV/m, allows us to sympathetically cool to the ultracold regime despite the presence of rf fields. Further, we present an outlook on interactions in an all-optical trap.

[1] Cetina, Marko, Andrew T. Grier, and Vladan Vuletić. "Micromotion-induced limit to atom-ion sympathetic cooling in Paul traps." *Physical review letters* 109.25 (2012): 253201
[2] Feldker, T., et al. "Buffer gas cooling of a trapped ion to the quantum regime." *Nature Physics* 16.4 (2020): 413-416.
[3] Weckesser, Pascal, et al. "Observation of Feshbach resonances between a single ion and ultracold atoms." *Nature* 600.7889 (2021): 429-433.
[4] M. Tomza et al. “Cold hybrid ion-atom systems”. *Reviews of Modern Physics* 91.3 (2019), p. 035001.

Large spin-orbit coupling as a source of Feshbach resonances in ultracold ion-atom mixtures

Agata Wojciechowska
Presented by Agata Wojciechowska (University of Warsaw, Poland)

Feshbach resonances are a crucial tool, enabling to control atoms' interactions in quantum gases, which have led to many significant breakthroughs. The following step to ultracold physics advancement is an observation of these resonances between ions and atoms. Until 2020, the ultracold regime was unattainable for ion-atom mixtures but desired for quantum simulation and computing. A quantum gas consisting of Li atoms and Ba^{+} ion is the first one, where Feshbach resonances were observed. What is more, we discovered that the resonances originate from a giant second-order spin-orbit interaction, which is a unique mechanism, compared to, for instance, neutral systems. Gaining a deep understanding of this phenomenon allows us to probe short-range interactions in ion-atom systems and precisely describe a deeply bound state of an excited electronic potential. I will present theoretical calculations to predict and describe Feshbach resonances, as well as our fit to the experimental results. The experiment is realized in Tobias Schaetz's group at the University of Freiburg, Germany.

A new ion trap for atom-ion experiments

Lucia Duca, Naoto Mizukami, Elia Perego, Massimo Inguscio, Carlo Sias
Presented by Carlo Sias (Istituto Nazionale di Ricerca Metrologica (INRIM) & European Laboratory for Nonlinear Spectroscopy (LENS), Italy)

I will report on the advancements in the realization of an experimental apparatus designed for immersing trapped Barium ions into an ultracold gas of fermionic Lithium. In particular, I will report on a number of technical advancements that we have realized in order to achieve a high level of control over the atom-ion quantum mixture, and especially on the unique design of our ion trap. The specific geometry of the electrodes makes it possible to continuously change the structure of the ion crystal from a one-dimensional string to a two-dimensional Coulomb crystal by changing a DC voltage. When the confining potential is made isotropic in the two-dimensional plane, we observe that the ions undergo a structural transition from a Coulomb crystal to a quantum rotor, in which the particles are no longer localized in space, but are rather delocalized along circular trajectories. Interestingly, for sufficiently large number of ions two or more concentric rings are populated, and the rings can exhibit independent dynamics. Notably, this experiment represents the first ion trapping experiment in Italy.

Chemical reactions between cold, trapped ions and neutral molecules

Heather Lewandowski
Presented by Heather Lewandowski (JILA, University of Colorado Boulder, USA)

Reactions between ions and radical molecules play an important role in the chemistry that drives dynamics in the interstellar medium and during combustion of hydrocarbons. Unfortunately, experimental measurements of these reactions are very challenging, and thus very rare. We use tools borrowed from the cold atom community to measure ion-molecule reactions in a well-controlled environment. Our high sensitivity allows us to study reactions where the reaction rate can be as low as one reaction per minute. I will present the capabilities of this cold ion-molecule reaction apparatus and some example reactions we have been able to study using this system, including ones that are relevant to chemistry in the interstellar medium and planetary atmospheres.

Interactions of trapped negative ions with ultracold atoms

Roland Wester
Presented by Roland Wester (University of Innsbruck, Austria)

The study of cold molecular ions and ionic complexes in traps has attracted a lot of interest for precision spectroscopy, quantum collision dynamics, and astrochemistry. Of particular interest is the study of interactions between ions and ultracold atoms to explore controlled collision dynamics at very low collision energies. In a close collaboration between Innsbruck and Heidelberg we have carried out several studies that focused on interactions between ultracold rubidium atoms and negative atomic and molecular ions using a hybrid ion-atom trap [1,2]. In associative electronic detachment collisions we observed a complex with the electron bound solely by dipolar forces. Comparison with ab initio calculations also revealed pronounced steric effects in the collision [3]. Collisions with atomic oxygen anions showed no associative detachment collisions with ground state rubidium [4]. This allowed us to explore elastic collisions and negative ion cooling by ultracold atoms [5], which may provide a pathway to negative ion temperatures below the minimum temperature of about 4 Kelvin reached by helium buffer gas cooling. Furthermore, optical control of the rubidium excited electronic state population allowed us to extend the measurements to cross sections of collisions involving excited state atoms [3,4].

[1] J. Deiglmayr, A. Göritz, T. Best, M. Weidemüller and R. Wester, Phys. Rev. A 86, 043438 (2012)[2] M. Nötzold, S. Z. Hassan, J. Tauch, E. Endres, R. Wester and M. Weidemüller, Appl. Sci. 10, 5264 (2020)
[3] S. Z. Hassan, J. Tauch, M. Kas, M. Nötzold, H. L. Carrera, E. S. Endres, R. Wester and M. Weidemüller, Nat. Commun. 13, 18 (2022)
[4] S. Z. Hassan, J. Tauch, M. Kas, M. Nötzold, R. Wester and M. Weidemüller, J. Chem. Phys. 156, 094304 (2022)
[5] J. Tauch et al., in preparation

Ion-molecule reactions near 0 K: the Lambda - doubling-mediated enhancement of the He^+ + NO reaction rate coefficient

Valentina Zhelyazkova, Serena Shilling, Fernanda B. V. Martins, and Frédéric Merkt
Presented by Valentina Zhelyazkova (Laboratory of Physical Chemistry, ETH Zurich, Switzerland)

Fast, exothermic and barrierless ion-molecule reactions drive rich chemistry in the cold environment of the interstellar medium [1,2]. These reactions proceed with high rate coefficients even at low temperatures, and are typically modelled by the classical Langevin model with a temperature- and collision-energy-independent reaction rate coefficient (k_L). At low temperatures and collision energies (E_coll), however, the rotational-state-dependent Stark shifts experienced by the molecule in the electric field of the ion can lead to a strong modification of the interaction potentials and reaction rate coefficients [3,4].

We study experimentally reactions between the He^+ ion and several small gas-phase molecules. To avoid heating by stray electric fields, the He^+ ion is replaced by a He atom in a Rydberg state [He(n)]. To reach low collision energies, we employ a merged-beam set-up [5]. The He(n) atoms are merged with a molecular supersonic beam, using a curved surface Rydberg-Stark deflector. The collision energy is varied by changing the velocity of the He(n) atoms with the deflector. The reaction product ions are collected in a time-of-flight mass spectrometer.

Although NO has only a small dipole moment (0.159 D), we observe a strong enhancement of the total reaction yield below ~k_B 1 K, with the total capture rate coefficient reaching a value of ~3 k_L at the lowest accessible energy (~k_B 100 mK). Our results are well described by calculations based on the adiabatic-channel model [3,4,6]. The observed enhancement is attributed to the Lambda-doubling in NO ($X^2Pi_{\frac{1}{2}}$ electronic ground state), which effectively amplifies the Stark effect more than tenfold. To emphasise this effect, we also present results on the He^+ + CO reaction. Carbon monoxide has a similar dipole moment to NO (0.112 D), but a X^1Sigma^+ ground electronic state and thus no Lambda-doubling. The total product ion yield of the He^+ + CO reaction exhibits a decrease with decreasing E_coll, attributed to the negative quadrupole moment of CO [7].

[1] D. Smith, Chem. Rev. 92, 1473 (1992).
[2] T. P. Snow and V. M. Bierbaum, Ann. Rev. Anal. Chem. 1, 229 (2008).
[3] J. Troe, Chem. Phys. 87, 2773 (1987).
[4] D. C. Clary, Ann. Rev. Phys. Chem. 41, 61 (1990).
[5] V. Zhelyazkova et al., Phys. Chem. Chem. Phys. 23, 21606 (2021).
[6] A. G. Wickman et al., J. Chem. Phys. 96, 1053 (1992).
[7] F. B. V. Martins et al., New J. Phys. 23, 095011 (2021).

Charge transfer reactions between rare gas ions and polar molecules

Andriana Tsikritea, Jake A. Diprose, Tim P. Softley, Brianna R. Heazlewood
Presented by Andriana Tsikritea (University of Liverpool, UK)

Laser-cooled Ca^+ ions, confined in a linear Paul trap, are used as a cold framework to undertake reactions studies between sympathetically cooled rare-gas ions (Xe^+, Kr^+ or Ar^+) and room-temperature polar molecules (NH_3, ND_3, H_2O or D_2O) [1-3]. The experimentally measured reaction rate coefficients, along with accompanying ab initio calculations, will be discussed in the context of capture theory models. For the ammonia reactions, capture theory predictions do not agree with our findings and, additionally, an inverse kinetic isotope effect (KIE) is observed; ND_3 reacts faster than NH_3. Conversely, capture theory predictions are in excellent agreement with the water reaction rate coefficients and no KIEs are observed.

A supersonic beam of NH_3 and ND_3 neutrals is employed to further study the reactions with sympathetically cooled ions. The low rotational state distribution and tuneable velocity of the ammonia beam will allow us to control more of the reaction parameters, and to probe the mechanism of charge transfer.

References
[1] L.S. Petralia et al., Nat. Commun., 11, 1, 2020
[2] A. Tsikritea et al., Chem. Sci., 12, 10005, 2021
[3] A. Tsikritea et al., ACS Phys. Chem. Au, 2022 (published online)

Quantum chemistry to quantum logic with molecular ions

Eric R. Hudson
Presented by Eric R. Hudson (University of California LA, USA)

Over the last few years, work in our field has shifted from the development of methods for preparing molecular ions with laser-cooled gases to using these systems as tools for science. We will discuss a recent experiment studying a reaction of astrophysical importance, C^+ + H2O. This reaction showcases how a reaction can be “statistical” even when its mechanism is not. We will then turn to new ideas for quantum logic using both dipolar and dipole-phonon mediated interactions between these cooled molecular ions. These protocols provide potentially attractive and scalable means for entangling molecular ions, as well as non-destructive read out of their internal states.

Ions in atomic Fermi gases and Bose-Einstein condensates

Georg Bruun
Presented by Georg Bruun (Aarhus University, Denmark)

We explore ions in degenerate atomic Fermi gases and Bose-Einstein condensates (BECs). First, we show that a mobile ion can form quasiparticle states, which are charged analogues of the neutral polarons observed in atomic gases. Several properties are however quite different due to the strength and long range nature of the atom-ion interaction. We furthermore demonstrate that a mobile ion in a BEC can form molecular ions by binding an increasing number of bosons. Then we turn our attention to the induced interaction between two trapped ions mediated by a surrounding Bose or Fermi gas. We derive several analytical results and show that the induced interaction can lead to substantial and observable shifts in the ion phonon frequencies.

Towards experimental ultracold ion-atoms investigations in Aarhus

Michael Drewsen
Presented by Michael Drewsen (Aarhus University, Denmark)

At the Center for Complex Quantum Systems, we recently decided to initiate an experimental activity with the aim of investigate many-body phenomena governed by ultracold ion-atoms interactions. In entering this intriguing and challenging research field with already several very well-established groups, we have in an initial phase decided to focus on how to design an experiment that can deal with the many already known obstacles, and key limiting processes. In the talk, I will discuss various issues in this context, which hopefully will contribute to the advancement of hybrid ion-atom research, and briefly comment on ideas to some specific future experiments.

Ultracold Ion-Neutral Experiments in Composite Optical Traps

Leon Karpa
Presented by Leon Karpa (Leibniz University Hannover, Germany)

The field of interactions between ions and neutral atoms has seen tremendous progress, and has now reached a point where quantum effects become visible and accessible. While for particularly favorable combinations of species this can be achieved by exploiting optimized radiofrequency(rf)-based ion traps, many envisioned applications require a more generic method, ideally not limited by the still inherently present heating stemming from the presence of rf fields. Trapping both species in composite optical potentials provides a way to study ultracold ion-neutral interactions, both in complete absence of rf-induced heating and for generic ion-neutral combinations. I will report on our recent demonstration of sympathetic cooling in such all-optical ion-atom traps, the limitations of this method and its prospects for future applications. In particular, I will discuss how these techniques allow going beyond the currently available ion-atom experiments by combining ions with quantum degenerate gases of polar molecules, an exciting new system expected to provide a rich and intricate interplay between long- and short-range interactions.

Quantum-limited thermometry of a Fermi gas with a charged spin particle

Lorenzo Oghittu and Antonio Negretti
Presented by Lorenzo Oghittu (University of Hamburg, Germany)

We investigate the sensitivity of an ion sensor in determining the temperature of an atomic Fermi gas. Our study extends to charged impurities the proposal by M. T. Mitchison et al. [Phys. Rev. Lett. 125, 080402 (2020)], where atomic neutral impurities were used as an in situ thermometer of the quantum gas. We find that the long-range character of the atom-ion interaction enhances the thermometer's sensitivity for certain system parameters. In addition, we investigate the impact of the ion quantum motional state on the sensitivity by assuming that it is confined in a harmonic trap. We observe that the temperature sensitivity of the ion is noticeably influenced by its spatial extension, making the latter a versatile tool to be manipulated for improving the thermometer performance. We finally discuss our findings in the context of current experimental atom-ion mixtures.

Reference: Phys. Rev. Research 4, 023069 (2022)

Observation of a molecular bond between ions and Rydberg atoms using a high-resolution pulsed ion microscope

Tilman Pfau
Presented by Tilman Pfau (University of Stuttgart, Germany)

Atoms with a highly excited electron, called Rydberg atoms, can form unusual types of molecular bonds. The bond differs from the well known ionic and covalent bonds not only by its binding mechanism, but also by its bond length ranging up to several micrometres. We report the observation a new type of molecular bond based on the interaction between the ionic charge and a flipping induced dipole of a Rydberg atom with a bond length of several micrometres. We measure the vibrational spectrum and spatially resolve the bond length and the angular alignment of the molecule using a high-resolution ion microscope. As a consequence of the large bond length, the molecular dynamics is extremely slow. These results pave the way for future studies of spatio-temporal effects in molecular dynamics, e.g., beyond Born- Oppenheimer physics.

Cold ion-molecule chemistry within the orbit of a Rydberg electron

Johannes Deiglmayr, Katharina Höveler, Frédéric Merkt
Presented by Johannes Deiglmayr (Univeristy of Leipzig, Germany)

Hydrogen is the most abundant element in the universe. Due to its apparent simplicity, reactions involving hydrogen play an important role in the development of quantum chemistry and have been studied extensively both by theory and experiment. Here, I will present work performed at ETH Zürich on the astrophysical important ion-neutral barrierless reaction $H_2^+ + H_2 \rightarrow H_3^+ + H$ and isotopologic variants. We study this reaction at collision energies below kB 1 K in a merged beam experiment by replacing the ion with the ionic core of a molecule in a highly-excited Rydberg state. The Rydberg electron does not influence the reaction for states with sufficiently high principal quantum number n but provides overall electric neutrality.

A detailed comparison of reactions of H_2, HD, and D2 with H_2^+, HD^+, and D_2^+ reveals that at low collision energies the product branching ratios cannot be explained by combinatorial or kinetic models. Instead, they follow closely a statistical model, derived from product state densities, which seems to contradict the established view of the reaction proceeding via a fast, direct reaction mechanism without intermediate short-lived complexes. In further experiments, we have studied the energy-dependent reaction rate coefficients for the reaction of H_2^+ and para H_2 (J = 0) at collision energies below k_B 1 K. We observe an enhancement at the lowest collision energies which is attributed to quantum enhancement as predicted 65 years ago by Vogt and Wannier. Measurements of the reaction $HD^+ + HD$ support this conclusion.

Quantum simulations with circular Rydberg atoms

Florian Meinert
Presented by Florian Meinert (University of Stuttgart, Germany)

Highly excited low-l Rydberg atoms in configurable mircotrap arrays have recently proven highly versatile for studying quantum many-body spin systems with single particle control. I will report on the advances of a new project pursuing to harness high-l circular Rydberg atoms for quantum simulation. When stabilized against black body radiation (BBR) in a suitable cavity structure, circular Rydberg states promise orders of magnitude longer lifetimes compared to their low-l counterparts and thus provide an appealing potential to strongly boost coherence times in Rydberg-based interacting atom arrays. To maintain excellent high-NA optical access we exploit a novel approach using an indium tin oxide (ITO) capacitor, capable of surpressing the parasitic microwave BBR even in a non-cryogenic environment while being transparent to visible light.

Quantum logic detection of single atom-ion collisions and the observation of trap-assisted formation of atom-ion bound states

Roee Ozeri
Presented by Roee Ozeri (Weizmann Institute of Science, Israel)

In this talk I will cover two recent experiments in our group. In the first I will describe the use of quantum logic techniques for the detection of collisions between trapped Sr^+ ions and ultracold Rb atoms. Using this technique we were able to compare Rb-Sr^+ spin-exchange cross-sections between all stable Sr^+ isotopes. We further used quantum logic to detect Rb-Rb^+ charge exchange cross-section. Our observations suggest s-wave effects; i.e. quantum interference; far outside the s-wave regime with up to 15 partial waves involved. In a different experiment we have found evidence that, unlike two free particles colliding, in atom-ion experiments where the ion is strongly trapped, energy and momentum can be exchanged between center-of-mass and relative motion. In this case a single collision can form a bound state where the binding energy is transferred into large motion of the molecule in the trap. By performing spin-exchange measurements as a function of the magnetic field and collision energy we are able to measure the molecule binding energy of 0.7(1) mK and a lifetime of 0.5(1) microsecond.

Dynamics and Bound State Formation of Charged Impurities in Ultracold Bosonic Gases

Peter Schmelcher
Presented by Peter Schmelcher (University of Hamburg, Germany)

Cold and ultracold atom-ion mixtures represent an intriguing platform for the formation of mesoscopic structures and their dynamics. This particularly due to the additional length scale which stems from the polarization interaction of the ions with the neutral atoms. The latter allow not only to polarize the immediate neighbourhood of ions but lead also to bound states which can be multiply occupied, depending on the quantum statistics (fermions or bosons) of the neutral species. We review aspects of our recent work in this direction addressing among others how a single ion can bind multiple atoms on mesoscopic scales, forming a correlated bound many-body compound. We explore these mesoscopic molecular ions from weak to strong atomic repulsion, thereby taking atom-ion and atom-atom correlations fully into account. Above a critical neutral atom number dissociation occurs resulting in an unbound fraction which forms a background gas for the mesoscopic bound molecule. Self-localization, and effective quasiparticle approaches are discussed and their limitations are revealed. The most recent developments and results of ongoing projects are summarized. Our study is carried out by means of the Multi Layer Multi-Configuration Time-Dependent Hartree method for Bosons (ML-MCTDHB), an ab initio approach to simulate the correlated quantum many-body dynamics and to compute the bound states of mixtures.

Prospects for quantum many-body physics studies utilizing cold ion-atom systems

Krzysztof Jachymski
Presented by Krzysztof Jachymski (University of Warsaw, Poland)

Owing to the comparatively large interaction range, ion-neutral systems should have vastly different many-body properties than short-range interacting impurities. However, studying them in experiments still represents a challenge. While there has been huge progress in observing and understanding ion-atom collisions as well as few-body phenomena, collective effects have so far been elusive. I will discuss the basic properties of a many-body ion-atom system under realistic conditions, describe the problems that one encounters and outline the research directions which seem to be the most promising.

Three-body Interactions in Ion Chains

Bárbara Andrade, Zohreh Davoudi, Tobias Graß, Mohammad Hafezi, Guido Pagano, Alireza Seif
Presented by Tobias Graß (ICFO Institute of Photonic Sciences, Spain)

We present a scheme which enables the engineering of three-spin interactions in chains of trapped ions. As in the standard Cirac-Zoller or Molmer-Sorensen scheme, the engineering is based on controlled ion-laser interactions which induce all-to-all interactions between the ions via their collective modes of motion. By extending the light-matter coupling to higher sidebands, tailored interactions between more than two ions are achieved. With this ingredient, the analog quantum simulation of a U(1) lattice gauge theory

becomes feasible through direct implementation of the quantum link model in the ion chain. The three-body scheme can also be used in the context of quantum computation for novel gates which entangle three qubits through a single gate operation.

Numerical treatment of an atom-ion pair in spatially displaced traps

Onyango Stephen Okeyo, Fabio Revuelta, Alejandro Saenz
Presented by Fabio Revuelta (Polytechnic University of Madrid, Spain)

We present a numerical method for describing two particles in spatially separated three-dimensional finite lattice potentials. The interatomic interaction potential between the particles is modeled using realistic Born-Oppenheimer potential curves obtained from ab initio quantum chemistry calculations. To check the correctness of our method, we consider a simple example of a hybrid system formed by an ultracold neutral atom and a single ion of Li^+ dimer trapped in two harmonic trap potentials. The results reveal the expected trap-induced resonances that manifest as avoided crossings between the least-bound molecular state and the trap states as a function of the separation distance between the two traps. In addition, other avoided crossings as a function of the interaction strength for fixed trap separations are also discussed.

Polyatomic ultralong range Rydberg molecules

Rosario González-Férez
Presented by Rosario González-Férez (Polytechnic University of Madrid, Spain)

In cold and ultracold mixtures of atoms and molecules, Rydberg interactions with surrounding atoms or molecules may, under certain conditions, lead to the formation of special long-range Rydberg molecules [1,2,3]. These exotic molecules provide an excellent toolkit for manipulation and control of interatomic and atom-molecule interactions, with applications in ultracold chemistry, quantum information processing and many-body quantum physics. In this talk, we will first discuss ultralong-range polyatomic Rydberg molecules formed when a heteronuclear diatomic molecule is bound to a Rydberg atom [3,4]. The binding mechanism appears due to anisotropic scattering of the Rydberg electron from the permanent electric dipole moment of the polar molecule. We propose an experimentally realizable scheme to produce these triatomic ultralong-range Rydberg molecules in ultracold KRb traps, which might use the excitation of potassium or rubidium [5]. By exploiting the Rydberg electron-molecule anisotropic dipole interaction, we induce a near resonant coupling of the non-zero quantum defect Rydberg levels with the KRb molecule in an excited rotational level. This coupling enhances the binding of the triatomic ultralong-range Rydberg molecule and produces favorable Franck-Condon factors. Another type of ultralong-range Rydberg molecule is formed in collisions between polar molecules in cold and ultracold settings [6]. The interaction of Λ-doublet nitric oxide (NO) with long-lived Rydberg NO molecules forms ultralong-range Rydberg bimolecules with GHz energies and kilo-Debye permanent electric dipole moments. The description includes both the anisotropic charge-molecular dipole interaction and the electron-NO scattering. The rotational constant for the Rydberg bimolecules is in the MHz range, allowing for microwave spectroscopy of rotational transitions in Rydberg bimolecules. The Rydberg molecules described here hold promise for studies of a special class of long-range bimolecular interactions.

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Collisions, exchange symmetry, and diffusion in ultra-cold ion-atom systems

Niranjan Myneni, Nishant Joshi, Amrendra Pandey, Olivier Dulieu, Robin Côté and S. A. Rangwala
Presented by Sadiq Rangwala (Raman Research Institute, India)

Ion-atom collisions at cold and ultra-cold temperatures have now been the object of several theoretical [1] and experimental investigations [2-5] for well over a decade. The basic problem is typically framed as the study of interactions of a single ion in a cold, dilute gas of ultra-cold atoms. In a majority of such studies,

the ion and atoms are of different species (heteronuclear) [3,5]. Our experiments, along with some others have focussed on interactions between ions and atoms of the same species (homonuclear), where the ion is the positively charged atom with which it is mixed [2,4,6,7]. Homonuclear ion-atom system allows for electron exchange in collision, with no resulting change in system energy. For the homonuclear ion-atom system, very low energy collision calculations have tended not to account for resonant charge exchange properly. We argue that at all energies, the proper way to account for the binary collision cross section between any homonuclear ion-atom pair (such as Li^+-Li) is by computing its total cross section, which includes the interference terms in the scattering amplitude, and use that to compute the total cross section [8]. In addition, at ultra-cold temperatures, the atoms and ion wavepacket delocalize, and because of exchange symmetry and under appropriate density conditions, charge hopping can result because of overlapping wavepackets of the ion with neighbouring atoms [9]. We analyse the diffusion of a single ion in a cloud of ultra-cold atoms for this homonuclear system. The diffusion of the ion is studied theoretically, as collisional and hopping based diffusion [10]. This leads to competition between diffusion mechanisms, which allows probablistic predictions for location of the ion with time. The status of the experiments to study the problems above will be presented.

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The Role of Long-range Pairwise Interactions in Ion-atom-atom Three-body Recombination

Marjan Mirahmadi, and Jesús Pérez Ríos
Presented by Marjan Mirahmadi (Fritz Haber Institute of the Max Planck Society, Germany)

In this work, we investigate the role of the long-range tail of pairwise interactions in ion-atom-atom direct three-body reaction $A+A+B^+$, based on a classical trajectory method in hyperspherical coordinates developed in Ref. [1]. We introduce an effective (hyper-) radial potential $V(\rho) \propto \rho^{\beta}$ in hyperspherical coordinates [2] and find the parameter β as a function of coefficients of the long-range two-body interactions $-C_6 r^{-6}$ (atom-atoms) and $-C_4 r^{-4}$ (ion-atom). In particular, we focus on the formation rate of molecular ions (AB^+) and neutral molecules (A_2) through this three-body recombination process over a wide range of temperatures.
As a result, we explain the previously derived threshold law (in Refs. [3,4]) for ion-neutral-neutral three-body recombination at low temperatures and establish a range for its validity. Similarly, we find new and intriguing scenarios in which the branching ratio of the product states after three-body recombination deviates from the expected threshold law in the cold regime.

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Universality in three-body collisions in ultracold hybrid ion-atom systems

J. Gębala, J. P. D'Incao, M. Tomza
Presented by Jacek Gębala (University of Warsaw, Poland)

We will introduce the concept of universality: a tool for efficient description of the scattering properties of ultracold three-body systems. Furthermore, we will discuss the motivations behind implementing universal potential models in order to calculate the recombination losses in ion-atom samples. We will proceed to showing how we can model an exemplary three-particle collision in a system interacting via the sum of two-body potentials. The presentation will include a reference to recent theoretical results in hybrid systems of Barium and Ytterbium ions immersed in Lithium gas -- where recently Feshbach resonances between a single ion and ultracold atoms were observed. We will show the limits of the universal approach in ion-atom systems: mainly the difficulties in proper description of weakly bound states as well as the differences in treating the atom-atom and atom-ion channels of scattering.

Molecular product distributions from three-body recombination of ultracold atoms

Paul S. Julienne
Presented by Paul S. Julienne (Joint Quantum Institute, NIST and the University of Maryland, USA)

Cold atoms and molecules in the nK regime offer extraordinary precision for preparing the reactants in specific quantum states with all quantized degrees of freedom specified and with a single partial wave contributing to a reactive collision. To take full advantage of the quantum control that such precise state preparation makes possible, it is necessary also to be able to predict and measure the product distribution of the reaction products. Detection of such products by ionizing them and detecting the ions is a promising experimental tool for this. This talk will describe theoretical methods for calculating three-body recombination rates and product distributions for the recombination of three cold atoms, A + A + A -> A_2 + A, and compare to experimental measurements on the recombination of Rb atoms to demonstrate the power of these methods. The calculations are based on realistic long-range potentials of the atoms with a repulsive wall added to limit the number of vibrational bound states in the potential. The three-body S-matrix is calculated by numerically solving the Schrodinger equation in an adiabatic hyperspherical representation. Pairwise additive two-body potentials are used at long range, adjusted to yield the known two-body scattering lengths for the singlet and triplet potentials. Good agreement is found between calculated and measured product vibrational-rotational distributions for the two isotopes ^{85}Rb [1] and ^{87}Rb [2], which differ by 4 orders of magnitude in total recombination rate constant. Over the range of product binding energy E_b surveyed, the product molecules conserve the initial spin character of the atoms, and the probability of formation drops off approximately as $1/E_b$. The talk will conclude by giving some opportunities and challenges for future studies.

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Signature of the s-wave scattering due to locking and unlocking of phase shifts in resonant-exchange processes

Robin Côté
Presented by Robin Côté (University of Massachusetts Boston, USA)

Resonant exchange is a general process playing a key role in many-body dynamics and transport phenomena, such as spin, charge, or excitation diffusion. A particular example of such a process is the resonant charge transfer between an ion and its parent atom. The underlying dynamics is described by the resonant exchange cross section. We show that the s-wave scattering, generally thought to contribute mainly in the ultracold (or Wigner) regime, dictates the overall cross section over a broad range of energies. In fact, this counter-intuitive behavior can be understood as an unexpected consequence of phase-shift locking; namely, all phase-shifts are “locked” relative to each other over a large range of energies, leading to a quasi-constant phase-shift difference and hence a simple expression for the

resonant exchange cross section. We also explore the regime when this is followed by a phase-shift "unlocking" taking place at higher energies. We derive an analytical expression and explain its applicability over a large range of collision energy, high above the Wigner regime; it accounts not only for the locking of phase shifts, but also for their gradual unlocking as the energy increases. We demonstrate the relationship to the classical capture (Langevin) cross section and apply it to three very different resonant processes: namely, resonant charge transfer, spin flip, and excitation exchange. Finally, we apply the expression to the case of resonant charge-transfer in ion–atom collisions over a large range of energies up to room temperatures and find good agreement between the computed (fully quantal) cross section and our newly obtained result. The s-wave signature also allows us to gain information about the Wigner regime from data obtained at much higher temperatures, which is especially advantageous for systems where the ultracold regime is not reachable. We show how one could use information at higher energies to gain insight into the s-wave regime.

Ion-Atom 2022 – Poster Abstract

P1: Quantum interference effects in cold Rb–Sr^+ collisions high above the ultracold regime

Maks Walewski, Matthew D. Frye, Michał Tomza
Presented by Maks Walewski (University of Warsaw, Poland)

The s-wave scattering regime in ion-atom systems is hard to reach using the currently available experimental techniques. However, in some systems the signatures of s-wave scattering can be seen high above the ultracold regime due to the “phase-locking” mechanism, by which the difference between the singlet and triplet scattering phases remains constant over a wide range of partial waves and collision energies. In effect, the s-wave scattering modulates the spin-exchange cross sections even at high temperatures. We are building a theoretical model for understanding the collisional properties of the Rb–Sr $^+$ system, investigated experimentally in the group of Prof. Roee Ozeri at the Weizmann Institute of Science, Israel. We demonstrate that the phase-locking mechanism plays an important role in determining the spin-exchange cross sections in the
Rb–Sr^+ system at temperatures much higher than 1 mK. We report the calibration of the a3Σ+ and A1Σ+ molecular potential curves based on the coupled-channel calculations and experimental data, and analyze the prospects for seeing the phase-locking mechanism at work in different ion-atom systems.

P2: Quantum simulation of the central spin model with a Rydberg atom and polar molecules in optical tweezers

Jacek Dobrzyniecki, Michał Tomza
Presented by Jacek Dobrzyniecki (University of Warsaw, Poland)

Central spin models, where a single spinful particle interacts with a spin environment, find wide application in quantum information technology and can be used to describe e.g. the decoherence of a qubit over time. We propose a method of realizing an ultracold quantum simulator for the central spin model. The proposed system consists of a single Rydberg atom (“central spin”) and surrounding diatomic molecules (“environment spins”), coupled to each other via dipole-dipole interactions. By mapping internal particle states to spin states, spin-exchanging interactions can be simulated. We demonstrate that this setup allows realizing a range of central spin models of high scientific interest. More precise control over the model can be exerted by directly manipulating the placement of environment spins. As an example, we consider a ring-shaped arrangement of environment spins, and show how the time evolution of the central spin is affected by the tilt angle of the ring.

P3: Interactions of alkaline-earth ions in ground and excited states with H2 and CO molecules: implications for collision induced decoherence and losses

Hela Ladjimi, Michał Tomza
Presented by Hela Ladjimi (University of Warsaw, Poland)

Collisions with residual H_2 and CO molecules remaining even in a high quality vacuum are one of the most important sources of decoherence and losses for quantum simulators and atomic clocks based on trapped ions. Here, to assess importance of these processes, we investigated interactions of alkaline-earth-(like) Ca^+, Sr^+, and Yb^+ ions in the ground and excited electronic states with H_2 and CO molecules using ab initio methods of quantum chemistry. We calculated potential energy surfaces for ground and excited states, and transition electric dipole moments between them using the coupled cluster and multireference configuration interactions methods. We assessed energetics and paths of possible chemical reactions and mechanisms of interaction- and collision-induce decoherence and deexcitation processes for ions in excited electronic states.

P4: Quantum simulation with ultracold atoms in a topological Rydberg lattice

João P. Mendonça, Krzysztof Jachymski
Presented by João P. Mendonça (University of Warsaw, Poland)

The main problem of quantum simulation is that it requires great experimental control over the system geometry, dimensionality, and interparticle interaction. Cold atoms in optical lattices have been shown to be very suitable for this task as the system parameters can be precisely tuned on fast optical timescales. This allows for realization of microscopic Hamiltonians with flexible onsite and long range interactions, tunnelling, and lattice geometry, including nonuniform potentials. The weak interaction between neutral atoms still poses a challenge and restricts the class of realizable systems. Meanwhile, ions can strongly interact with each other via Coulomb repulsion, while Rydberg atoms exhibit van der Waals forces acting on micrometer scales, allowing for much larger energy scales and thus reduction of operation times. The proposed platform is to combine, in a single experimental setup, laser cooled trapped ions or Rydberg atoms with ultracold neutral atoms. Such a hybrid system is expected to have the best of both worlds, namely the long coherence time, great atomic scalability, high controllability with spatial localization, and tunable interactions in an intermediate range. We study many theoretical possibilities for the Rydberg platform from 1D to 3D systems and distinct feasible interaction potentials. In particular, the zig-zag Rydberg lattice brings to light the possibility to get topological phonons which will be coupled to the atomic gas. We find that the phonon dispersion can feature edge modes, flat bands, and Dirac points. This system works like a crystal for the ultracold neutral atoms, giving us a perfect platform for quantum simulation of many-body and condensed matter systems such as high-Tc superconductors.

P5: Compound atomic systems: ionic Bose polaron dynamics

Ubaldo Cavazos Olivas, Krzysztof Jachymski
Presented by Ubaldo Cavazos Olivas (University of Warsaw, Poland)

Ultracold quantum many-body systems constitute an interesting research playground due to their wide range of applications, from precision measurements to simulating condensed matter phenomena. One particular example are hybrid systems of atoms and ions, which are rapidly developing [1]. A distinctive property of impurity systems at ultralow temperature is the emergence of the so-called polaron. For bosonic atoms at weak coupling, their behavior can be understood by means of Bogolubov (mean field) theory. Nevertheless, this approach is no longer valid as soon as the strong coupling regime is taken into account. Ion-atom systems feature long-range interactions which drive the system to form a many-body bound state with high density and large atom number [2]. In order to explore this physics,
inspired by the study performed in [3], a variational approach is adopted. Employing a regularized potential that retains the correct long-distance behavior, we study the properties of the ionic Bose polaron, such as its energy and the number of bosons that takes part in the cloud formation, which is tunable by the potential parameters. This approach also allows to access the system dynamics.

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P6: Ultracold interactions of alkali-metal and alkaline-earth-metal ions with spin-polarized metastable helium atoms

Marcin Gronowski, Michał Tomza
Presented by Marcin Gronowski (Institute of Physical Chemistry, Polish Academy of Sciences, Poland)

Promising systems to reach the quantum regime of ion-atom collisions are samples of heavy-ion immersed into an ultracold gas of light atoms like ultracold spin-polarized metastable helium (3S). Helium in 3S state possesses enough internal energy to ionize various chemicals. However, ultra-low temperatures allowed for mitigation of such process, as demonstrated by creating the Bose-Einstein condensates of 4He*, Fermi gases of 3He*, and a mixture of neutral ^{87}Rb and ^{4}He*.
We investigated interactions and collisions in spin-polarized samples composed of metastable helium atoms and alkali-metal or alkaline-earth-metal ions. We computed potential energy curves for electronic states of the highest possible multiplicity. Lighter ions (Li^+, Na^+, Be^+, Mg^+) exhibit a potential energy curve not deeper than 1500 cm-1 with minima at an interatomic distance larger than 11 bohr. The

remaining ions (K^+, Rb^+, Ca^+, Sr^+) interact stronger with He*; well depths are between 6000 and 8000 cm-1, and equilibrium distances are between 7.5 and 7.9 bohr. The charge transfer process leading to He^+ (2S) and neutral metal atom is energetically possible for lighter ions, even assuming spin polarization of the system. Only alkaline-earth-metal ions are subject to the Penning ionization. The core-electron excitation is energetically possible only for

Rb^+. All systems studied here can be subject to spin relaxation. We computed transition dipole moments and evaluated the rate constants of charge transfer collisions. We also analyzed prospects for using magnetically tunable Feshbach resonances to control charge transfer and Penning ionization processes. When it was possible, we predicted scattering lengths.

P7: Feshbach resonances in ultracold atom-ion collisions

Piotr Kulik, Krzysztof Jachymski
Presented by Piotr Kulik (University of Warsaw, Poland)

Feshbach resonances are crucial phenomena in studies of ultracold gases. It is an essential tool to control collisions between atoms, which is currently a dynamically developing field. We describe ultracold atom-ion collisions using the multichannel quantum-defect formalism and apply the model derived in [1] to simulate systems composed of alkali atoms and alkaline earth metal ions and investigate the occurrence of magnetic Feshbach resonances.

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P8: Dynamics of a trapped ion in a quantum gas: effects of particle statistics

Lorenzo Oghittu, Melf Johannsen, Antonio Negretti, Rene Gerritsma
Presented by Antonio Negretti (University of Hamburg, Germany)

We study the quantum dynamics of an ion confined in a radio-frequency trap in interaction with either a Bose or spin-polarized Fermi gas. To this end, we derive quantum optical master equations in the limit of weak coupling and the Lamb-Dicke approximations. For the bosonic bath, we also include the so-called “Lamb-shift” correction to the ion trap due to the coupling to the quantum gas as well as the extended Fröhlich interaction within the Bogolyubov approximation that have been not considered in previous studies. We calculate the ion kinetic energy for various atom-ion scattering lengths as well as gas temperatures by considering the intrinsic micromotion and we analyze the damping of the ion motion in the gas as a function of the gas temperature. We find that the ion’s dynamics depends on the quantum statistics of the gas and that a fermionic bath enables to attain lower ionic energies.

P9: Cold ion chemistry between the He^+ ion and small molecules with a quadrupole moment

Fernanda B. V. Martins, Francesca van Swaaij, Valentina Zhelyazkova, Frédéric Merkt
Presented by Fernanda B. V. Martins (ETH Zurich, Switzerland)

Exothermic, barrier-free ion-molecule reactions proceed with high rate coefficients even at very low temperatures. These reactions are typically described using the Langevin model, which predicts the rate coefficient to be independent of the temperature or the collision energy (Ecoll). At near-zero collision energies, however, a strong Ecoll dependence of the capture rate coefficients can arise because of the interaction between the charge of the ion and the electric dipole or quadrupole moments of the neutral molecule. To reach such low collision energies, we use a merged-beam approach and study ion-molecule reactions within the orbit of a highly excited Rydberg electron, which prevents the heating up of the ions by stray electric fields without influencing the reaction.

In previous studies of reactions between He^+ and either linear or symmetric top molecules, we found that for polar reactants, such as NH3, a pronounced increase in the rate coefficient is observed with decreasing Ecoll [1,2], whereas for N2, which has no dipole moment but a negative quadrupole moment, the reaction yield decreases with decreasing Ecoll [3]. In this contribution, we will present the results of recent investigations at low Ecoll of the reactions of He^+ with molecules that have a quadrupole moment, with particular emphasis on the He^+ + CO and the

$He^+ + C_2H_4$ reaction systems. In the former case, we examine in detail the role of the charge-dipole and charge-quadrupole interactions. The dipole moment of CO is small, and it is not obvious to predict whether the Ecoll behavior of the rate coefficients is dominated by the charge-dipole or the charge-quadrupole interaction. In the latter case, we examine for the first time an ion-molecule reaction involving a nonpolar asymmetric molecule with a large quadrupole moment.

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P10: Electronic structure and prospects for the formation of ionic-molecular alkali-metal-barium: $BaAlk^+$ (Alk=Li, Na, K, Rb, Cs and Fr)

Sana Akkari, Wissem Zrafi, Hela Laadjimi, Mohamed Bejaoui, Hamid Berriche
Presented by Hamid Berriche (American University of RAK (UAE) & University of Monastir (Tunisia))

Accurate knowledge of electronic properties is important for creating and manufacturing ultracold molecules. Here, we report ab initio quantum chemistry calculations on the properties of alkali-metal-barium Ba-Alk^+ (Alk= Li, Na, K, Rb, Cs and Fr) molecular ions for their electronic ground state. The potential energy curves (PECs) and permanent dipole moments (PDMs) are calculatedon the basis of multi-reference configuration interaction MRCI/MRCI-CBS(complete basis set) and the coupled cluster simple double and tripled excitation CCSD(T) level of theories, where the core-valence correlations and relativistic effect are included. The related spectroscopic constants are extracted and compared with available reference [1-4]. The results exhibit that the dissociation energies, equilibrium distances, and PDMs of Ba-Alk^+ have an interesting trend depending on the mass of the alkali-metal-atom [5-6]. Stimulated black body (T= 300 K) and spontaneous transition rates are calculated and used to compute radiative lifetimes of vibrational states of the electronic ground states of the Ba-Alk^+ molecular ionic systems. This work provides favorable information for the experimental study of forming ultra-cold molecules via photoassociation technique [7].

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P11: Using a hybrid atom-ion setup as a flexible platform for cold chemistry experiments

Markus Deiß, Shinsuke Haze, Dominik Dorer, Eberhard Tiemann, Jose P. D'Incao, Paul S. Julienne, Johannes Hecker Denschlag
Presented by Markus Deiß (Ulm University, Germany)

In recent years we have studied a variety of chemical processes in a hybrid atom-ion setup. Here, we present an overview of our results regarding
- state-to-state investigations of three-body recombination of neutral atoms,
- an analysis of the evolution of molecular ions in the presence of collisions and light fields,
- the formation of neutral ultralong-range Rydberg molecules,
- the prediction of a novel atom-ion Rydberg molecule.

P12: Distortion of the mercury 1S0-3P0 clock line in two-species atomic clock

Linek A., Ciuryło R., Żuchowski P., Witkowski M.
Presented by Adam Linek (Nicolaus Copernicus University in Torun, Poland)

Determining the accuracy of an atomic clock is non-trivial. There are many effects that perturb the clock line transition, the impact of which is difficult to estimate. The use of a two-species atomic clock opens the possibility for a better determination of the clock line frequency due to the ability to use the second atomic species as a tool to determine the magnitude of the perturbation effect. On the other hand, the very nature of the composite system itself provides new systematic effects whose impact must be estimated. Therefore, implementing a two-species atomic clock, it is desirable to perform diagnostics to determine if this is feasible.

Our work focuses on theoretical calculations for the Hg-Rb mixture. Here we show how the frequency and shape of the mercury clock line 1S0-3P0 are distorted if overlapped with rubidium atoms. When rubidium atoms (S = 1/2) interact with mercury in excited states (S = 1) the resulting potential energy curve can be either S = 3/2 or 1/2. In the latter case, this is the same symmetry as the HgRb molecular ground-state. Since the interaction potential which correlates with 3P0 state of Hg contains an admixture of S = 1/2 state, transitions to molecular states of Hg(3P0)—Rb are no longer forbidden. This might affect the line shape of the mercury clock line.

Our ab initio calculations allowed us to determine how the spectral line parameters, both its shift and shape, are perturbed by collision with another atomic species. This approach was general, yet it eventually allowed us to apply this to a Hg-Rb mixture, where we investigated how the 1S0-3P0 mercury clock line is perturbed upon collisions with the rubidium atoms. These results are crucial for diagnosing whether it is possible to construct a two-species atomic clock that includes mercury and rubidium.

P13: Generation of symmetry adapted spherical harmonics for molecular collision processes

Jan Franz, Franco A. Gianturco
Presented by Jan Franz (Gdansk University of Technology, Poland)

In the majority of the numerical simulations of the collisions between atoms and molecules the potential is expanded in products of radial coefficients and Legendre potentials (see e. g. López-Duran et al. [1]). In most applications the spatial symmetry of the collision partners is not taken into account. In cross section calculations of collisions between electrons or positrons with molecules it is standard to make use of the molecular point group and expand the interaction potential and scattering wavefunction into symmetry adapted linear combinations of spherical harmonics (see e. g. Sanna and Gianturco [2]). In these cases the computer time for the calculation of cross section can be reduced by several orders of magnitude. Here we present an algorithm to generate symmetry adapted linear combinations of spherical harmonics.

References
[1] D. López-Durán, E. Bodo, F. A. Gianturco, ASPIN: An all spin scattering code for atom-molecule rovibrationally inelastic cross sections, Computer Physics Communications, 179 (2008) 821 - 838.
[2] N. Sanna, F. A. Gianturco, Differential cross sections for electron/positron scattering from polyatomic molecules, Computer Physics Communications, 114 (1998) 142 - 167.

P14: Interactions of alkaline earth metal ions with diatomic molecules

Piotr Gniewek, Michał Tomza
Presented by Piotr Gniewek (University of Warsaw, Poland)

We investigated interactions of polar and apolar diatomic molecules (NO, OH, NH, CO, O_2, N_2) with alkaline-earth ions (Ca^+, Sr^+) using state-of-the-art ab inito methods of quantum chemistry. We also derived the general long-range form of ion-molecule interactions up to R^{-6} contributions for molecules in degenerate and non-degenerate electronic states. In case of degenerate diatomic molecules the interaction with atomic ions removes the degeneracy of the electronic terms. The resulting interaction energies are obtained as the eigenvalues of a 2x2 perturbation matrix. The off-diagonal terms appear for the first time for n = 1 + 2 Λ, n = 2 + 2 Λ, and n = 4 + 2 Λ in case of electrostatic, induction, and dispersion energies, respectively. Here n gives the asymptotic decay rate of the given energy contribution,

R^{-n}, and Λ is the angular momentum projection number for the diatomic molecule. Among the investigated systems, the interaction energy minima of the Ca^+ complexes are deeper than those of the corresponding Sr^+ complexes (by about 10% - 20%). Not unexpectedly, interactions of ions with dipolar molecules are strongly anisotropic. The Ca^+ - OH complex has a deep minimum (De of about 50 000 cm-1) corresponding to the charge-transfer state Ca^{2+} - OH^-.

P15: Isotope exchange equilibrium in the OH^- + HD <-> OD^- + H2 reaction at low temperatures

Š. Roučka, S. Rednyk, E. Vanko, J. Palacký, O. E. Hernandez Alvarez, P. Dohnal, R. Plašil, J. Glosík
Presented by Štěpán Roučka (Charles University)

We measured the rate coefficients of the reaction OH^- + HD -> OD^- + H_2 and its reverse OD^- + H_2 -> OH^- + HD in a cryogenic radiofrequency 22-pole trap. The experiment was carried out with buffer-gas-cooled ions at temperatures down to 10 K. The knowledge of both forward and reverse reaction rate coefficients allowed us to evaluate the equilibrium constants. These experimental data were used to validate the equilibrium constants calculated from spectroscopic data.

This work was supported by the Czech Science Foundation projects 20-22000S and 21-28560S and Charles University Grant Agency 37672.

P16: State transfer protocols using a dragged impurity

Daniel Bosworth, Maxim Pyzh and Peter Schmelcher
Presented by Daniel Bosworth (University of Hamburg)

We propose protocols for preparing an initially non-interacting one-dimensional gas of trapped bosons in both pure and mixed excited trap states. The protocols rely on dragging an external potential, such as an ion, through the gas. This breaks the system's parity symmetry and leads to avoided crossings between neighbouring single-particle states. We exploit these avoided crossings in order to dynamically transfer the atomic state diabatically from the ground state up to a desired excited state or mixture of neighbouring states. Our calculations are performed using the exact ab initio Multi-Layer Multi-Configuration Time-Dependent Hartree Method for Mixtures. This serves as a basis for future studies on quench dynamics of excited atomic gases.

P17: Compact laser system for experiments with isotopic mixtures of ultracold potassium

Mateusz Bocheński, Mariusz Semczuk
Presented by Mateusz Bocheński (University of Warsaw)

We present our work on building a compact laser setup capable of laser cooling of all stable potassium isotopes (^{39}K, ^{40}K, ^{41}K) consisting of a master laser, frequency distribution module and an amplifying stage. The core of our setup is a master laser stabilized to the $2^2S_{1/2}$ (F=1,F=2)→$2^2P_{3/2}$(F=2,F=3) crossover of the most abundant potassium isotope, ^{39}K. The beam is then sent via a single mode, polarization maintaining fiber to the frequency distribution module, where it is split into a cooling and a repumping path. In each path, one acousto-optic modulator (AOM) in a double pass configuration is used per isotope to tune the frequency to create beams detuned by +80 MHz and -80 MHz from the cooling and repumping transitions, respectively. The beams are fiber coupled to seed dedicated tapered amplifiers and the amplified light is then frequency shifted into resonance with cooling and repumping transitions. We obtain near 1 W of cooling and repumping light, more than enough for typical ultracold applications.
The setup incorporates additional master laser stabilized to a transition of the D1 line of potassium 39K, which utilizes the same frequency distribution module and the amplifying stage to prepare coherent cooling and repumping beams for sub-doppler cooling of all stable potassium isotopes with gray molasses. For this purpose, only the frequency of the AOMs used for D2-line cooling needs to be changed.

The switching between isotopes is done without any moving parts, is computer controlled and can be reliably performed in less than 1 ms, limited only by the settling time of the tapered amplifiers used in the setup. With this setup we have demonstrated sequential loading of magneto-optical traps of 41K and 39K as well as simultaneous loading of both isotopes, which paves the way for future studies of ultracold isotopic mixtures.
Our design circumvents the common problem of setting up multiple laser systems simplifying the experimental setup while maintaining the flexibility of working with all isotopes, in particular with the 41K and 40K mixture, where the bosonic isotope (41K) can be used to sympathetically cool fermionic 40K to obtain a quantum degenerate Bose-Fermi mixture.

P18: Towards Non-destructive Heterodyne Atom Number Measurement In An Ultracold Cesium And Potassium Mixture

Jakub Dobosz, Mariusz Semczuk
Presented by Jakub Dobosz (University of Warsaw)

Many experiments in ultracold physics rely on destructive detection, in particular absorption imaging. This limits the typical data acquisition rate to one measurement every 10-20 seconds, limited by the sample preparation time. Here, we present an alternative method of detection that exploits the phase shift induced by atoms on an off-resonance probe beam with respect to a co-linear reference beam of different frequency, resulting in a phase shift of the detected beat note. The change in the density of the trapped atomic cloud and hence the atom number can be detected by such heterodyne interferometer with negligible heating of the sample. Based on the observation that in many experiments the only figure of merit is the change in the trapped atom number, cameras typically used for detection can be replaced, or at least supplemented, by photodiodes. The method can shorten the data acquisition time by removing the need for multiple repetitions of the experimental sequence. It should allow measurements with high time resolution reaching several microseconds in a single experimental realization thanks to the implementation of photodiodes as detectors. The scheme presented here is particularly useful when the studied processes lead to atom loss or change of population to a state not interacting with the light used in the interferometer. Typical examples of application are photoassociation spectroscopy, temperature and lifetime measurements.

P19: Observation of missing lowest levels of the 0^-_g purely-long-range state of Cs_2

Koray Dinçer, Mariusz Semczuk
Presented by Koray Dinçer (University of Warsaw)

We use photoassociation (PA) of spin polarized (F=3,M_F=3) ultracold cesium atoms confined in a 1D optical lattice to confirm the existence of two lowest lying vibrational levels in the 0^-_g purely long-range state of Cs_2. The observation of these two levels confirms the theoretical predictions of Bouloufa et al. [1] postulating that the numbering of vibrational levels of this state needs to be shifted by two in order to agree theory with experimental data. We also provide unambiguous evidence that the work of Zhang et al. [2], which claimed priority of observing these new levels, in fact observed levels belonging to the 0^+_u molecular potential. Due to the expected low molecular formation rate we have investigated the possibility of enhancing the association of molecules in v=0 and v=1 levels with Feshbach resonances. Several of them are present at fields below 70 G but the two lowest levels could be detected only in the vicinity of the Feshbach resonance at 19.9 G [3]. We have determined the binding energies of the (v,J)=(0,2), (1,0), (1,2) and (1,4) with absolute accuracy better than 1 MHz by referencing the photoassociation laser to a frequency comb. For the v= 1 level we have extracted the rotational constant of ~56 MHz.

[1] Bouloufa, N., Crubellier, A., & Dulieu, O. Phys. Rev. A, 75(5), 052501. (2007).
[2] Zhang, Y., Ma, J., Wu, J., Wang, L., Xiao, L., & Jia, S. . Phys. Rev. A, 87(3), 030503.(2013).
[3] Tolra, B. Laburthe, et al. EPL (Europhysics Letters) 64.2 (2003): 171.

	June 8th Wednesday	June 9th Thursday	June 10th Friday
	Session A1	**Session B1**	**Session C1**
08:30	**Registration**		
09:00	**Welcome**	Georg Brunn	Peter Schmelcher
09:15	Stefan Willitsch		
09:30		Michael Drewsen	Krzysztof Jachymski
09:45	Olivier Dulieu		
10:00		Leon Karpa	Tobias Graß
10:15	Shinshuke Haze	Lorenzo Oghittu	Fabio Revuelta
10:30	**Coffee break**	**Coffee break**	**Coffee break**
	Session A2	**Session B2**	**Session C2**
11:00	Rene Gerritsma	Tilman Pfau	Rosario González Férez
11:15			
11:30	Thomas Walker	Johannes Deiglmayr	Sadiq Rangwala
11:45			
12:00	Agata Wojciechowska	Florian Meinert	Marian Mirahmadi
12:15	Carlo Sias	**Group Photo**	Jacek Gębala
12:30	**Lunch break**	**Lunch break**	**Lunch break**
	Session A3	**Session B3**	**Session C3**
14:00	Heather Lewandowski	Roee Ozeri	Paul Julienne
14:15			remote
14:30	Roland Wester	**Discussion panel on future of ion-atom**	Robin Côté
14:45			remote
15:00	Valentina Zhelyazkova	**COST Meeting - WG4**	**Concluding remarks**
15:15	Andriana Tsikritea		
15:30	**Coffee break**	**Coffee break**	**Coffee break**
	Session A4		
16:00	Eric Hudson remote	**Old Town Sightseeing***	*** For details please refer to page 29**
16:30	**Poster Session**		
18:30			
19:30	**Workshop Garden Pub***	**Workshop dinner***	

Organisational matters for evening activities:

- ### Workshop Garden Pub

We are pleased to invite you to pub **"Lolek Grill&Bar"**
The **drinks** will be served from **18:15**
The **main courses** will be served from **19:20**

Venue adress:
Lolek Grill&Bar, Rokitnicka 20, Warsaw

Connection from workshop venue:
It is within 10 min walking distance from Workshop venue, in the park "Pole Mokotowskie"

- ### Old Town Sightseeing

The sightseeing starts **at 16:30.**

Staring point:
Central Campus
of the University of Warsaw, **Krakowskie Przedmieście 26/28**

Connection from workshop venue:
The most convenient connection to the starting point is with **bus 128**, **bus 175**.

- ### Workshop Dinner

We are pleased to invite you to restaurant **"Kuźnia Smaku Restaurant"**
The **dinner** starts at **19:30**

Venue adress:
Kuźnia Smaku Restaurant, Mazowiecka 10, Warsaw

Connection from workshop venue:
The most convenient connection to the restaurant is with **tram 15**.