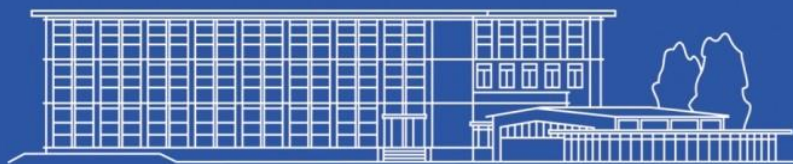




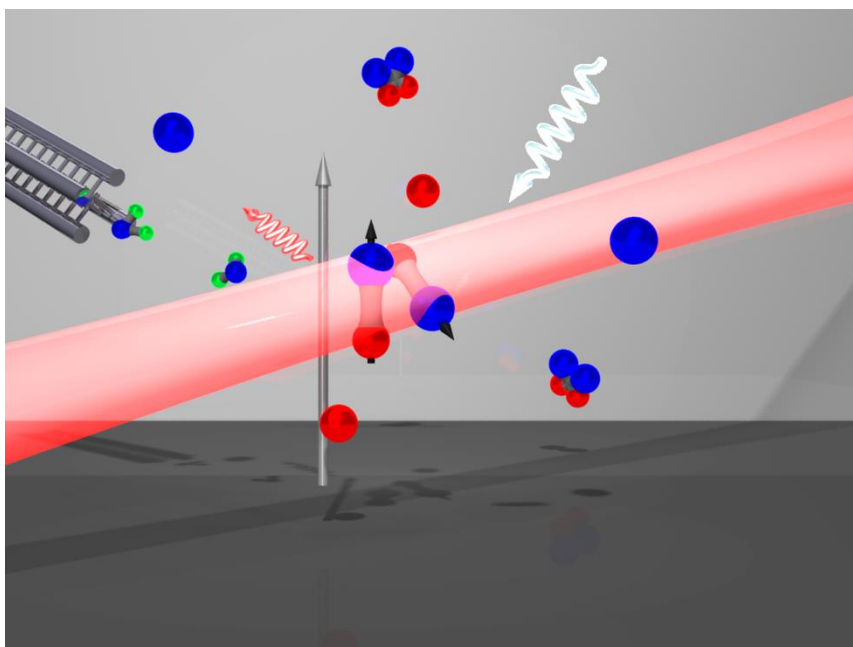
# FRIAS

FREIBURG INSTITUTE  
FOR ADVANCED STUDIES  
ALBERT-LUDWIGS-  
UNIVERSITÄT FREIBURG



## FRIAS Junior Researcher Conference

# COLD AND ULTRACOLD CHEMISTRY



Freiburg, February 21-22, 2022 (online)

Organized by

Katrin Dulitz

Leon Karpa

Fabian Thielemann

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
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# 1. PROGRAM OVERVIEW

PROGRAM - "COLD AND ULTRACOLD CHEMISTRY"			
DAY 1	DAY 2		
12:00	Welcome	12:00	Andreas Buchleitner
12:10	Get-to-know I	12:20	Florian Meinert
12:25:00	Stefan Willitsch	12:40:00	Baruch Margulis
12:45:00	Christiane Koch	12:55:00	Coffee / Lab tour "NaK"
13:05:00	Get-to-know II	13:15:00	Tijs Karman
13:20:00	Olivier Dulieu	13:35:00	Vikram Plomp
13:40:00	J. Hecker Denschlag	13:50:00	Discussion
14:00:00	Tim Langen	14:30:00	Poster karaoke B
14:15:00	Coffee / Lab tour "BaLi"	14:50:00	Poster B
14:35:00	Piotr Żuchowski	15:30:00	Coffee / Award committee*
14:55:00	Omar A. Khedaoui	15:50:00	Rene Gerritsma
15:10:00	Discussion	16:10:00	Michał Tomza
15:50:00	Poster karaoke A	16:30:00	Adrien Devolder
16:10:00	Poster A	16:45:00	Discussion
16:50:00	Coffee / Lab tour "HeLi"	17:25:00	Krzysztof Jachymski
17:10:00	Hendrick L. Bethlem	17:40:00	Silke Ospelkaus
17:30:00	Robert Wild	18:00:00	Conference awards
17:45:00	Open discussion	18:15:00	Open discussion

Invited talk   
 Hot-topic talk 

Hours are given in Central European Time (Berlin – Amsterdam – Paris).

## \* POSTER AWARD COMMITTEE:

Brianna Heazlewood  
 Krzysztof Jachymski  
 Tijs Karman  
 Tim Langen  
 Timothy Softley

## 1.1 INVITED TALKS

SPEAKER	TITLE
Stefan Willitsch	<i>Probing complex chemical reactions with cold and controlled molecules</i>
Christiane Koch	<i>Quantum effects in cold collision</i>
Olivier Dulieu	<i>Ion loss events in a cold Rb-Ca<sup>+</sup> hybrid trap: photodissociation, black-body radiation and non-radiative charge exchange</i>
Johannes Hecker Denschlag	<i>Life and death of a cold BaRb<sup>+</sup> molecule inside an ultracold cloud of Rb</i>
Piotr S. Żuchowski	<i>Toward the accurate prediction of low-energy collision properties</i>
Hendrick L. Bethlem	<i>Cold Molecules for precision tests of fundamental physics</i>
Andreas Buchleitner	<i>Controlled many-particle dynamics: interference vs. interaction</i>
Florian Meinert	<i>Ions and Rydberg atoms under the microscope</i>
Tijs Karman	<i>Shielding ultracold molecules with microwaves</i>
Rene Gerritsma	<i>The quantum physics of interacting atoms and ions</i>
Michał Tomza	<i>Accurate ab initio molecular calculations for ultracold scattering experiments</i>
Silke Ospelkaus	<i>Collisions in ultracold gases of <sup>23</sup>Na<sup>39</sup>K molecules</i>

## 1.2 HOT-TOPIC TALKS

SPEAKER	TITLE
Tim Langen	<i>Self-bound dipolar droplets and supersolids in molecular Bose-Einstein condensates</i>
Omar Abdelkader Khedaoui	<i>Determination of branching ratios of bimolecular reactions of astrochemical interest using chirped pulse Fourier transform microwave spectroscopy</i>
Robert Wild	<i>Measurement of the quantum tunneling reaction <math>H_2 + D^- \rightarrow HD + H^-</math></i>
Baruch Margulis	<i>Quantum Tomography of Feshbach Resonance States</i>
Vikram Plomp	<i>High-resolution imaging of C-He and C-H<sub>2</sub> collisions using a Zeeman decelerator</i>
Adrien Devolder	<i>Coherent control of ultracold molecular collisions: Generalized Optical theorem</i>
Krzysztof Jachymski	<i>Collisional losses of ultracold molecules due to intermediate complex formation</i>

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### 1.3 OVERVIEW OF POSTER CONTRIBUTIONS & MATCHES FOR KARAOKE

PRESENTER (POSTER #)	TITLE
Daniel Bosworth (A1)	<i>Novel trimer states and tunable dynamics in long-range atom-ion Ryberg <b>molecules</b></i>
Markus Deiß (A2)	<i>Spin-conservation propensity rule for three-body recombination of ultracold Rb atoms</i>
Simon Hofsäss (A3)	<i>Buffer gas cooling and optical cycling of AlF molecules</i>
Adam Koza (A4)	<i>Towards collisional cooling of polyatomic <b>molecules</b></i>
Christine Maria Lochmann (A5)	<i>Complex formation in the three-body reaction of Cl<sup>-</sup> with H<sub>2</sub></i>
Rianne Lous (A6)	<i>Buffer gas cooling of ions in time-dependent traps using ultracold atoms</i>
Marijn Peter Man (A7)	<i>Ab initio study of the reactivity of ultracold RbSr + RbSr collisions</i>
Dhritabrata Pal (A8)	<i>Selenium, another chalcogen in the array of hydrogen bonding: a cold matrix isolation infrared spectroscopic study</i>
Caleb Rich (A9)	<i>Collisions between ultracold molecules and atoms in a magnetic trap</i>
Andriana Tsikritea (A10)	<i>Charge transfer reactions between rare gas ions and polar molecules</i>
Marcin Umiński (A11)	<i>Tuning ultracold collisions of He<sup>*</sup>-Li with external magnetic <b>field</b></i>
Pascal Weckesser (A12)	<i>Feshbach resonances between a single ion and ultracold atoms</i>
Zhenlin Wu (A13)	<i>Towards Ultrafast Single Photon Spectroscopy with Trapped Molecular Ions</i>
Krzysztof Zamarski (A14)	<i>Towards Ultracold Ground-State KCs Molecules</i>
Volker Karle (B2)	<i>Topological phases with kicked <b>molecules</b></i>

JuHyeon Lee (B3)	<i>Quantum State Control of Chiral <b>Molecules</b></i>
Mara Meyer zum Alten Borgloh (B4)	<i>Preparing and characterizing ultracold bosonic <sup>23</sup>Na<sup>39</sup>K spin polarized ground state molecules</i>
Chloe Miossec (B5)	<i>Cryogenic ion trap to study cold and controlled ion-radical reactions</i>
Bijit Mukherjee (B6)	<i>Feshbach resonances and molecule formation in ultracold mixtures of Rb and Yb(3P) <b>atoms</b></i>
Tobias Sixt (B7)	<i>Spin-state-controlled Penning collisions between metastable helium atoms and ground-state lithium <b>atoms</b></i>
Alexandra Tsoukala (B9)	<i>Towards controlled reactive collisions between S atoms and D<sub>2</sub> <b>molecule</b></i>
Kai Konrad Voges (B10)	<i>Probing photoinduced two-body loss on nonreactive bosonic ground-state <b>molecules</b></i>
Lok Yiu Wu (B11)	<i>Producing a Cold, Controlled Source of Radicals</i>
Lei Xu (B12)	<i>Conformationally-selected ions for reactions with conformationally-selected molecules</i>

## MATCHES FOR POSTER KARAOKE:

A1 - A14  
A2 - A13  
A3 - A4  
A4 - A3  
A5 - A7  
A6 - A8  
A7 - A5  
A8 - A6  
A9 - A11  
A10 - A12  
A11 - A9  
A12 - A10  
A13 - A2  
A14 - A1  
B2 - B4  
B3 - B7  
B4 - B2  
B5 - B6  
B6 - B5  
B7 - B3  
B9 - B10  
B10 - B9  
B11 - B12  
B12 - B11

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## **2. ABSTRACTS**

### 2.1 INVITED TALKS

## Probing complex chemical reactions with cold and controlled molecules

Stefan Willitsch

*Department of Chemistry, University of Basel*

Recent advances in the development of experimental methods for the manipulation, cooling and trapping of molecules and ions in the gas phase have opened up new avenues for precise studies of the dynamics and mechanisms of chemical reactions. Using electrostatic deflection of molecular beams, molecules can be spatially separated based on their effective dipole moments enabling the isolation of individual rotational states and molecular conformations. Employing this methodology, we have recently developed new experimental approaches for studies of rotational and conformational effects in both ionic and neutral chemical reactions involving polyatomic molecules.

First, we report on the combination of electrostatically deflected beams with Coulomb-crystallised ions in traps for the investigation of conformationally specific reactivities in complex ion-molecule reactions. We discuss recent studies in which we have applied this method to the precise characterisation of the reaction mechanism of polar cycloadditions, i.e., ionic Diels-Alder (DA) reactions, which constitute one of the key routes for the formation of cyclic compounds in synthetic chemistry.

Second, we have recently developed a novel crossed-molecular-beam experiment for investigating reactions of rotationally and conformationally selected strong-field-seeking molecules. The apparatus combines an electrostatically deflected beam which was crossed in a first series of experiments with a beam of metastable rare-gas atoms. Here, we report first results on the rotational and conformational specificities of chemi-ionisation reactions with the examples of OCS and hydroquinone, respectively.

## Quantum effects in cold collision

Christiane Koch

*Freie Universität Berlin*

In cold collisions, where only a few partial waves contribute to the scattering dynamics, the wave nature of matter emerges, becoming observable in e.g. diffraction patterns, interference effects, or scattering resonances. The latter help build an intuitive understanding of the collision process, due to the spatial localization of the resonance wavefunctions. For resonances that are localized behind the centrifugal barrier and thus in the reaction region, sharp peaks in the reaction rates are the characteristic signature. If, however, the localization occurs outside of the reaction region, mostly the elastic scattering is modified. This may occur due to above-barrier resonances, the quantum analogue of classical orbiting. Resonances of both types are found in the example of metastable helium colliding with deuterium molecules [1].

In addition to building intuition, scattering resonances can be exploited to magnify quantum effects in cold collisions. Probing, for example, the resonances with molecules that are rotationally state-selected allows for disentangling the isotropic and anisotropic contributions to the inter-particle interaction [2]. Angle-resolved measurements of the quantum scattering resonances may reveal asymmetric resonance lineshapes, characteristic for Fano interference of a quasi-bound state with a continuum of states [3]. A similar interference effect can also be observed in the product channel of cold reactive collisions populating Fano-Feshbach resonances. These resonances may be protected against decay despite resonant coupling to a scattering continuum if a phase condition is fulfilled. For rare gas diatomic ions, the corresponding phase dependence results in predissociation lifetimes spanning four orders of magnitude, found to be in good agreement with experimental measurements [4].

[1] P. Paliwal et al., *Nature Chemistry* 13, 94 (2021)

[2] A. Klein et al., *Nature Physics* 13, 35 (2017)

[3] P. Paliwal et al., *Nature Commun.* 12, 7249 (2021)

[4] A. Blech et al., *Nature Commun.* 11, 999 (2020)

## **Ion loss events in a cold Rb-Ca<sup>+</sup> hybrid trap: photodissociation, black-body radiation and non-radiative charge exchange**

Xiaodong Xing<sup>1</sup>, Humberto da Silva Jr<sup>1,2</sup>, Romain Vexiau<sup>1</sup>, Nadia Bouloufa-Maafa<sup>1</sup>, and Olivier Dulieu<sup>1</sup>

<sup>1</sup> *Université Paris-Saclay, CNRS, Laboratoire Aimé Cotton, Orsay, France*

<sup>2</sup> *Department of Chemistry and Biochemistry, University of Nevada, Las Vegas, Nevada 89154, USA*

We theoretically investigate the collisional dynamics of laser-cooled <sup>87</sup>Rb ground-state atoms and <sup>40</sup>Ca<sup>+</sup> ground-state ions in the context of the hybrid trap experiment of Ref. [Phys. Rev. Lett. 107, 243202 (2011)], leading to ion losses. Cold <sup>87</sup>Rb<sup>40</sup>Ca<sup>+</sup> ground-state molecular ions are created by radiative association, and we demonstrate that they are protected against photodissociation by black-body radiation and by the <sup>40</sup>Ca<sup>+</sup> cooling laser at 397 nm. This study yields an interpretation of the direct observation of <sup>87</sup>Rb<sup>40</sup>Ca<sup>+</sup> ions in the experiment, in contrast with all other hybrid trap experiments using other species. Based on novel molecular data for spin-orbit interaction, we also confirm that the non-radiative charge-exchange is the dominant ion-loss process and obtain rates in agreement with experimental observations and a previous calculation.

*X. X. acknowledges support from the Chinese Scholarship Council (Grant No. 201706240178).*

## Life and death of a cold BaRb<sup>+</sup> molecule inside an ultracold cloud of Rb

Johannes Hecker Denschlag

*Institut für Quantenmaterie, Universität Ulm*

We study the evolution of a cold single BaRb<sup>+</sup> molecule while it continuously collides with ultracold Rb atoms [1]. The initially weakly bound molecule can undergo a sequence of elastic, inelastic, reactive, and radiative processes. We investigate these processes by developing methods for discriminating between different ion species, electronic states, and kinetic ion energy ranges. By analyzing the experimental data while taking into account theoretical insights, we obtain a consistent description of the typical trajectory through the manifold of available atomic and molecular states. Monte Carlo simulations describe the measured dynamics well.

[1] Amir Mohammadi, Artjom Krüchow, Amir Mahdian, Markus Deiß, Jesús Pérez-Ríos, Humberto da Silva Jr., Maurice Raoult, Olivier Dulieu, and Johannes Hecker Denschlag, *Phys. Rev. Research* **3**, 013196 (2021)

## **Toward the accurate prediction of low-energy collision properties.**

Piotr S. Żuchowski

*Faculty of Physics, Astronomy and Applied Informatics,*

*Institute of Physics, Nicolaus Copernicus University in Torun*

*Centre of Excellence Astrophysics and Astrochemistry*

In the past several years, we have witnessed how theoretical chemistry, when combined with quantum scattering theory, can support the newly designed experiments in the ultracold matter. Thanks to these tools, it was possible:

1. To find new mechanisms of Feshbach resonances in collisions.
2. Predict the feasibility of sympathetic or evaporative cooling.
3. Address individual features in molecular beams experiments in a low kinetic energy regime.
4. Find routes toward the formation of molecules from ultracold atoms.

In this contribution, I will provide a brief account of the achievable accuracy of quantum chemistry. The accuracy of methods translates into the accuracy of the interaction potentials, and I will briefly discuss how the accuracy affects the scattering cross-sections and how sensitive they are for inaccuracies of ab initio quantum chemistry potentials. I will discuss more complex systems what potential problems we fall into while dealing with them. Finally, I will provide some examples of recent experimental works which greatly benefitted from accurate calculations of interaction potentials between atoms and molecules.

## **Cold Molecules for precision tests of fundamental physics**

Hendrick L. Bethlem

*Vrije Universiteit Amsterdam and University of Groningen, The Netherlands*

Polar molecules in general, and heavy polar molecules in particular, have a number of properties that make them highly attractive for experiments that search for new physics. Unfortunately, the same properties that make them attractive, make them difficult to cool and manipulate.

I will discuss two experiments on polar molecules: the first experiment is aimed at measuring a possible variation of the fundamental constants using vibrational transitions in ammonia molecules. The ammonia molecules are decelerated, trapped and adiabatically cooled using a series of ring electrodes to which sinusoidally varying voltages are applied. The electric fields can be rapidly switched off to perform field free spectroscopy with interaction times exceeding one millisecond. I will present results on high resolution spectroscopy of cold ammonia around 1.5 micron.

The second experiment, conducted by the NL-eEDM consortium, is aimed at measuring CP-violating interactions in a barium-monofluoride (BaF) molecules. I will present recent results on deceleration and trapping of SrF and BaF molecules using a 4,5 meter long traveling wave decelerator.

## **Controlled many-particle dynamics: interference vs. interaction**

Andreas Buchleitner

*Physikalisches Institut and EUCOR Centre for Quantum Science and Quantum Computing  
Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg*

State of the art experiments on controlled ensembles of identical particles exhibit a rapidly increasing complexity as the number of constituents is increased. Distinct sources of this complexity are many-particle interferences and interactions, i.e., indistinguishability and dynamical instability, which, however, are rarely discriminated against each other. This appears surprising, e.g., in the debate on many-particle analogues of (single particle) Anderson localization, since the latter is a pure (single particle) interference effect. We'll discuss the interplay of interference and interaction in controlled many-particle dynamics (mostly in a Bose-Hubbard-like setting), and briefly touch upon related issues in spectral and open system theory.



## **Ions and Rydberg atoms under the microscope**

Florian Meinert

*5. Physikalisches Institut, Universität Stuttgart*

Optical quantum gas microscopes have allowed in-situ probing of ultracold matter on an unprecedented level of spatial resolution. This resolution, however, is typically limited by the wavelength of the imaging light. I will report on our endeavor to image individual ultracold atoms by means of an ion microscope to overcome this limit. We demonstrate a spatial resolution of approximately 200 nm and the capability to perform 3D imaging in a pulsed-mode operation.

In a first experiment, we have performed microscopy of a single cold ion interacting with a single Rydberg atom. Our instrument allowed us to observe a novel and only recently predicted molecular bond between the ion and the Rydberg atom, which differs from the well-known ionic and covalent bonds. The bond results from the Rydberg atom's flipping induced dipole moment in the electric field of the ion and ranges up to micrometer distances. We measure the vibrational spectrum, and study the molecule's spatial alignment using our ion microscope. These results pave the way for spatio-temporal studies of molecular dynamics, e.g. beyond Born-Oppenheimer physics or cold collisions and chemistry.

## Shielding ultracold molecules with microwaves

Tijs Karman

*Radboud University Nijmegen, the Netherlands*

In this talk, I will discuss how we can use microwaves to engineer repulsive long-range interactions between ultracold polar molecules [1]. The repulsive interactions prevent molecules from coming close together and thereby suppresses various loss mechanisms. At the same time, "microwave shielding" leads to large elastic cross sections required for thermalization and evaporative cooling -- an elusive milestone in the field. I will discuss the first experimental realization of microwave shielding using cold CaF molecules trapped in optical tweezers [2], demonstrating a factor of six suppression of the inelastic loss. I will also show recent results on microwave shielding a bulk gas of NaK molecules realizing efficient evaporative cooling to a degenerate Fermi gas [3].

[1] Phys. Rev. Lett. **121**, 163401 (2018)

[2] Science **373**, 779 (2021)

[3] arXiv:2201.05143 (2022)

## **The quantum physics of interacting atoms and ions**

Rene Gerritsma

*University of Amsterdam*

In recent years, a novel field of physics and chemistry has developed in which trapped ions and ultracold atomic gases are made to interact with each other. In our experiment, we overlap a cloud of ultracold  ${}^6\text{Li}$  atoms in a dipole trap with a  ${}^{171}\text{Yb}^+$  ion in a Paul trap. We buffer gas-cooled a single  $\text{Yb}^+$  ion to temperatures close to the quantum (or s-wave) limit for  ${}^6\text{Li}$ - $\text{Yb}^+$  collisions. I will discuss recent experiments in which we observed collisions between trapped ions and  $\text{Li}_2$  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 discuss strategies and prospects for reaching deeper into the quantum regime.

## **Accurate *ab initio* molecular calculations for ultracold scattering experiments**

Michał Tomza

*Faculty of Physics, University of Warsaw, Poland*

I will present how molecular electronic structure and quantum scattering calculations can support and explain ultracold quantum physics experiments. Quantum-chemical calculations of potential energy curves, permanent and transition electric dipole moments, fine and hyperfine coupling constants provide parameters for effective Hamiltonians describing nuclear dynamics. Multichannel quantum scattering calculations give scattering lengths, elastic, inelastic, and reactive rate constants. I will discuss the capabilities and limits of state-of-the-art methods applied to neutral and ionic systems based on alkali-metal and alkaline-earth-metal atoms, and present our recent results for ongoing experimental efforts.

## Collisions in ultracold gases of $^{23}\text{Na}^{39}\text{K}$ molecules

P. Gersema, K. K. Voges, M. Meyer zum Alten Borgloh, L. Koch, A. Zenesini, L. Karpa, and S. Ospelkaus

*Institut für Quantenoptik, Leibniz Universität Hannover, Germany*

Understanding and controlling collisions in ultracold gases of all-ground state molecules is of great importance in view of possible applications of the molecules for quantum-many-body physics and precision measurements. Here, we report the preparation of an ultracold gas of bosonic polar  $^{23}\text{Na}^{39}\text{K}$  molecules in a specific hyperfine state of their rovibronic ground state. We analyze the two-body decay of a pure molecular sample and in various atom-molecule mixtures. We find an unexpectedly low two-body decay coefficient for collisions between molecules and  $^{39}\text{K}$  atoms in a selected hyperfine state [1]. Finally, we report about our recent studies of photoinduced-loss processes for the chemically stable  $^{23}\text{Na}^{39}\text{K}$  molecules [2].

[1] K. K. Voges et al. PRL 125, 083401 (2020)

[2] P. Gersema et al. PRL 127, 163401 (2021)

## 2.2 Hot-topic talks

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## **Self-bound dipolar droplets and supersolids in molecular Bose-Einstein condensates**

M. Schmidt<sup>1</sup>, L. Lassablière<sup>2</sup>, G. Quéméner<sup>2</sup> and T. Langen<sup>1</sup>

<sup>1</sup>*Physikalisches Institut and Center for Integrated Quantum Science and Technology, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany*

<sup>2</sup>*Université Paris-Saclay, CNRS, Laboratoire Aimé Cotton, 91405 Orsay, France*

We numerically study the many-body physics of molecular Bose-Einstein condensates with strong dipole-dipole interactions. We observe the formation of self-bound droplets, and explore phase diagrams that feature a variety of exotic supersolid states. In all of these cases, the large and tunable molecular dipole moments enable the study of unexplored regimes and phenomena, including liquid-like density saturation and universal stability scaling laws for droplets, as well as pattern formation and the limits of droplet supersolidity.

We discuss a realistic experimental approach to realize both the required collisional stability of the molecular gases and the independent tunability of their contact and dipolar interaction strengths using a combination of microwave and DC electric fields. Our work provides both a blueprint and a benchmark for near-future experiments with bulk molecular Bose-Einstein condensates.

## **Determination of branching ratios of bimolecular reactions of astrochemical interest using chirped pulse Fourier transform microwave spectroscopy**

Omar Abdelkader Khedaoui, Brian M. Hays, Ilsa R. Cooke, Thomas S. Hearne, Theo Guillaume, Divita Gupta, Myriam Drissi and Ian R. Sims

*Univ Rennes, CNRS, IPR (Institut de Physique de Rennes) - UMR 6251, F-35000 Rennes, France*

The aim of this work is to study gas-phase collisional processes and determine the branching ratios of astrochemically relevant bimolecular reactions taking place in the interstellar medium where the temperatures range from 10 to 100 K, using a combination of the CRESU (Reaction Kinetics in Uniform Supersonic Flow) technique with the chirped pulse Fourier transform micro-(mm-) wave (CPFTMW) spectroscopic technique. The CRESU technique uses a Laval nozzle, through which a gas expands from a high to low pressure environment creating a low temperature flow with uniform conditions that can last for hundreds of microseconds allowing the study of fast and medium rate reactions. To detect reaction products, two microwave spectrometers have been built, one operating in the E band (60-90) GHz and the second covering the Ka band (26.5-40) GHz.

Although CPFTMW spectroscopy is well suited to study cold processes, the technique is highly sensitive to pressure and the recorded signals can be considerably attenuated by collisions. Reducing the collision rate helps creating a favourable environment for the signal detection. One solution developed to achieve this uses a skimmer to sample a small portion of the CRESU flow to undergo a secondary expansion into a higher vacuum established in a secondary turbo-pumped chamber, where both the temperature and pressure of the gas are lowered. A second technique involves the use of pulsed instead of continuous flows to increase the effective pumping capacity by using a perforated disk rotating at the entrance of the nozzle which prevents the gas from expanding until its orifice meets with the nozzle entry, thus reducing the overall flow rate being pumped creating more vacuum and therefore fewer collisions.

Quantitative results on the branching ratios of reactions of CN radicals with alkenes at low temperatures will be presented, and future perspectives discussed



## Measurement of the quantum tunneling reaction $\text{H}_2 + \text{D}^- \rightarrow \text{HD} + \text{H}^-$

Robert Wild<sup>1</sup>, Markus Nötzold<sup>1</sup>, Malcolm Simpson<sup>1</sup>, Thuy Dung Tran<sup>2</sup>, Roland Wester<sup>1</sup>

<sup>1</sup>*Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Innsbruck*

<sup>2</sup>*Department of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University, Prague*

Hydrogen is the most abundant element in the universe, and collisions of hydrogen and its charged forms are important in the chemistry and evolution of the interstellar medium (ISM). Additionally, binary collisions of atomic with molecular hydrogen belong to the most fundamental molecular systems and are simple enough to be theoretically investigated using first-principle methods, providing suitable benchmark systems for quantum calculations.

The rate of the tunneling reaction  $\text{H}_2 + \text{D}^- \rightarrow \text{HD} + \text{H}^-$ , for which the collision complex is closely related to the  $\text{H}_3^-$  anion, has been calculated but has lacked verification. Here we present high-sensitivity measurements of the reaction rate carried out in a cryogenic 22-pole ion trap. We model the effect of a high-energy tail in the velocity distribution to investigate its influence on the reaction rate. Our measured value agrees with quantum tunneling calculations, serving as a benchmark for molecular theory.

## Quantum Tomography of Feshbach Resonance States

Baruch Margulis<sup>1</sup>, Karl Horn<sup>2</sup>, Daniel Reich<sup>2</sup>, Meenu Upadhyay<sup>3</sup>, Mariusz Pawlak<sup>4</sup>, Markus Meuwly<sup>3</sup>, Piotr S. Żuchowski<sup>5</sup>, Christiane Koch<sup>2</sup> and Ed Narevicius<sup>1</sup>

<sup>1</sup>*Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot, Israel.*

<sup>2</sup>*Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, Arnimallee Berlin, Germany*

<sup>3</sup>*Department of Chemistry, University of Basel, Basel, Switzerland*

<sup>4</sup>*Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Toruń, Poland*

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Quantum phenomena that lead to a formation of long-lived collision complexes, such as scattering resonances play a central role to the outcome of cold molecular collisions. These resonances are fundamental probes of the fine details of internuclear interactions and serve as a benchmark for current computational methods.

Here we present a joint experimental and theory study where we are able to generate and investigate the multi-channel decay of a Feshbach resonance state with quantum state-to-state resolution. Our method is based on the coincidence detection of electron/ion momenta in Penning ionization collisions between metastable noble gas atoms and neutral molecules. At the ionization step of the dynamics, the molecular ion-neutral atom system is generated in a specific Feshbach resonance state which is identified by the kinetic energy of the ejected electron. The kinetic energy of the product ions provide information about the decay of each resonance state to a manifold of states which differ by the final vibrational state of the molecular ion. Here, in a single measurement, we obtain both the energy and the composition at the continuum of each resonance state. Such a tomography of the Feshbach resonance states provides several tens of quantum numbers per measurement.

The experimental results pose a formidable challenge to current computational methods. We show that Feshbach state tomography allows us to probe both the short range interactions that are responsible for rovibrational and reactive dynamics as well as the long range part of the potential effecting the energy location of resonances states.

We also present an experimental scheme for control of tomography of the Feshbach states which based on the initial constraint of total angular momentum at the Ionization step of the dynamics. The latter is motivated by our recent observation of a partial wave resonance at the lowest state of relative angular momentum.

## High-resolution imaging of C-He and C-H<sub>2</sub> collisions using a Zeeman decelerator

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The technique of Zeeman deceleration to control collision partners in combination with velocity map imaging (VMI) to probe collision products enables controlled and high-resolution scattering studies for a large class of chemically relevant paramagnetic species [1]. In this work, we combine our Zeeman decelerator and VMI setup with an improved near-threshold resonance-enhanced multiphoton ionization scheme for carbon atoms employing VUV-light. The resulting high-resolution measurements of both C-He and C-H<sub>2</sub> collisions reveal fine details of the state-to-state angular scattering distributions, providing a stringent test for ab initio calculations of the cross sections and complementing previous experimental studies that were insensitive to the angular distributions [2,3].

For both scattering systems narrow spaced diffraction oscillations were resolved. Furthermore, we observed rapid variations in the angular distributions for the C-H<sub>2</sub> scattering system at low collision energies, which can be interpreted in terms of the occurrence of scattering resonances, as well as the consecutive addition of partial waves as the energy increases. Our combination of techniques will allow for a detailed investigation of scattering resonances in low-energy C-He collisions and offers new and exciting prospects to study reactive scattering processes.

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# Coherent control of ultracold molecular collisions: Generalized Optical theorem

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Coherent control is based on coherent superposition of initial internal states, inducing interference of scattering amplitudes to a final state. This method does not require the presence of magnetic (or electric) dipole moments and is complementary to current control methods, based on external fields. In our previous work [1], we have shown that ultracold temperature are ideal conditions for coherent control, thanks to the smaller number of involved partial waves. Via destructive interference, a process can be completely suppressed.

However, this previous study focused on state-to-state cross sections, which unfortunately need complicated coincidence measurements of the two scattered molecules. On the other hand, observation of coherent control would be easier by measurement of total cross section. In standard scattering theory, the total cross-section is related to the imaginary part of the elastic forward scattering amplitude via the optical theorem. We present a generalization of the multichannel optical theorem for the scattering of initial coherent superpositions. Using the generalized optical theorem, we show extensive control of the total cross-section for  $O_2$ - $O_2$  and  $^{85}Rb$ - $^{85}Rb$  collisions (see figure).

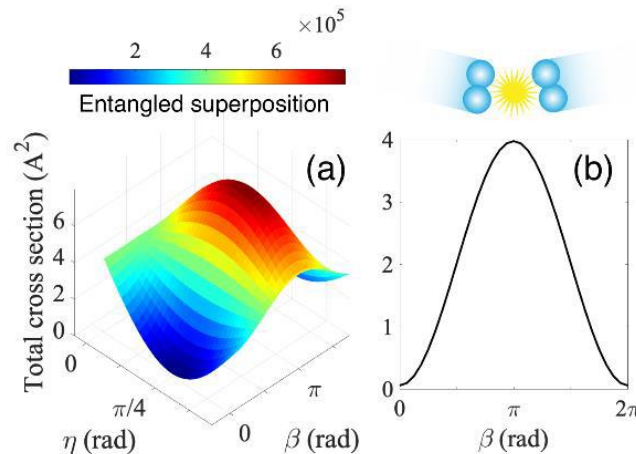


Figure: Coherent control of the total integral cross section for the cold  $O_2+O_2$  collisions at  $10 \mu K$

[1] A. Devolder, P. Brumer, and T. V. Tschberbul, Phys. Rev. Lett. 126, 153403 (2021).

## **Collisional losses of ultracold molecules due to intermediate complex formation**

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Understanding the sources of losses and chemical reactions of ultracold alkali-metal molecules is among the critical elements needed for their application in precision measurements and quantum technologies. Recent experiments with nonreactive systems have reported unexpectedly large loss rates, posing a challenge for theoretical explanation. Here, we examine the dynamics of intermediate four-atom complexes formed in bimolecular collisions. We calculate the nuclear spin-rotation, spin-spin, and quadrupole coupling constants for alkali tetramers using ab initio quantum-chemical methods. We show that the nuclear spin-spin and quadrupole couplings are strong enough to couple different rotational manifolds to increase the density of states and lifetimes of the collision complexes, which is consistent with experimental results.

## 2.3 Poster contributions

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## Novel trimer states and tunable dynamics in long-range atom-ion Ryberg molecules

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We consider a hybrid atom-ion system consisting of a pair of bosons interacting with a single ion in a quasi-one-dimensional trapping geometry. Building upon a model potential for the atom-ion interaction developed in earlier theoretical works [1], we investigate the behavior of the low-energy eigenstates for varying contact interaction strength  $g$  among the atoms. In particular, we contrast the two cases of a static ion and a mobile ion. Our study is carried out by means of the multilayer multiconfiguration time-dependent Hartree method for bosons (MCTDHB) [2], a numerically exact *ab initio* method for the efficient simulation of entangled mixtures. We find that repulsive atom interactions induce locally distinct modifications of the atomic probability distribution unique to each eigenstate. While the atoms on average separate from each other with increasing  $g$ , they do not necessarily separate from the ion. The mobility of the ion leads in general to greater separations among the atoms as well as between the atoms and the ion. Notably, we observe an exchange between the kinetic energy of the atoms and the atom-ion interaction energy for all eigenstates, which is both interaction and mobility induced. For the ground state, we provide an intuitive description by constructing an effective Hamiltonian for each species, which aptly captures the response of the atoms to the ion's mobility. Furthermore, the effective picture predicts enhanced localization of the ion, in agreement with our results from exact numerical simulations.

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[2]: Krönke et al. New J. Phys. 15 063018 (2013)

[3]: Bosworth et al. PRA 103 033303 (2021)

## Spin-conservation propensity rule for three-body recombination of ultracold Rb atoms

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Three-body recombination is a fundamental reaction process where in a collision of three atoms a diatomic molecule is produced. We investigate three-body recombination in a state-to-state resolved way using an ultracold gas of Rb atoms. Our experiments show that the hyperfine state of the atom pair forming the molecule is conserved. Interestingly, this spin propensity rule holds for both, samples of <sup>87</sup>Rb atoms and samples of <sup>85</sup>Rb atoms, despite the fact that the two species have drastically different scattering properties. We explore the physical origin and the general validity of the spin propensity rule. This allows us to formulate criteria in order to assess whether the hyperfine spin state is conserved in three-body recombination or not, for different parameter regimes, collision channels and reactant species.



## Topological phases with kicked molecules

Volker Karle

*IST Austria*

During the last decades technological advances have made possible unprecedented coherent control of molecules. Improved control of the duration and temporal shape of laser pulses opens up new possibilities to create platforms for quantum simulation and information processing. In my work I propose to use molecules kicked by lasers as a non-hermitian topological system to probe topological modes. Exploiting non-trivial topological properties is considered to be one promising pathway for quantum computation, since topological modes are protected against decoherence.

My theoretical work lays the foundation for experiments feasible already now. This poses a thrilling opportunity, in so far as controlling topological transitions in materials usually requires changing the material or structural properties. Whereas topological states in condensed matter systems often show up as macroscopic properties, the topological states of a quantum optical system can be probed directly in a non-destructive way.

Specifically, I show how it is possible to simulate topological insulators with chiral and time-reversal symmetries using quantum resonances. At triple resonance the  $C_2$  and time-reversal symmetry leads to topological Dirac cones, which give rise to integer Euler invariants. These non-Abelian topological invariants open the possibility of braiding the Dirac cones with each other. Changing the strength and the shape of the laser potential, topological phase transitions are observed and new Dirac cones emerge. Further, I outline how at a critical strength an anomalous Floquet Dirac cones appear, which connects the first with the third band over the periodic boundary. Finally, I outline how immersing the kicked molecule into a quantum bath turns the system into a many-body system. The question how entanglement changes the topological properties of quasi-particles is of current interest in topological physics and can be explored with this system in a novel way.

## **Towards collisional cooling of polyatomic molecules**

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The last decades have been the time of intensive development of chemistry and physics of ultracold matter, both in terms of theoretical description and experimental methods. Currently, finding effective methods of cooling polyatomic molecules has become a significant challenge. One possibility is sympathetic cooling, based on cooling the pre-cooled system by interactions with ultracold atomic gas. Invaluable help in this regard is the possibly accurate quantumchemical description of the molecular systems under consideration, including intermolecular interactions.

In this project, the system consisting of a formaldehyde molecule interacting with metal atoms of groups 1 and 2 of the periodic table of elements was considered. Particular attention has been paid to the CH<sub>2</sub>O+Rb system. Calculations of the electronic structure were carried out using the coupled-clusters method in the CCSD(T) variant within the Born-Oppenheimer approximation. The results obtained with the use of different functional basis sets were compared. For final calculations, the aug-cc-pwC5Z-PP basis sets were used for the metal atoms and aug-cc-PV5Z basis sets for the H, C and O atoms. Core electrons were replaced with pseudopotentials for heavier atoms. Based on the obtained results, interaction curves for various geometries were obtained, and in the case of rubidium, two 2D cuts of the potential energy hypersurface. Both cuts were expanded into a Legendre polynomial basis. The chemical reactivity between metal atoms in ground and excited electronic state was studied to identify the most promising system for experimental implementation.

## Complex formation in the three-body reaction of Cl<sup>-</sup> with H<sub>2</sub>

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Dihydrogen halide clusters are the subject of various theoretical and experimental studies. In their anionic state they are weakly bound complexes and can provide insight into dynamical processes in chemical reactions [1]. Here we report the three-body reaction rate of Cl<sup>-</sup> with H<sub>2</sub> forming the Cl<sup>-</sup>(H<sub>2</sub>) complex, as well as the temperature dependence of this reaction in the range of 10 – 26K [2]. Furthermore, we observe the back-reaction with an unexpected dependence to the third power of the H<sub>2</sub> density. Comparisons of the experiment in a 22-pole rod and a newly installed 16-pole wire trap [3] are presented and show that the ions reach lower temperature in the 16-pole trap.

We recently also observed a three-body process in the reaction of C<sub>2</sub><sup>-</sup> with two H<sub>2</sub> which leads to the product C<sub>2</sub>H<sup>-</sup>. In the future, we plan on expanding the research of three-body reactions at low temperatures. One focus will be the influence of the nuclear spin state of Hydrogen on the three-body rate of Cl<sup>-</sup> with H<sub>2</sub>.

[1] F. Dahlmann, et al., J. Chem. Phys. (in press) (2021); <https://doi.org/10.1063/5.0073749>

[2] R. Wild, et al., J. Phys. Chem. A 2021, 125, 39, 8581–8586

[3] K. Geistlinger, et al., Rev. Sci. Instrum. 92, 023204 (2021)

## **Buffer gas cooling of ions in time-dependent traps using ultracold atoms**

Rianne S. Lous

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For exploration of quantum effects with hybrid atom-ion systems, reaching ultracold temperatures is the major limiting factor. In this work, we present results on numerical simulations of trapped ion buffer gas cooling using an ultracold atomic gas in a large number of experimentally realistic scenarios. We explore the suppression of micromotion-induced heating effects through optimization of trap parameters for various radio-frequency (rf) traps and rf driving schemes including linear and octupole traps, digital Paul traps, rotating traps and hybrid optical/rf traps [1]. We find that very similar ion energies can be reached in all of them even when considering experimental imperfections that cause so-called excess micromotion. Moreover we look into a quantum description of the system and show that quantum mechanics cannot save the ion from micromotion-induced heating in an atom-ion collision. The results suggest that buffer gas cooling can be used to reach close to the ion's groundstate of motion and is even competitive when compared to some sub-Doppler cooling techniques such as Sisyphus cooling. Thus, buffer gas cooling is a viable alternative for ions that are not amenable to laser cooling, a result that may be of interest for studies into quantum chemistry and precision spectroscopy.

[1] Trimby et al., arXiv:2109.15195

## Ab initio study of the reactivity of ultracold RbSr + RbSr collisions

Marijn P. Man

*(Radboud University) (Based on work co-authored by Tijs Karman and Gerrit C. Groenenboom)*

We perform ab initio calculations in order to assess the reactivity of ultracold RbSr ( $^2\Sigma^+$ ) + RbSr ( $^2\Sigma^+$ ) collisions occurring on the singlet as well as the triplet potential. At ultracold energies reactions are energetically possible if they release energy, i.e., they are exoergic.

We find that, in addition to the formation of Rb<sub>2</sub>+2Sr and Rb<sub>2</sub>+Sr<sub>2</sub> in singlet collisions, also the formation of Sr<sub>2</sub>Rb+Rb and Rb<sub>2</sub>Sr+Sr in both singlet and triplet collisions is exoergic. Hence, the formation of these reaction products is energetically possible in ultracold collisions. We find barrierless qualitative reaction paths leading to the formation of the Rb<sub>2</sub>Sr+Sr, Sr<sub>2</sub>Rb+Rb, and singlet Rb<sub>2</sub>+2Sr reaction products and show that a reaction path with at most a submerged barrier exists for the creation of the singlet Rb<sub>2</sub>+Sr<sub>2</sub> reaction product. Because of the existence of these reactions we expect ultracold RbSr collisions to result in almost universal loss even on the triplet potential.

## **Preparing and characterizing ultracold bosonic $^{23}\text{Na}^{39}\text{K}$ spin polarized ground state molecules**

Mara Meyer zum Alten Borgloh

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Recently, ultracold polar molecules have become the focus of interest for research in quantum chemistry and metrology. Heteronuclear molecules have a large electric dipole moment, which allows the study of long-range and anisotropic dipole-dipole interactions. Moreover, their large number of degrees of freedom, such as rotation and vibration, opens up new possibilities for quantum simulations.

We report the preparation of ground-state bosonic spin-polarized NaK molecules with a large electric dipole moment of 2.7 D. Starting from an ultracold quantum gas mixture of K and Na atoms, we first generate weakly bound molecules near a Feshbach resonance. The Feshbach molecules are then transformed into strongly bound molecules in the absolute molecular ground state by stimulated Raman adiabatic passage (STIRAP). The STIRAP pulse is performed within 12  $\mu\text{s}$  and has an efficiency of about 70 %, preparing up to 4200 molecules at a temperature of about 300 nK. Finally, we report the dependence of the energy structure of the vibrational ground state manifold on the electric field and the manipulation of the molecular hyperfine and rotational state.

## **Cryogenic ion trap to study cold and controlled ion-radical reactions**

Chloé Miossec

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Ion-radical reactions are an important part of the gas phase chemistry that takes place in extreme environments such as the interstellar medium or outer regions of our atmosphere. However, their complexity and high reactivity makes them difficult to study in isolation.

We have built an ion trap which, combined with a Zeeman decelerator[1], will give us enough control to study ion-radical reactions under cold, controlled conditions. To achieve such control, the ion trap is cryogenically cooled to less than 10 K, and features an anti-vibration system, a new optical system designed for the imaging of Coulomb crystals, and a flight tube to record TOF mass spectra at selected reaction times. The optical system has previously been tested ex-vacuo at room temperature [2]. We now characterize it in vacuo, under both room temperature and at low temperature conditions.

Analysis of our experimental characterisation studies confirms that the ion trap reaches the low temperatures expected ( $\approx 10$  K). It also shows that the resolution of the images recorded with the new optical system is not impacted by the cryogenic temperatures of the ion trap, nor by the vibrations from the cryocooler, which are very effectively damped.

These results confirm that the cryogenic ion trap apparatus meets all requirements for the study of ion-radical reactions using Coulomb crystals.

**Acknowledgments:** This work was supported by the EPSRC (Engineering and Physical Sciences Research Council of the UK) and the ERC (European Research Council).

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## Feshbach resonances and molecule formation in ultracold mixtures of Rb and Yb( $^3P$ ) atoms

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We have investigated magnetically tunable Feshbach resonances in ultracold collisions of Rb with Yb in its metastable  $^3P_2$  and  $^3P_0$  states, using coupled-channel scattering and bound-state calculations [1]. For the  $^3P_2$  state, we find sharp resonances when both atoms are in their lowest Zeeman sublevels. However, these resonances are decayed by inelastic processes that produce Yb atoms in  $^3P_1$  and  $^3P_0$  states. The molecules that might be formed by magnetoassociation at the  $^3P_2$  thresholds have lifetimes typically of the order of few microseconds. For the  $^3P_0$  state, by contrast, there are resonances that are promising for magnetoassociation. The patterns of the bound states that cause resonances here are closely analogous to those for Yb( $^1S$ ) [2].

However, there are additional couplings for Yb( $^3P_0$ ) that arise directly from the electrostatic potential-energy curves and spin-orbit coupling, and do not rely on the distance-dependence of the hyperfine coupling. These couplings produce resonances due to both rotating and non-rotating molecular states that are significantly stronger than the analogous resonances for Yb( $^1S$ ) [2-3]. The ones due to rotating states are denser in magnetic field; in contrast to Yb( $^1S$ ), they exist even for bosonic isotopes of Yb( $^3P_0$ ). Molecules formed by magnetoassociation of Yb( $^3P_0$ ) can decay only by processes that form Yb( $^1S$ ), with or without excitation of Rb to its  $^2P$  state, so are expected to be long-lived.

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3. D. A. Brue and J. M. Hutson, Phys. Rev. A, **87**, 052709 (2013).



## **Probing photoinduced two-body loss on nonreactive bosonic ground-state molecules**

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Recently, ultracold molecular quantum gases have been found to suffer from rapid two-body losses. These losses are caused by the formation of so-called sticky tetramer complexes, which are then destroyed by collisions or photoinduced processes.

Here we report on our investigations of photoinduced losses of  $(\text{NaK})_2$  tetramers in bosonic quantum gases of NaK molecules. The predicted lifetime of the  $(\text{NaK})$  complexes of  $6 \mu\text{s}$  should allow us to keep the molecules in the dark for a considerable time and to significantly suppress the two-body decay of the NaK molecules. However, we do not observe any suppression in the parameter range that is achievable for us. Our results suggest that either the lifetime of the complex is drastically underestimated and could be up to two orders of magnitude higher than previously thought, or that other, as yet unknown, loss mechanisms prevail in our system.

## **Selenium, another chalcogen in the array of hydrogen bonding: a cold matrix isolation infrared spectroscopic study**

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With the modification of the definition of hydrogen bonding in 2011 by the IUPAC committee [1], there has been a pursuit of broadening the hydrogen bonding horizon. Along the chalcogen series, oxygen (O) has been known to participate in hydrogen bonding for ages. Sulphur (S) has also been added to the list of hydrogen bonding motifs, with almost equivalent H-bond strength compared to O [2]. The next element to S is Selenium (Se), having an electronegativity of 2.55 compared to S (2.58) on the Pauling scale. Hence, it is expected to engage in hydrogen bonding. Se is an essential element due to its presence in selenocysteine, the 21<sup>st</sup> amino acid, and selenomethionine. Although Se is present in amino acids, the domain of hydrogen bonding of Se has been rarely investigated. Only a few experimental and theoretical reports are available in the literature owing to the hydrogen bonding property of Se.

Herein, the hydrogen bonding acceptor property of Se has been explored using the cold condition of Matrix Isolation combined with Infrared spectroscopy. The experiments have been performed at 8 K with Dimethyl Selenide [(CH<sub>3</sub>)<sub>2</sub>Se] as acceptor and different O-H donors (Water, Methanol, and Ethanol) in argon and nitrogen matrices. The formation of the complexes is monitored by changes in the infrared spectral patterns compared to the monomer spectra. The nature of the intermolecular complexes formed has been characterised using quantum chemical calculations. Comparing the theoretical and experimental results, it is concluded that the complexes formed under the cold condition are stabilised by O-H...Se hydrogen bonding interaction. Finally, the strength of the selenium-centered hydrogen bonding has been compared with two of the analogous chalcogens, i.e., Oxygen and Sulphur. Surprisingly, it is found that Se forms a hydrogen bond of almost equal strength of that of O and S.

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## Feshbach resonances between a single ion and ultracold atoms

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The fields of ultracold atoms and trapped ions are important pillars of experimental quantum optics. Recently the expertise of both fields has been combined in hybrid trapping setups [1] with the aim to prepare atom-ion mixtures at low temperatures close to the few-partial wave regime. There, new quantum phenomena such as atom-ion Feshbach resonances and the formation of mesoscopic, weakly bound molecules have been predicted. However, reaching the ultracold regime in hybrid setups is a challenging task, as intrinsic micromotion heating effects of conventional radio-frequency (rf) traps [2] limit most experiments.

In our experiments in Freiburg, we follow two pathways to overcome these heating effects allowing us to enter the few-partial wave regime. On the one hand, we choose an atom-ion mixture with high mass imbalance – <sup>6</sup>Li atoms and <sup>138</sup>Ba<sup>+</sup> ions – as comparably heavy ions are subject to less heating [2,3]. On the other hand, we have developed optical dipole traps for ions allowing us to probe atom-ion interactions in complete absence of rf fields [4].

In this talk, I demonstrate the first observation of Feshbach resonances between Ba<sup>+</sup> ions and Li atoms [5]. We find a total of 11 resonances by magnetic-field dependent ion loss spectroscopy and identify four of them as s-wave resonances. Operating with lower densities we can suppress inelastic three-body recombination, allowing us to apply Feshbach resonances to control the ion's sympathetic cooling rate. In the future, we want to apply these findings to store atoms and ions in a combined optical dipole trap while operating in the s-wave limit.

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## Buffer gas cooling and optical cycling of AIF molecules

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Ultracold, polar molecules promise many new applications in fundamental physics and chemistry. In particular, aluminium monofluoride (AIF) is a promising candidate to produce a dense, ultracold gas through laser cooling.

We show that AIF can be produced very efficiently in a bright, pulsed cryogenic buffer gas molecular beam, and demonstrate rapid optical cycling on the Q rotational lines of the  $A^1\Pi \leftrightarrow X^1\Sigma^+$  transition near 228 nm.<sup>1</sup> This is the first step towards cooling the molecules to ultracold temperatures in a magneto-optical trap (MOT). We measure the brightness of the molecular beam to be  $>10^{12}$  molecules per steradian per pulse in a single rotational state and present a new method to determine its velocity distribution accurately using a single molecular pulse. The photon scattering rate is compared to theoretical predictions of the optical Bloch equations and a rate equation model. An exceptionally high scattering rate can be sustained despite the large number of Zeeman sublevels (up to 216 for the Q(4) transition) involved in the optical cycle. We demonstrate that losses from the optical cycle due to vibrational branching to  $X^1\Sigma^+, v = 1$  can be addressed efficiently with a repump laser, allowing us to scatter about  $10^4$  photons using two lasers. Further, we investigate two other loss channels, photo-ionisation and parity mixing by stray electric fields. The upper bounds for these effects are sufficiently low to allow loading the molecules into a MOT.

We also present our recent progress in creating a dense and cold cloud of cadmium (Cd) atoms using the  $^1P_1 \leftarrow ^1S_0$  transition near 229 nm. Cd is an excellent test species for our MOT apparatus as it shares many properties with the more complex case of AIF.

<sup>1</sup>S. Hofsäss, et al. "Optical cycling of AIF molecules." *New Journal of Physics* (2021)

## Quantum State Control of Chiral Molecules

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The two non-superimposable mirror images of a chiral molecule are referred to as enantiomers. Even though most physical properties of enantiomers are identical – which makes them intrinsically challenging to separate – their handedness often determines their functionality. There is a plethora of scientific methods to study chirality; however, chiral analysis, particularly for complex samples, is still challenging. Recently, the enantiomer-specific state transfer (ESST) method [1] was demonstrated using tailored microwave fields. This method allows to populate or depopulate a rotational state of a chosen enantiomer, providing a way of quantum-controlled chiral separation. Thus far, the transfer efficiency of ESST has been limited by thermal population of the energy levels participating in ESST [1,2] and by  $M_J$  degeneracy [3].

To address these prior limitations, we developed a new experimental scheme which increases the efficiency of ESST by over a factor of ten compared to previously reported values [4]. This scheme enables a quantitative comparison between experiment and theory for the transfer efficiency in what is the simplest ESST triangle for any chiral molecule, that is, the one involving the absolute ground state level,  $|JK_aK_c\rangle = |000\rangle$ . Starting with a racemic mixture, a straightforward extension of this scheme should be able to create a molecular beam with an enantiomer-pure rotational level, holding great prospects for future spectroscopic and scattering studies.

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## Spin-state-controlled Penning collisions between metastable helium atoms and ground-state lithium atoms

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Ultracold trapped mixtures of different atomic species are the starting point to obtain ultracold heteronuclear molecules, which may feature long-range and anisotropic interactions. Such interactions allow for new physics and chemistry studies in a regime which is purely dominated by quantum effects. To achieve the co-trapping of ultracold alkali atoms and metastable rare-gas atoms, Penning-ionizing collisions must be efficiently suppressed. As a first step towards co-trapping, we study quantum-state-controlled Penning collisions between metastable helium atoms ( $\text{He}^*$ ) and ground-state lithium atoms (Li) in order to investigate efficient ways of controlling the outcome of such ionizing collisions. For this, we have combined a supersonic-beam source for  $\text{He}^*$  with a magneto-optical trap (MOT) for Li [1]. In order to distinguish in between the contributions of  $\text{He}(2^3\text{S}_1)$  and  $\text{He}(2^1\text{S}_0)$  to the reaction rate, we deplete the population in the  $2^1\text{S}_0$  level using a novel optical-excitation scheme [2]. Furthermore, we use laser-optical pumping to prepare both  $\text{He}(2^3\text{S}_1)$  and  $\text{Li}(2^2\text{S}_{1/2})$  in selected magnetic sub-levels prior to the collision [3].

In this contribution, we demonstrate the efficient control of  $\text{He}(2^3\text{S}_1)\text{-Li}(2^2\text{S}_{1/2})$  Penning ionization by spin-state preparation. Our results imply a strong suppression (enhancement) of Penning-ionizing collisions for non-spin-conserving (spin-conserving) reaction channels. Our results are in good agreement with a model based on spin angular momentum coupling of the prepared atomic states to the molecular reaction channels. Small deviations from the model indicate the contribution of quartet states to the reaction rate, which is in violation of spin-conservation rules.

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## Collisions between ultracold molecules and atoms in a magnetic trap

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Recent work has demonstrated direct laser cooling of diatomic molecules to temperatures of around 5  $\mu\text{K}$ . A promising route to increase the phase-space density is sympathetic cooling with evaporatively cooled atoms. This requires a favourable ratio of elastic to inelastic collisions rates.

We demonstrate a dual species magneto-optical trap of CaF molecules and Rb atoms. After a stage of sub-Doppler cooling and quantum state preparation both species are transferred into a magnetic quadrupole trap. When the molecules are prepared in the first rotationally-excited state, we observe rapid loss due to rotation-changing collisions with the atoms [1]. By contrast, when the molecules are in the ground rotational state we see no inelastic loss. Comparing these measurements to the results of a single-channel loss model based on quantum defect theory, we find a short-range loss parameter close to unity for rotationally excited molecules, but below 0.04 for molecules in the rotational ground state. These results are promising for the prospects of sympathetic cooling of molecules using ultracold atoms.

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## Charge transfer reactions between rare gas ions and polar molecules

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Ca<sup>+</sup> Coulomb crystals are used as a cold framework to undertake reactions between sympathetically cooled rare gas ions (Xe<sup>+</sup>, Kr<sup>+</sup> or Ar<sup>+</sup>) and polar molecules (NH<sub>3</sub>, ND<sub>3</sub>, H<sub>2</sub>O or D<sub>2</sub>O) [1-3]. The experimentally calculated reaction rate coefficients are compared with predictions from capture theory models. For the ammonia reactions, capture theory predictions do not agree with our findings. Additionally, an inverse kinetic isotope effect (KIE) is observed; ND<sub>3</sub> reacts faster than NH<sub>3</sub>. Conversely, capture theory predictions are in excellent agreement with the water reaction rate coefficients and no KIEs are observed. The success of capture theories in predicting the behaviour of these reactions, and future experiments to further probe the mechanism of the charge transfer reactions, will be discussed.

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## Towards controlled reactive collisions between S atoms and D<sub>2</sub> molecule

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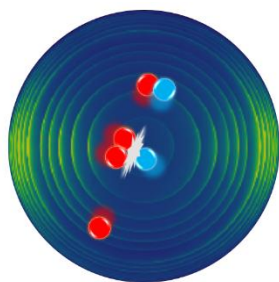
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One of the greatest challenges in the field of molecular reaction dynamics is the ability to control the reagents' degrees of freedom towards selective product formation. Studying such selectively driven reactions in the cold regime is of particular scientific importance, since the wave nature of the atoms governs the reactivity and quantum effects reveal themselves.

In our lab we combine a Zeeman decelerator with the Velocity Map Imaging technique. The decelerator allows for full velocity and quantum state control of the atomic or molecular beam prior to collisions, while Velocity Map Imaging together with near-threshold ionization can be used to probe the reaction products with high precision. This combination of techniques thus enables scattering experiments with extraordinary resolution, revealing intimate details of molecular collisions that are washed out otherwise.

So far, this experimental approach has only been used in inelastic scattering experiments, where we have been able to observe quantum phenomena such as diffraction oscillations and scattering resonances. In the near future, we plan to use our powerful techniques to study reactive scattering for the very first time, starting with the prototypical insertion reaction between sulfur atoms (S) and molecular deuterium (D<sub>2</sub>).

In this contribution I will describe our experimental approach and report the progress we have made so far concerning the control of this reaction.



## Tuning ultracold collisions of He\*-Li with external magnetic field

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One of the main goals of studying cold matter is to broaden our knowledge of mechanisms underlying chemical reactions. Recent advances in the field of cold matter experiments bring us closer to observing how chemical reactions may be precisely controlled. Feshbach resonances, which we observe in cold regime, are a quantum phenomenon playing a crucial role in the results of atom and molecule collisions. Alkali atoms and helium are good examples to observe due to their simple structures. Here we are examining a model system in which chemical reaction controlled by external field can be studied: the cold collisions of Li atoms with metastable helium (labelled as He\*) in magnetic field.

He\*-Li molecules may come in one of two spin states: a stable, spin-polarized quartet state and unstable, low-spin doublet state, in which we observe the Penning ionization. The bound states are mixtures of these two states.

To describe them we use two interaction potentials: a real, published before Morse/Long-Range potential describing quartet state and a predicted, theoretical complex potential of doublet state. To characterize the low-energy collisions we use the renormalized Numerov method and discrete variable representation.

As we are interested in dependency on external magnetic field, we also consider Zeeman effect, which allows us to carefully shift Energy levels. Using this, we may tune our system to allow Feshbach resonances to happen. In proximity of resonances, we expect to observe increased rate of inelastic reactions, and thus ion production. Depending on the composition of these two states, the Feshbach resonances, which originate from them, might have different loss rates and shapes. Taking advantage of the mentioned properties we may, for the first time, observe chemical reactions induced by magnetic field.

## Producing a Cold, Controlled Source of Radicals

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Producing a pure, state-selected beam of gas-phase radicals – with a tuneable velocity – in the laboratory is rife with challenges. Yet, it is one of the most important tools we need in our arsenal to precisely study ion-radical reactions that are astrochemically and atmospherically relevant.<sup>1</sup> Taking advantage of the paramagnetic behaviour of radicals, we can use external magnetic fields to filter out only the target species (that are travelling at a selected velocity) from a beam containing a mixture of other species. A CMA-ES evolutionary algorithm<sup>2</sup> has been applied to optimise the passage of a beam of H atoms, starting from a source with a mixture of species present through to the detection region, passing through a 12-stage Zeeman decelerator and a magnetic guide composed of 4 Halbach arrays and 2 skimming blades. The combined optimised switching sequence and vertical displacements of the arrays and blades from the central beam axis significantly improves on previous best<sup>3</sup> methods, achieving a 3.4-fold increase in particle numbers and a narrower velocity distribution of transmitted particles. Based on these findings, a second-generation magnetic guide is being designed to act as a stand-alone radical filter. The second-generation guide will feature additional Halbach arrays, to improve transverse focusing of the beam and to target O and OH radicals. This will be interfaced with a liquid surface, expanding the scope of relevant chemical reactions that can be studied with exceptional control over the properties of the reaction.

This work was supported by the Engineering and Physical Sciences Research Council (EPSRC), the European Research Council (ERC) and the Community for Analytical Measurement Science (CAMS).

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## **Towards Ultrafast Single Photon Spectroscopy with Trapped Molecular Ions**

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Over the past decades, trapped atomic ions have developed into one of the most promising platforms for realizing quantum simulation and quantum computation. The highly controllable atomic qubits can also be used to probe and control co-trapped single molecular ion. Recently impressive progress has been achieved in diatomic molecular ions like  $\text{CaH}^+$  and  $\text{N}_2^+$ , realizing non-demolition state detection of molecular ions by coupling them to an atomic logic ion via a common motional mode.

We aim to introduce entanglement enhanced single photon absorption spectroscopy to study ultrafast molecular dynamics on the platform. By preparing the auxiliary atomic ion in a non-classical cat state, the recoil signal produced by single photon absorption events on the target molecular ion can be amplified and read out. In this way, we plan to investigate intramolecular behaviours in time domain using ultrafast laser pulses. This may pave the way to the study of polyatomic molecules with complex vibrational structure at the single molecule level.

The experimental system we are building consists of a linear Paul trap from AQT at room temperature, compact rack-based laser systems for manipulating  $\text{Ca}^+$  qubits and a high-power pulsed laser for performing spectroscopy. The laser can generate ultrafast pulses at the femtosecond scale for studying molecule vibration and has a wide tuning range from 210 to 16000 nm that allow us to explore most vibrational modes in molecules. Currently we are at the stage of setting up the system for trapping our first  $\text{Ca}^+$  ion and we will start with proof of concept experiments on simple diatomic ions like  $\text{CaH}^+$ .

## Conformationally-selected ions for reactions with conformationally-selected molecules

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The different effective dipole moment of conformational isomers allows for their spatial separation by means of electrostatic deflection, enabling their individual reactivity to be investigated<sup>1</sup>. Recently, the conformerspecific polar cycloaddition of dibromobutadiene (DBB) with trapped propene ions has shown that both gauche and s-trans DBB conformers display capture-limited reaction rates<sup>2</sup>. The reaction was found to occur through both a concerted and a stepwise reaction mechanism, despite the spatial rearrangement of atoms necessary in s-trans DBB for the latter to take place.

These results were obtained by selectively aiming the molecular beam containing either one of the two conformers at a static target of propene ions embedded within a laser-cooled Coulomb crystal of calcium ions. In order to gain further control over the reaction partners, we now wish to also select the conformational isomer of the ionic reactant. Here, we discuss the generation of conformationally--selected ionic targets of meta-methoxystyrene to enable the study of fully-conformationally-selected ion–molecule reactions. Following the detailed study of the isomer-selective ionisation of the four different m-methoxystyrene conformers, we aim to individually load them into a Coulomb crystal to determine their stability to such environment.

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## **Towards Ultracold Ground-State KCs Molecules**

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Ultracold atomic gases have proven to be a versatile tool for the study of many-body quantum mechanics, but despite a wide variety of exhibited phenomena, single alkali atoms interact only via short-range, isotropic contact interactions. One of the most common methods of introducing long-range dipolar interactions into the system is replacing single atoms with heteronuclear diatomic molecules, which carry a significant electric dipole moment and can be prepared in their absolute ground state. The focus of our project is the KCs molecule, which has not yet been observed in the ultracold regime. Its main advantages are a large dipole moment (1.92 Debye), chemical stability, and the option to switch between bosonic and fermionic isotopes. In our current setup, we are researching possible cooling and mixing schemes for potassium and cesium. Simultaneously, we are building an upgraded version of the setup, in which we are planning to produce KCs molecules using the technique of Feshbach association, followed by a stimulated Raman adiabatic passage (STIRAP), which has been shown to transfer molecules to their absolute ground state with up to 90% efficiency. Once an ultracold molecular sample is prepared, we will be able to control the dipolar interactions using high electric fields, load the molecules into an optical lattice, and image individual lattice sites using a high-resolution objective. Such a well-controlled system will provide an excellent platform for studying lattice spin models, exotic phases of matter and the possibility of implementing a molecule-based qubit.

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## 4. ACKNOWLEDGMENTS & LIST OF SPONSORS

The organizers of this workshop gratefully acknowledge support from the following organizations and companies:



The organizers would like to thank the event management team of FRIAS, in particular Mrs. Kyra Vogt and Mr. Attilio Ferrarese.