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05-08 September 2023, Warsaw, Poland

Workshop on ultracold molecules 2023
Program and abstracts

ultracold-molecules-2023.fuw.edu.pl

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Excellence Initiative – Research University (2020-2026)

EXCELLENCE INITIATIVE RESEARCH UNIVERSITY

Faculty of Physics, University of Warsaw

FACULTY OF PHYSICS
UNIVERSITY OF WARSAW

Chairs of the conference

Michał Tomza, University of Warsaw, Poland

Piotr Żuchowski, Nicolaus Copernicus University, Poland

Organising commitee

Krzysztof Jachymski, University of Warsaw, Poland

Marcin Gronowski, University of Warsaw, Poland

Mariusz Semczuk, University of Warsaw, Poland

Matthew Frye, University of Warsaw, Poland

Kacper Cybiński, University of Warsaw, Poland

Invited Speakers

Loic Anderegg, Harvard University, USA

Thomas Bilitewski, Oklahoma State University, USA

Mateusz Borkowski, Columbia University, USA

Simon Cornish, Durham University, United Kingdom

Matthew Eiles, Max Planck Institute for the Physics of Complex Systems, Germany

Kaden Hazzard, Rice University, USA

Jeremy Hutson, Durham University, United Kingdom

Alan Jamison, University of Waterloo, Canada

Tijs Karman, Radboud University, the Netherlands

Christiane Koch, Free University of Berlin, Germany

Tim Langen, University of Stuttgart, Germany

Mikhail Lemeshko, IST Austria, Vienna, Austria

Maxence Lepers, University of Burgundy, Dijon, France

Xin-Yu Luo, Max-Planck-Institute for Quantum Optics, Germany

Bas van de Meerakker, Radboud University, the Netherlands

Edvardas Narevicius, TU Dortmund University, Germany

Silke Ospelkaus-Schwarzer, Leibniz University Hannover, Germany

Gabriel Patenotte, Harvard University, USA

Gerhard Rempe, Max-Planck-Institute for Quantum Optics, Germany

Florian Schreck, University of Amsterdam, the Netherlands

Michael Tarbutt, Imperial College London, United Kingdom

Stefan Truppe, Imperial College London, United Kingdom

Timur Tscherbul, University of Nevada, Reno, USA

Sebastian Will, Columbia University, USA

Aleksander Woźniak, University of Warsaw, Poland

Calder Miller, JILA, University of Colorado Boulder, USA

Hot-Topic Speakers

Roman Bause, University of Groningen, the Netherlands

Luke Caldwell, University College London, United Kingdom

Yuly Andrea Chamorro Mena, University of Groningen, the Netherlands

Anna Dawid, The Flatiron Institute, USA

Kai Dieckmann, Centre for Quantum Technologies, National University of Singapore, Singapore

Matthew Frye, University of Warsaw, Poland

Marcin Gronowski, University of Warsaw, Poland

Baraa Shammout, Leibniz Universität Hannover, Germany

Ashwin Singh, University of California, Berkeley, USA

Giacomo Valtolina, Fritz Haber Institute of the Max Planck Society, Germany

Piotr Wcisło, Nicolaus Copernicus University, Toruń, Poland

Hannah Williams, Durham University, United Kingdom

05 September 2023 - Tuesday

Session A1

Chaired by Michał Tomza from Faculty of Physics, University of Warsaw, Poland

12.30 - 14.00	**Registration & Welcome Coffee**	
13.55 - 14.00	**Welcome**	
14.00 - 14.30	**Sebastian Will**	Microwave shielding and cooling of ultracold dipolar NaCs molecules
14.30 - 15.00	**Xin-Yu Luo**	Creation of ultracold tetratomic molecules from a Fermi gas of microwave-shielded polar molecules
15.00 - 15.30	**Tijs Karman**	Thermalization of microwave-shielded molecules
15.30 - 16.00	**Coffee break**	

Session A2

Chaired by Anna Dawid from The Flatiron Institute, USA

16.30 - 17.00	**Maxence Lepers**	Two-photon optical shielding of collisions between ultracold polar molecules
17.00 - 17.30	**Timur Tscherbul**	Magnetic Feshbach resonances in ultracold atom-molecule collisions from converged coupled-channel calculations
17.30 - 17.45	**Baraa Shammout**	Modeling photoassociative spectra of ultracold NaK+K
17.45 - 18.00	**Anna Dawid**	Automated detection of laser cooling schemes for ultracold molecules
18.00- 18.30	**Coffee break**	
18.30- 19.00		
19.00 - ...	**Welcome Dinner**	For details please refer to **page 39**

06 September 2023 - Wednesday

Session B1

Chaired by Mateusz Borkowski from Columbia University, USA

09.00 - 09.30	**Michael Tarbutt**	Testing fundamental physics using laser cooled molecules
09.30 - 10.00	**Tim Langen**	Laser cooling of barium monofluoride
10.00 - 10.15	**Matthew Frye**	High-spin molecules from high-spin atoms: spin-spin coupling and Feshbach resonances in Cr+Yb
10.15 - 10.30	**Luke Caldwell**	Electron EDM measurement with trapped molecular ions
10.30 - 11.00	**Coffee Break**	

Session B2

Chaired by Hannah Williams from Durham University, United Kingdom

11:00 - 11.30	**Florian Schreck**	Tuning interactions in Rb-Sr mixtures by reduced dimensions and Feshbach resonances
11:30 - 12.00	**Gabriel Patenotte**	Dipolar interactions in a molecular tweezer array controlled by tweezer polarization
12.00 - 12.30	**Mikhail Lemeshko**	Angular momentum of small molecules: quasiparticles and topology
12.30 - 14.00	**Lunch Break**	

Session B3

Chaired by Tijs Karman from Radboud University, the Netherlands

14:00 - 14.30	**Alan Jamison**	Feshbach Resonances and Ultracold Chemistry
14:30 - 15.00	**Calder Miller**	Controlling a Many-Body Spin System of Polar Molecules
15.00 - 15.30	**Thomas Bilitewski**	Single-particle control over long-range interacting quantum spin systems in controllable geometries is opening new opportunities for quantum simulation and metrology.
15.30 - 16.00	**Coffee Break**	

Session B4

Chaired by Giacomo Valtolina from Fritz Haber Institute of the Max Planck Society, Germany

16:00 - 16.30	**Simon Cornish**	Full quantum control of ultracold polar molecules
16.30 - 17.00	**Jeremy Hutson**	Making Molecules by Merging Tweezers
17.00 - 19.00	**Poster Session**	

07 September 2023 - Thursday

Session C1

Chaired by Simon Cornish from Durham University, United Kingdom

09.00-09.30	**Silke Ospelkaus-Schwarzer**	Understanding and controlling collisions in quantum gases of NaK molecules
09.30-10.00	**Stefan Truppe**	Laser cooling the alkaline-earth-like diatomic molecule AlF
10.00-10.15	**Hannah Williams**	Zeeman Sisyphus Deceleration of Molecules
10.15-10.30	**Marcin Gronowski**	Ab initio electronic and scattering properties of the NaLi molecule in the $a^3\Sigma^+$state
10.30-11.00	**Coffee Break**	

Session C2

Chaired by Tim Langen from University of Stuttgart, Germany

11:00-11.30	**Christiane Koch**	TBA
11:30-12.00	**Kaden Hazzard**	Ultracold molecule synthetic dimensions
12.00-12.15	**Kai Dieckmann**	Efficient Creation of Ultracold Polar LiK Molecules
12.15-12.30	**Giacomo Valtolina**	Experiments with magnetic mixtures and molecules in Berlin
12.30-14.00	**Lunch Break**	

Session C3

14:00-15.00	**Panel discussion**	Future of ultracold molecules
15.00-15.30	**Coffee Break**	
15.30-16.00	Transfer to Old Town	By public transport. We advise taking **bus** line **175** or **128** headed downtown.
16.00-19.00	**Old Town Sightseeing**	
19.30 - ...	**Workshop Dinner**	For details please refer to **page 39**

08 September 2023 - Friday

Session D1

Chaired by Silke Ospelkaus-Schwarzer from Leibniz University Hannover, Germany

09.00-09.30	**Gerhard Rempe**	Collisions and coherences in ensembles of cold polyatomic molecules
09.30-10.00	**Loïc Anderegg**	Laser Cooled Molecules for Fundamental Physics and Quantum Science
10.00-10.15	**Piotr Wcisło**	Cold molecular hydrogen
10.15-10.30	**Ashwin Singh**	Progress towards optically trapping ground-state, small, chemically stable molecules
10.30-11.00	**Coffee Break**	

Session D2

Chaired by Mikhail Lemeshko from IST Austria, Vienna, Austria

11:00-11.30	**Edvardas Narevicius**	Quantum state tomography of Feshbach resonances in molecular ion collisions via electron-ion coincidence spectroscopy
11:30-12.00	**Bas van de Meerakker**	Cold and controlled collisions using tamed molecular beams
12.00-12.15	**Roman Bause**	Laser-cooling BaF for measuring the electric dipole moment of the electron
12.15-12.30	**Yuly Andrea Chamorro Mena**	New Physics searches with molecules
12.30-14.00	**Lunch Break**	

Session D3

Chaired by Piotr Żuchowski from Nicolaus Copernicus University, Poland

14:00-14.30	**Mateusz Borkowski**	Searching for new physics with next-generation molecular lattice clocks
14.30-15.00	**Aleksander Woźniak**	Towards a new physics with ultracold strontium molecules by state-of-the-art fully relativistic calculations
15.00-15.30	**Matthew Eiles**	A more quantitative theory of ultralong-range Rydberg molecules
15.30-16.00	**Coffee Break**	
16.00	**Farewell**	

Poster Session – list of accepted contributions

P1	**Niccolo Bigagli**	Collisionally Stable Gas of Bosonic Dipolar Ground State Molecules
P2	**Robert Bird**	Tunable Feshbach resonances in collisions of ultracold molecules in $^2\Sigma$ states with alkali-metal atoms
P3	**Shrestha Biswas**	Ultracold Field-Linked Tetratomic Molecules
P4	**Mateusz Bocheński**	Ultra-cold potassium-cesium mixtures in an optical dipole trap
P5	**Ubaldo Cavazos-Olivas**	Polaron and bipolaron formation in a Bose gas
P6	**Arthur Christianen**	From polarons to molecules in a Bose-Einstein condensate
P7	**Jakub Dobosz**	Loading dynamics of a dual-species magneto-optical trap of cesium and potassium
P8	**Jacek Dobrzyniecki**	Quantum simulation of the central spin model with a Rydberg atom and polar molecules in optical tweezers
P9	**Tim de Jongh**	A New Lithium 6 Quantum Gas Microscope : Exploring the Projection of a Many-Body Wavefunction onto Single Atoms
P10	**Yimeng Wang**	Generation of entanglement in ultracold collision processes
P11	**Tobias Franzen**	Towards ground state CsYb molecules
P12	**Marta Gałyńska**	The low-lying excited states of $LiYb^+$
P13	**Sangami Ganesan Santhi**	Interactions and cold collisions of AlF in the ground and excited states with He: implications for buffer gas cooling
P14	**Axel Görlitz**	1- and 2-Photon Photoassociation Spectroscopy of RbYb near the Yb intercombination line
P15	**Jingxuan He**	Selection and control of cryogenically-cooled (bio)nanoparticle beams with external fields
P16	**Jule Heier**	Collisions in a quantum gas of bosonic $^{23}Na^{39}K$ molecules
P17	**Hubert Jóźwiak**	Magic wavelength for a rovibrational transition in molecular hydrogen
P18	**Charbel Karam**	Two-photon optical shielding of collisions between ultracold polar molecules
P19	**Adam Koza**	Parity violation in laser-coolable chiral molecules
P20	**Hela Ladjimi**	Chemical reactions of ultracold alkaline-earth-metal diatomic molecules
P21	**Marijn Man**	Modest electric fields lead to enormously larger sticking times in ultracold molecular collisions.
P22	**João Pedro Mendonça**	Quantum simulation of extended electron-phonon-coupling models in a hybrid Rydberg atom setup

P23	**Bijit Mukherjee**	Shielding collisions of ultracold CaF molecules with static electric fields
P24	**Prerna Paliwal**	Quantum-logic control of complex molecular ions for applications in molecular and chemical physics
P25	**Sakthikumaran Ravichandran**	Exploring Kitaev model with Rydberg Atoms: Probing Exotic Spin States through Dipole-Dipole Interactions
P26	**Andreas Schindewolf**	Field-Linked Resonances
P27	**Leonid Shirkov**	Dynamics of complexes of aromatic molecules with alkali-metal and alkaline earth-metal atoms with application to spectroscopy and ultracold studies
P28	**Ritika Soni**	Rotational quenching of C_2 with ^{3}He and ^{4}He collisions at ultracold temperatures.
P29	**Michał Suchorowski**	Rotation of a molecule in two-dimensional condensate: angulon properties and spontaneous vortex formation
P30	**Jacek Szczepkwoski**	Excited electronic states of Sr_2: ab initio predictions and experimental observation of the $2^1\Sigma_u^+$ state
P31	**Marek Tylutki**	Superfluid Bose and Fermi gases and their mixtures
P32	**Matej Veis**	Many-body Perturbation Theory formulated in terms of physically motivated parameters for 1D atomic chains
P33	**Alexandre Voute**	Charge transfer of polyatomic molecules in ion-atom hybrid traps: Stereodynamics in the millikelvin regime
P34	**Maks Walewski**	Quantum resonant control of cold Rb–Sr^+ collisions high above the ultracold regime
P35	**Agata Wojciechowska**	Mercury Rydberg molecules
P36	**Eduardo Padilla**	Testing deep ultraviolet laser cooling of AlF molecules with cadmium atoms
P37	**Yanning Yin**	A hybrid trap of cold ions and cold neutral molecules for ion-molecule reaction studies
P38	**Krzysztof Zamarski**	Progress towards ultracold KCs molecules
P39	**Michael Ziemba**	An Experiment to Measure the Electron's Electric Dipole Moment Using an Ultracold Beam of YbF Molecules

Ultracold Molecules 2023 – Talk Abstracts

05 September 2023 - Tuesday

Microwave shielding and cooling of ultracold dipolar NaCs molecules

Sebastian Will
Presented by Sebastian Will (Columbia University, USA)

We have recently demonstrated microwave shielding and evaporative cooling for bosonic NaCs ground state molecules [1,2]. Dressing the molecules with a circularly polarized microwave field, we observe a suppression of inelastic loss by a factor of 200 and reach lifetimes of 1 second in dense molecular ensembles. We have demonstrated evaporative cooling for bosonic molecules and reached a phase-space density of 0.1, on the verge of BEC [3].

In this talk, I will share our latest insights on the collisional properties of this strongly dipolar system. NaCs has a large dipole moment (4.6 Debye) and offers exciting scientific prospects for many-body physics, both in the classical and the quantum regime.

References:
[1] Warner, et al., Overlapping Bose-Einstein condensates of Na and Cs, PRA 104, 033302 (2021)
[2] Stevenson, et al., Ultracold gas of dipolar NaCs ground state molecules, PRL 130, 113003 (2023)
[3] Bigagli, et al., Collisionally stable gas of bosonic dipolar ground state molecules, arXiv:2303.16845 (2023)

Creation of ultracold tetratomic molecules from a Fermi gas of microwave-shielded polar molecules

Xin-Yu Luo
Presented by Xin-Yu Luo (Max-Planck-Institute for Quantum Optics, Germany)

Stable molecular Fermi gases with strong dipolar interactions provide unique opportunities for studying exotic quantum matter such as p-wave superfluidity and extended Fermi-Hubbard models. I will first show our endeavors in understanding and controlling collisions of ultracold molecules, which eventually allow us to stabilize the molecular gas by microwave shielding. This technique enables the evaporation of polar molecules to temperatures well below the Fermi temperature [1]. The intermolecular potential can be flexibly tuned by the microwave field, allowing us to observe field-linked resonances in collisions of polar molecules. It provides a universal tuning knob to independently control the dipolar interaction and contact interaction [2]. In the end, I will present the creation of ultracold field-linked tetratomic molecules by electroassociation in a degenerate Fermi gas of microwave-shielded polar molecules [3]. Additionally, I will discuss several exciting new possibilities associated with these field-linked molecules.

References:
[1] A. Schindewolf et al., Evaporation of microwave-shielded polar molecules to quantum degeneracy, Nature 607, 677 (2022)
[2] X.-Y. Chen* and A. Schindewolf* et al., Field-linked resonances of polar molecules, Nature 614, 59 (2023)
[3] X.-Y. Chen et al., Ultracold field-linked tetratomic molecules, arXiv preprint arXiv:2306.00962 (2023)

Thermalization of microwave-shielded molecules

Tijs Karman
Presented by Tijs Karman (Radboud University, the Netherlands)

Rapid progress is made in suppressing collisional loss of ultracold molecules by microwave shielding.
The success of evaporative cooling of molecules, however, does not only require suppressed loss but also fast thermalization by elastic collisions.
It turns out the elastic collisional properties of the molecules are also affected by microwave dressing, which induces dipole-dipole interactions.
I will discuss thermalization of microwave shielded molecules, which has implications for efficient evaporative cooling, but also provides opportunities to explore dipolar physics in thermal molecular gases.

Two-photon optical shielding of collisions between ultracold polar molecules

Maxence Lepers
Presented by Maxence Lepers (University of Burgundy, Dijon, France)

We propose a method to engineer repulsive long-range interactions between ultracold ground-state molecules using optical fi elds, thus preventing short-range collisional losses. It maps the microwave coupling recently used for collisional shielding onto a two-photon transition, and takes advantage of optical control techniques. In contrast to one-photon optical shielding [Phys. Rev. Lett. 125, 153202 (2020)], this scheme avoids heating of the molecular gas due to photon scattering. The proposed protocol, exemplified for $^{23}Na^{39}K$, should be applicable to a large class of polar diatomic molecules.

Magnetic Feshbach resonances in ultracold atom-molecule collisions from converged coupled-channel calculations

Timur Tscherbul, Masato Morita, Paul Brumer, Piotr Zuchowski, and Maciej Kosicki
Presented by Timur Tscherbul (University of Nevada, Reno, USA)

We report converged coupled-channel calculations on ultracold Rb + SrF collisions in a magnetic field based on ab initio singlet and triplet potential energy surfaces of the Rb-SrF trimer. The calculations fully incorporate the hyperfine and Zeeman structure of the colliding species in the rigid-rotor approximation using the total rotational angular momentum representation for molecular collisions in a magnetic field (T.V. Tscherbul and J.D. D'Incao, arXiv:2306.05563). We calculate the spectra of magnetic Feshbach resonances in ultracold Rb + SrF collisions for the various initial hyperfine-Zeeman states of Rb and SrF.

Modeling photoassociative spectra of ultracold NaK+K

Baraa Shammout, Leon Karpa, Silke Ospelkaus, Eberhard Tiemann, and Olivier Dulieu
Presented by Baraa Shammout (Leibniz U niversität Hannover, Germany)

A model for photoassociation of ultracold atoms and molecules is presented, and applied to the case of ^{39}K and $^{23}Na^{39}K$ bosonic particles. The model relies on the assumption that photoassociation is dominated by long-range atom-molecule interactions, well outside the chemical bond region. The frequency of the photoassociation laser is chosen close to a bound-bound rovibronic transition from the $X^1\Sigma+$ ground state toward the metastable $b^3\Pi$ lowest excited state of $^{23}Na^{39}K$, allowing to neglect any other excitation which could hinder the photoassociation detection. The energy level structure of the long-range $^{39}K...^{23}Na^{39}K$ excited super-dimer is computed in the space-fixed frame by solving coupled- channel equations, involving the coupling between the $^{23}Na^{39}K$ internal rotation with the mechanical rotation of the super-dimer complex. A quite rich structure is obtained, and the corresponding photoassociation rates are presented. Other possible photoassociation transitions are discussed in the context of the proposed model.

High-spin molecules from high-spin atoms: spin-spin coupling and Feshbach resonances in Cr+Yb

Matthew Frye, Piotr Żuchowski, Michał Tomza
Presented by Matthew Frye (Faculty of Physics, University of Warsaw, Poland)

We investigate interactions and ultracold collisions of Cr with Yb. This combination of a high-spin but spherical atom with a closed-shell atom could form a molecule which would inherit the large magnetic dipole moment from Cr but also gain an electric dipole moment, allowing new modes of control and interaction. This system has only one potential curve, but the many unpaired electrons on Cr give rise to a substantial intra-atomic spin-spin interaction which creates Feshbach resonances due to rotationally excited states. We find such resonances are guaranteed below 250 Gauss, and can reach widths of 10s of Gauss in favourable circumstances. We consider the effects of hyperfine and isotopic substitution, and find that this system is remarkably robust to unlucky scattering lengths. These results show this is a promising system for both molecule formation and studying mixtures including dipolar species.

Testing fundamental physics using laser cooled molecules

Michael Tarbutt
Presented by Michael Tarbutt (Imperial College London, United Kingdom)

I will present progress on two experiments that use laser-cooled molecules to test fundamental physics. In the first, we are developing a clock based on vibrational transitions in CaF molecules confined in a magic wavelength lattice. Pure vibrational transitions have little sensitivity to external perturbations so can make highly accurate clocks. By comparing to an optical atomic clock, we aim to measure variations in the electron-to-proton mass ratio. The molecular lattice clock could also provide improved frequency standards in the infra-red. In the second experiment, we aim to measure the electron's electric dipole moment using ultracold YbF molecules. I will present the construction of this experiment which features a slow-moving beam cooled below 100 μK in an extremely low magnetic noise environment.

Laser cooling of barium monofluoride

Tim Langen
Presented by Tim Langen (University of Stuttgart, Germany)

In the first part of my talk I will report on our progress towards laser cooling of BaF molecules. Due to its high mass, resolved hyperfine structure in the excited state and branching losses through intermediate states, this molecular species is notoriously difficult to cool, but it shows high promise for various types of precision measurement applications. In the second part, I will discuss the new possibilities that bulk molecular Bose-Einstein condensates may open up for dipolar many-body physics in the near future. Building on our work on dipolar droplets and supersolids that form from weakly dipolar atoms, I will show how ultracold molecules and microwave shielding can provide fundamentally new insights into these exotic states of matter.

Automated detection of laser cooling schemes for ultracold molecules

Anna Dawid, Niccolò Bigagli, Daniel Savin, Sebastian Will
Presented by Anna Dawid (The Flatiron Institute, USA)

Ultracold molecules offer exciting prospects for quantum sciences, including quantum chemistry, sensing, and simulations. Their applications are, however, limited by the challenges in their cooling. So far, there were two main approaches to producing ultracold molecules: either by combining already ultracold atoms (resulting in, e.g., KRb and NaCs) or by laser cooling species with quasidiagonal Franck-Condon factors (like SrF, CaF, and YO). Those ultracold species are far from being chemically typical, and thus their applications are limited outside fundamental physics.

Recently, a laser cooling scheme was found for the carbon dimer [1], proving that laser cooling is possible for species with strongly off-diagonal Franck-Condon factors. A manual search for such schemes across complex molecular energy levels is challenging. Here, we report the development of a graph-based algorithm allowing for the automated detection of laser cooling schemes out of energy levels and allowed transition data accessible for a range of molecular species in the Exomol database. We rediscovered found laser cooling schemes for the carbon dimer and proposed more that, interestingly, occur in higher rotational branches. We also report discovery of new laser cooling schemes for CN, YO, carbon dioxide, and more. This work paves the way for ultracold molecules with new applications, in particular in astrochemistry.

References:
[1] N. Bigagli, D. W. Savin, & S. Will. Laser cooling scheme for the carbon dimer (12C2). Phys. Rev. A 105, L051301 (2022)

Electron EDM measurement with trapped molecular ions

Luke Caldwell
Presented by Luke Caldwell (University College London, United Kingdom)

We recently made the most precise measurement yet of the electron's electric dipole moment using HfF molecular ions. This is the first time the record has been set by an experiment using trapped molecules. I will discuss some of the advantages and challenges that come with this approach.

Tuning interactions in Rb-Sr mixtures by reduced dimensions and Feshbach resonances

Florian Schreck
Presented by Florian Schreck (University of Amsterdam, the Netherlands)

We present interaction tuning in ultracold Rb-Sr mixtures by reducing the effective dimension in which the gas lives and by magnetic Feshbach resonances. These schemes may lead to the controlled creation of RbSr molecules, which have large electric and magnetic dipole moments when transferred to their rovibronic ground state. Interaction tuning in this mixture of alkali and alkaline-earth atoms may also enable the study of interesting many-body physics in optical lattices.

Dipolar interactions in a molecular tweezer array controlled by tweezer polarization

Gabriel Patenotte
Presented by Gabriel Patenotte (Harvard University, USA)

Tunable electric dipole-dipole interactions and an abundance of long-lived rotational states make polar molecules an attractive platform for quantum simulation and computation. Recently, coherent exchange of the rotational states of adjacent polar molecules has been observed in our optical tweezer array. Our system consists of an AOD-based programmable array of individual NaCs molecules in the ground state of their internal and motional degrees of freedom. We adjust the ellipticity of the tweezer polarization to cancel the first-order differential polarizability of a rotational transition. The stabilized transition is then used to observe dipolar interactions whose rate is controlled by array spacing and orientation of the tweezer polarization. We observe several coherent oscillations of the |gg> population with a 2 ms pi time at an inter-particle spacing of 2 μm. Finally, we present progress on removing defects from the molecular tweezer array by indirect state-selective imaging of Cs in a large magnetic field. A higher density molecular array will enable quantum simulation and computation applications reliant on interparticle interactions.

Angular momentum of small molecules: quasiparticles and topology

Mikhail Lemeshko
Presented by Mikhail Lemeshko (IST Austria, Vienna, Austria)

I will present our recent findings on small molecules kicked by laser pulses. First, I will describe a technique that allows to probe highly excited molecular states in the presence of an environment, such as superfluid ^{4}He, and a corresponding theory based on angulon quasiparticles that is capable of describing such states, in good agreement with experiment [1].

Second, I will show how that even the simplest of existing molecules - closed-shell diatomics not interacting with one another - host topological charges when driven by periodic far-off-resonant laser pulses. A periodically kicked molecular rotor can be mapped onto a "crystalline" lattice in angular momentum space. This allows to define quasimomenta and the band structure in the Floquet representation, by analogy with the Bloch waves of solid-state physics. In such a momentum space we predict the occurrence of Dirac cones with topological charges, protected by reflection and time-reversal symmetry. These Dirac cones -- and the corresponding edge states -- are broadly tunable by adjusting the laser strength and can be observed in present-day experiments by measuring molecular alignment and populations of rotational levels. This paves the way to study controllable topological physics in gas-phase experiments with small molecules as well as to classify dynamical molecular states by their topological invariants.

References:
[1] I. Cherepanov et al. Phys. Rev. A 104, L061303 (2021); New J. Phys. 24 075004 (2022)
[2] V. Karle, A. Ghazaryan, M. Lemeshko. Phys. Rev. Lett. 130, 103202 (2023)

Feshbach Resonances and Ultracold Chemistry

Alan Jamison
Presented by Alan Jamison (University of Waterloo, Canada)

For many years, it was believed that Feshbach resonances would be unobservable in chemically reactive ultracold systems due to the absence of short-range coherence in collisions at the universal loss limit. I will report our work observing a rich set of Feshbach resonances in the NaLi + Na system at ultracold temperatures. We also observe a single, isolated Feshbach resonance in the NaLi + NaLi system. Combining theory and experiment, we analyze the spectrum of Feshbach resonances found in two different reactant states for the atom-molecule system. We are able to uncover details of collision complexes and reaction mechanisms for short-ranged chemical dynamics.

Controlling a Many-Body Spin System of Polar Molecules

Calder Miller
Presented by Calder Miller (JILA, University of Colorado Boulder, USA)

Rotational states of polar molecules natively realize a long-range Heisenberg XXZ Hamiltonian, tunable with microwave and DC electric fields. I will present the dynamics of a system of ultracold $^{40}K^{87}Rb$ molecules in itinerant and pinned geometries. In the itinerant regime, the short-time dynamics are captured by a collective spin model, while at longer times collisions couple spin to motion, resulting in dephasing. We also vary the electric field strength and explore its effect on the dynamics of the molecules as we increase the confinement potential in a 3D lattice. Finally, I will discuss progress developing experimental tools to enable observation of further physics, such as spin squeezing and spin transport.

Single-particle control over long-range interacting quantum spin systems in controllable geometries is opening new opportunities for quantum simulation and metrology.

Thomas Bilitewski
Presented by Thomas Bilitewski (Oklahoma State University, USA)

I will discuss recent theoretical work on the temporal growth and spatial propagation of quantum correlations and entanglement in two-dimensional bi- and multi-layers realising spin 1/2 quantum XXZ models with couplings mediated by long range interactions.

In the collective regime at the Heisenberg point this realises the paradigmatic two-mode squeezing Hamiltonian, resulting in exponential generation of metrologically useful entanglement from initially prepared unentangled product states. Generically, the dynamic instability generates spatially separated correlated pairs with specific momenta, controllable via the dipole orientation or applied field gradients.

Polar molecule arrays not only allow the observation of the generated entanglement via collective measurements, but also single-particle control over the spatially separated entangled particles.

References:
[1] arXiv:2302.09059,
[2] arXiv:2211.12521

Full quantum control of ultracold polar molecules

Simon Cornish
Presented by Simon Cornish (Durham University, United Kingdom)

Ultracold polar molecules are an exciting new platform for quantum science and technology. The combination of rich internal structure of vibration and rotation, controllable long-range dipole-dipole interactions and strong coupling to applied electric and microwave fields has inspired many applications. These include quantum simulation of strongly interacting many-body systems, the study of quantum magnetism, quantum metrology and molecular clocks, quantum computation, precision tests of fundamental physics and the exploration of ultracold chemistry. Many of these applications require full quantum control of both the internal and motional degrees of freedom of the molecule. In Durham, we study ultracold ground-state RbCs molecules formed by associating Rb and Cs atoms using a combination of magnetoassociation and stimulated Raman adiabatic passage (STIRAP) [1].

This talk will report our work on the development of full quantum control of the molecules. Specifically, we will discuss how we have mastered the ac Stark shift due to the trapping light [2] to demonstrate robust storage qubits in the molecule [3] and will describe the development of magic traps [4] that support second-scale rotational coherences giving access to controllable dipole-dipole interactions [5]. Finally, we will describe new experiments that produce single molecules in optical tweezers starting from a single Rb and a single Cs atom [6]. Using this platform, we prepare the molecules in the motional ground state of the trap and can perform addressing and detection of single molecules [7]. Moreover, we demonstrate a new hybrid platform that combines single ultracold molecules with single Rydberg atoms [8], opening a myriad of possibilities.

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Making Molecules by Merging Tweezers

Jeremy Hutson
Presented by Jeremy Hutson (Durham University, United Kingdom)

Ultracold molecules may be formed in optical tweezers by either magnetoassociation or photoasssociation. We have collaborated with Kang-Kuen Ni’s group at Harvard to form an NaCs molecule by magnetoassociation from Na and Cs atoms in a tweezer [1], and with Simon Cornish’s group at Durham to form an RbCs molecule [2].

For RbCs, we were surprised to discover that a molecule can be formed when tweezers are merged without needing magnetoassociation. This occurs because there is an avoided crossing (as a function of tweezer separation z0) between states of the confined atom pair and a weakly bound state of the molecule. An RbCs molecule is formed by adiabatic passage over this avoided crossing as the tweezers are merged. We refer to this as mergoassociation.

We have modelled mergoassociation with coupled-channel calculations for both isotropic and anisotropic tweezers and find good agreement between experimental and theoretical probabilities of molecule formation. We have also developed an approximate approach that offers insight into the strength of the avoided crossing and thus the efficiency of mergoassociation.

Mergoassociation offers a route to forming ultracold molecules in systems that do not possess Feshbach resonances suitable for magnetoassociation. It can be effective when there is a near-threshold molecular state bound by up to a few times the harmonic frequency of the trap.

More generally, optical tweezers offer a rich platform for highly selective studies of atomic and molecular collisions and reactions. Configurable tweezer arrays offer further possibilities for quantum science, ranging from fundamental studies of few-body dipolar physics to quantum simulation and quantum computing [4]. They present many fascinating challenges for theory at both the single-particle and few-particle levels.

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Understanding and controlling collisions in quantum gases of NaK molecules

Silke Ospelkaus-Schwarzer
Presented by Silke Ospelkaus-Schwarzer (Leibniz University Hannover, Germany)

In this talk, I will report about recent experiments with quantum gases of polar bosonic $^{23}Na^{39}K$ molecules. I will first discuss inelastic atom-molecule and molecule-molecule collisions and their origin [1,2,3]. Afterwards I will discuss the control of atom-molecule collisions by Feshbach resonances as well as a proposal for blue shielding of collisions of polar molecules using optical photons at Raman resonance [4].

References:
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[4] Charbel Karam, Mara Meyer zum Alten Borgloh, Romain Vexiau, Maxence Lepers, Silke Ospelkaus, Nadia Bouloufa-Maafa, Leon Karpa, Olivier Dulieu: Two-photon optical shielding of collisions between ultracold polar molecules, arxiv:2211.08950

Laser cooling the alkaline-earth-like diatomic molecule AlF

Stefan Truppe
Presented by Stefan Truppe (Imperial College London, United Kingdom)

We present our recent progress on laser cooling AlF molecules using deep UV lasers. AlF is distinctively different from the molecular species that have been laser-cooled so far: it is a stable molecule that can be produced in large quantities, and it has a strong $A^1\Pi \leftarrow X^1\Sigma+$ transition near 227.5 nm that can be used for rapid slowing and cooling in a magneto-optical trap (MOT) with a large capture velocity. The electronic structure allows using a Zeeman slower to significantly enhance the number of molecules in the MOT.

Similar to alkaline-earth and alkaline-earth-like atoms, AlF has narrow, spin-forbidden $a^3\Pi \leftarrow X^1\Sigma+$ transitions near 367 nm for precision spectroscopy and narrow-line cooling. We aim to study collisions between AlF molecules and use the narrow line to explore direct laser cooling to the μK regime.

Zeeman Sisyphus Deceleration of Molecules

Bethan Humphreys, Hannah Williams
Presented by Hannah Williams (Physics Department, Durham University, United Kingdom)

Laser cooling has proved to be a hugely successful technique for producing slow samples of molecules. The large number of photon scattering events leads to limitations in terms of both the efficiency of slowing and the variety of suitable molecular species. At Durham University, we are building a new molecular beam experiment to test a static field, Zeeman-Sisyphus decelerator. We will present theoretical predictions for the performance of the decelerator for different molecular species as well as an update on the status of the calcium fluoride beam line.

Ab initio electronic and scattering properties of the NaLi molecule in the $a^3\Sigma^+$ state

Marcin Gronowski, Adam Koza, Michał Tomza
Presented by Marcin Gronowski (Faculty of Physics, University of Warsaw, Poland)

The significance of spin-spin and spin-rotation couplings in atom-molecule collisions has been recently demonstrated by combined experimental and theoretical studies on Feshbach resonances in the complex composed of the ultracold polar and magnetic $^{23}Na^6Li$ molecule in the rovibrational ground state of the lowest triplet $a^3\Sigma+$ electronic and sodium atom. Here, we focus on the prediction of the electronic, rovibrational, and hyperfine structure of $^{23}Na^6Li$ in $a^3\Sigma+$. We obtained spectroscopic accuracy ($<0.5 cm^{-1}$) in these 14-electron

molecules using state-of-the-art ab initio quantum chemistry methods. We explore the role of higher-level excitations, core-electron correlation, relativistic, QED, adiabatic, and nonadiabatic corrections on alkali-metal systems' scattering and spectroscopic properties.

TBA

Christiane Koch
Presented by Christiane Koch (Free University of Berlin, Germany)

TBA

Ultracold molecule synthetic dimensions

Kaden Hazzard
Presented by Kaden Hazzard (Rice University, USA)

Rotational states in ultracold molecules can be used as effective lattice sites, forming a so-called synthetic dimension when they are coupled with microwaves to mimic tunneling between lattice sites. Recent experiments on Rydberg atoms, a similar dipolar interacting system, have realized topological band structures [1] and seen interaction-stabilized strings in dynamics [2]. I will review this and discuss exciting possible next steps for dipolar interacting synthetic dimension platforms. A particularly intriguing one is that they are predicted to harbor exotic new quasiparticles known as paraparticles that are neither fermions or bosons, and which, in contrast to anyons, can exist in systems with more than two spatial dimensions. I will also discuss some of the unique possibilities molecules offer this research.

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Efficient Creation of Ultracold Polar LiK Molecules

C. He, X. Nie, S. Botsi, S. Kumar, V. Avalos, A. Yang, and K. Dieckmann
Presented by Kai Dieckmann (Centre for Quantum Technologies, National University of Singapore, Singapore)

We report the creation of ultracold polar LiK molecules. While adapting our previously reported pathway via a singlet intermediate state we achieve 98% efficiency for stimulated Raman adiabatic passage (STIRAP) to the rovibrational ground state. This high efficiency was achieved after characterizing and improving the level of phase noise of the STIRAP lasers. Two-photon spectroscopy was performed to measure the Stark shift of the ground state and the permanent electric dipole moment. The measured 3.6 debye is in among the highest among the bi-alkali molecular species. The measure 5.6 ms life time of optically trapped the molecules consistent with chemically reactive collisional loss of the molecules. The qbit transition to the first excited rotational state was measured with resolved hyperfine structure. We further discuss our plans to study dipolar physics based on this transition in an optical lattice at a magic wavelength that allows for long coherence times.

Experiments with magnetic mixtures and molecules in Berlin

Giacomo Valtolina
Presented by Giacomo Valtolina (Fritz Haber Institute of the Max Planck Society, Germany)

Our group is studying the unique features of lanthanide atoms, such as dysprosium, for molecular quantum science.

We are building a new apparatus for controlling ultracold reactions between dysprosium atoms and dimers using an optical cavity. We report on the realization of a MOT of dysprosium and how we plan to achieve cavity-controlled chemistry.

On the side, we are exploring the optical spectra of dysprosium-bearing molecules and discovered a new properties that enables quantum-state-resolved creation of internally cold molecular ions. We discuss the new opportunities from this effect, in particular related to eEDM experiments.

Collisions and coherences in ensembles of cold polyatomic molecules

Gerhard Rempe
Presented by Gerhard Rempe (Max-Planck-Institute for Quantum Optics, Germany)

Polyatomic molecules offer research possibilities not shared by atoms or simple dimers, ranging from fundamental physics to quantum science. The experimental challenge is to produce cold and dense samples that are trappable for long times. We have reached these goals with a combination of cryogenic buffer-gas cooling, centrifuge deceleration and electric trapping, and have observed for the first time the dipolar interaction between fluormethane molecules [Koller et al., Phys. Rev. Lett. 128, 203401 (2022)]. We have also implemented a state-selective laser-induced fluorescence detection and used it to observe coherences between symmetry-protected rotational states in cold formaldehyde molecules. The insensitivity of our new qubit against external perturbations makes polyatomic molecules promising candidates for a quantum-information-processing platform.

Laser Cooled Molecules for Fundamental Physics and Quantum Science

Loïc Anderegg
Presented by Loïc Anderegg (Harvard University, USA)

Ultracold molecules have a wide range of potential applications spanning from fundamental physics to quantum simulation and computation. Motivated by potential discoveries in these areas, significant advances in controlling molecules at the single-quantum-state level have occurred over the past decade. Progress in direct laser-cooling of molecules has led to the first molecular magneto-optical traps, which have allowed for optical trapping of ultracold molecules. Optical tweezer arrays have allowed both high-fidelity readout as well as quantum control of individual molecules. In this talk, we will discuss using optical tweezer arrays of CaF molecules to study ultracold collisions and quantum bits based on rotational states. We show greatly improved rotational coherence times for molecular qubits in optical tweezer traps, which parametrizes the potential performance of polar-molecule-based quantum simulators or computers. Finally, we show progress towards realizing the goal of high-fidelity molecular qubits by demonstrating dipolar interactions and entanglement between CaF molecules.

Extending the tools of quantum control beyond the rich structure of diatomic molecules to polyatomic molecules leads to powerful new scientific avenues. Notably, polyatomic molecules generically possess low-lying, closely spaced energy levels of opposite parity. This results in long-lived, fully polarizable quantum states with minimal sensitivity to external perturbations suitable for a broad range of scientific applications. These states promise significant improvements to searches for physics beyond the Standard Model, including probing for the electron's electric dipole moment (eEDM). Here we present results on laser-cooling and optical trapping of the polyatomic molecule CaOH. We establish coherent control of individual quantum states in CaOH and perform electron spin precession of an eEDM sensitive state. We demonstrate extended coherence times by utilizing eEDM sensitive states with tunable, near-zero magnetic field sensitivity. These results establish a path for eEDM searches with trapped polyatomic molecules, towards orders-of-magnitude improved experimental sensitivity to time-reversal-violating physics. Finally, we present recent results on single particle control by loading CaOH molecules into optical tweezer arrays which will allow future quantum simulations and collision studies.

Cold molecular hydrogen

Piotr Wcisło
Presented by Piotr Wcisło (Nicolaus Copernicus University, Poland)

Due to its simplicity, H_2 constitutes a perfect tool for testing fundamental physics: testing quantum electrodynamics, determining fundamental constants, or searching for new physics beyond the Standard Model. H_2 has a huge advantage over the other simple calculable systems of having a set of a few hundred ultralong living rovibrational states, which implies the ultimate limit for testing fundamental physics with H_2 at a relative accuracy level of 10^{-24}. The present experiments are far from this limit. I will present our so far results and ongoing projects aimed at exploring this huge potential with cold H_2.

Progress towards optically trapping ground-state, small, chemically stable molecules

Ashwin Singh, Lothar Maisenbacher, Ziguang Lin, Jeremy J. Axelrod, Cristian D. Panda, Holger Müller
Presented by Ashwin Singh (University of California, Berkeley, USA)

Despite a diversity of interest in studying cold molecules, access to cold, trapped molecule samples has been limited to only a few select species. To this end, we have recently designed an experiment aimed at trapping a variety of small, closed-shell molecules, such as N_2, O_2, CO, and HCl, in their ground state [1]. The molecules will be directly buffer-gas loaded at 1.5 K into a ~10-K deep optical dipole trap produced by a tightly-focused, 1064-nm buildup cavity operating at ~300 GW/cm^2. The very far-off-resonant, quasi-electrostatic trapping mechanism is insensitive to a molecule's internal state, energy level structure, and its electric and magnetic dipole moment, and can therefore trap multiple chemical species, even simultaneously. Here, we discuss experimental progress made towards realizing this trap, including building test cavities and parts of the cryogenic system.

References:
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Quantum state tomography of Feshbach resonances in molecular ion collisions via electron-ion coincidence spectroscopy

Edvardas Narevicius
Presented by Edvardas Narevicius (TU Dortmund University, Germany)

During collisions coupling between relative and internal atomic and molecular degrees of freedom leads to the formation of Feshbach resonances. The large phase space volume that particles explore in this metastable scattering state supports interference between many different quantum pathways that include inelastic and reactive processes. We present a new method that allows us to measure simultaneously all the quantum channels for Feshbach resonances that appear in collisions between vibrationally excited H2+ ion and noble gas atoms. Our quantum state mapping is based on ion-electron coincidence velocity map imaging spectroscopy.

Cold and controlled collisions using tamed molecular beams

Bas van de Meerakker
Presented by Bas van de Meerakker (Radboud University, the Netherlands)

The study of molecular collisions with the highest possible detail has been an important research theme in physical chemistry for decades. Experimentally, the level of detail obtained in these studies depends on the quality of preparation of the collision partners before the collision, and on how accurately the products are analyzed afterward.

Over the last years, methods have been developed to get improved control over molecules in a molecular beam. With the Stark decelerator, a part of a molecular beam can be selected to produce bunches of molecules with a computer-controlled velocity and with longitudinal temperatures as low as a few mK [1]. The molecular packets that emerge from the decelerator have small spatial and angular spreads, and have almost perfect quantum state purity. These tamed molecular beams are excellent starting points for high-resolution crossed beam scattering experiments.

I will illustrate the possibilities this technology offers to study molecular collisions with unprecedented precision and at low collision energies. I will discuss our most recent results on the combination of Stark deceleration and velocity map imaging. The narrow velocity spread of Stark-decelerated beams results in scattering images with an unprecedented sharpness and angular resolution. This has facilitated the observation several quantum effects in state-to-state cross sections, such as diffraction [2,3], scattering resonances [4-6] and product pair correlations in bimolecular collisions [7]. Finally, I will present recent results on bimolecular collisions at collision energies down to 0.1 cm^{-1} obtained by merged beam configurations [8].

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[3] J. Onvlee et al., Imaging quantum stereodynamics through Fraunhofer scattering of NO radicals with rare gas atoms, Nature Chemistry 9, 226 (2017)
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Laser-cooling BaF for measuring the electric dipole moment of the electron

Roman Bause
Presented by Roman Bause (University of Groningen, the Netherlands)

Most beyond-Standard-Model theories contain new sources of CP violation. If one of these were true, the electron would very likely exhibit an electric dipole moment much larger than what the Standard Model predicts. By measuring energy shifts in heavy polar molecules, the experimental upper bound on this dipole moment has been lowered by three orders of magnitude within the last decade, excluding new physics at TeV energy scales.

In the NL-eEDM collaboration, we attempt to perform a new dipole-moment measurement with the BaF molecule on the level of 10^{-30} e cm. To obtain bright and slow molecular beams, we use a combination of a cryogenic molecule source, electrostatic focusing, Stark deceleration, and laser cooling, which will yield pulses of 10^6 molecules at a repetition rate of 10 Hz, and a spin-precession time of 15 ms.

I will report on our recent progress in laser cooling BaF. This species is much harder to cool than, for example, CaF, due to its high mass and long excited-state lifetime. However, electrostatic focusing and Stark deceleration can be used to overcome these disadvantages and improve the cooling scheme.

New Physics searches with molecules

Yuly Chamorro, Johan Polet, Lukas Pasteka, Anastasia Borschevsky
Presented by Yuly Andrea Chamorro Mena (University of Groningen, the Netherlands)

The Standard Model (SM) of particle physics describes the matter and radiation in the universe in terms of fundamental particles to high precision. Although no discrepancies between SM predictions and laboratory experiments have been found so far, we know the SM is incomplete. For example, the observed matter-antimatter asymmetry in the universe requests more time-reversal symmetry-violating mechanisms than the one included in the SM. Recent advances in experimental and theoretical techniques have led to promising searches for the parity and time-reversal symmetry-violating electric dipole moment of the electron (eEDM) in molecules to probe new physics. The complex electronic, vibrational and rotational structure in molecules gives access to an enhanced energy shift due to the eEDM (d_e), $\Delta E = d_e W_d$. The electronic molecular parameter Wd increases with the atomic number as Z^3, and therefore systems with a heavy atom are favorable for eEDM measurements. Additionally, the use of ultracold molecules increases the statistical sensitivity of the experiment. In this contribution, I will present two cases of study. The symmetric top molecules $BaCH_3$ and $YbCH_3$; and the YbCu and YbAg proposed ultracold-assembled molecular candidates (2020 Phys. Rev. Lett. 125 153201). We calculate W_d using high-accuracy relativistic coupled cluster methods and systematically evaluate the uncertainties of our computational approach. We report enhancements up to 10^{10} for the eEDM signal at electric fields of 1~V/cm.

Searching for new physics with next-generation molecular lattice clocks

Mateusz Borkowski
Presented by Mateusz Borkowski (Columbia University, USA)

Molecular lattice clocks enable the search for new physics, such as fifth forces or temporal variations of fundamental constants, in a manner complementary to atomic clocks. Here we present the operation of a vibrational lattice clock operating on a 32-THz Raman transition between the most weakly- and most deeply-bound vibrational levels of ultracold strontium molecules. We study the major systematic effects and determine the absolute frequency of the clock transition at the Hz level. In particular, we employ Stark-shift spectroscopy and modern quantum chemistry methods to characterize the polarizabilities of the Sr_2 molecule from dc to infrared. Using this description, we determine the static and dynamic blackbody radiation shifts for all possible vibrational clock transitions to the 10–16 level. This constitutes an important step towards mHz-level molecular spectroscopy in Sr_2, and provides a framework for evaluating BBR shifts in other homonuclear molecules. Finally, we determine the sensitivities of isotope shifts in a molecular lattice clocks to Yukawa-type fifth forces. In the future, a next-generation molecular lattice clock could enable searches for new physics at unprecedented sensitivity.

Towards a new physics with ultracold strontium molecules by state-of-the-art fully relativistic calculations

Aleksander Woźniak, Robert Moszyński
Presented by Aleksander Woźniak (Quantum Chemistry Laboratory, University of Warsaw, Poland)

Cutting-edge ab initio techniques of the electronic structure theory and quantum dynamics of nuclear motions have found diverse applications spanning atomic, molecular, nuclear, and material physics. This presentation reports a groundbreaking application related to non-Newtonian gravity. To this end, advanced all-electron ab initio calculations have been performed for the ground state of the strontium diatomic molecule. These calculations employed a state-of-the-art four-component relativistic Dirac-Coulomb coupled cluster method with single, double, and non-iterative triple excitations. This method was further enhanced with the full configuration interaction correction, providing a precise description of the valence-valence electronic correlation.

Moreover, the Born-Oppenheimer Dirac-Coulomb potential was supplemented by including contributions from the two-electron Darwin and orbit-orbit interactions, along with the QED radiative correction. Additionally, the potential was fine-tuned by accounting for the leading-order mass-dependent terms. Finally, the long-range Van der Waals coefficients for all contributions to the mass dependent potential have been computed.

Although the ab initio results are subject to ongoing refinements, the current findings reveal an $^{88}Sr_2$ potential well depth of 1080.83 cm^{-1}, as compared with the best empirical value of 1081.64 cm^{-1} [1]. The numerical results for a wide range of interatomic distances have been fitted with suitable analytical expressions opening the possibility to study the QED retardation in the long-range. The present mass-dependent potential applicable to all bosonic Sr_2 molecules — including the mixed dimers — combined with the Hertz precision measurements of the group of Tanya Zelevinsky at Columbia University will allow for the search of the non-Newtonian mass dependent interactions mediated by the exchange of hypothetical gauge bosons.

References:
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A more quantitative theory of ultralong-range Rydberg molecules

Matthew Eiles
Presented by Matthew Eiles (Max Planck Institute for the Physics of Complex Systems, Germany)

Ultralong-range Rydberg molecules comprised of one or more ground state atoms bound within the orbit of a Rydberg atom display many exaggerated features when compared to typical ultracold molecules. Their dipole moments and bond lengths exceed those of “typical” ultracold molecules by several orders of magnitude, and their oscillatory adiabatic potential curves have local minima and exhibit narrow avoided crossings at many internuclear distances. The detection of these molecules through precision spectroscopy has improved rapidly in recent years, motivating improvements the theoretical description of these molecules. The standard approach to compute potential energy curves is to diagonalize the generalized Fermi/Omont pseudopotential in a basis of atomic Rydberg orbitals, which cannot yield quantitatively accurate results as the calculation does not converge as the basis size is increased. This attempt at quantitative calculations is further challenged by divergences stemming from resonant electron-atom scattering, which must be renormalized, and the lack of accurately calculated electron-atom scattering phase shifts to use as inputs. In this talk I will present potential energy curves computed using a fully spin-dependent Green’s function method and their vibrational states, which are free of these convergence problems and contain all relevant spin degrees of freedom. With these, we can fit model-independent electron-atom scattering phase shifts to use in later quantitative studies.

Ultracold Molecules 2023 – Poster Abstracts

P1: Collisionally Stable Gas of Bosonic Dipolar Ground State Molecules

Niccolò Bigagli, Claire Warner, Weijun Yuan, Siwei Zhang, Ian Stevenson, Tijs Karman, Sebastian Will
Presented by Niccolo Bigagli (Physics, Columbia University, USA)

Stable ultracold ensembles of dipolar molecules hold great promise for many-body quantum physics, but high inelastic loss rates have been a long-standing challenge. Recently, it was shown that gases of fermionic molecules can be effectively stabilized through external fields. However, many quantum applications will benefit from molecular ensembles with bosonic statistics. We report on the stabilization of a bosonic gas of strongly dipolar NaCs molecules against inelastic losses via microwave shielding, decreasing losses by more than a factor of 200 and reaching lifetimes on the scale of 1 second. We also measure high elastic scattering rates, a result of strong dipolar interactions, and observe the anisotropic nature of dipolar collisions. Finally, we demonstrate evaporative cooling of a bosonic molecular gas to a temperature of 36(5) nK, increasing its phase-space density by a factor of 20. This work is a critical step towards the creation of a Bose-Einstein condensate of dipolar molecules.

P2: Tunable Feshbach resonances in collisions of ultracold molecules in $^2\Sigma$ states with alkali-metal atoms

Robert C. Bird, Michael R. Tarbutt, and Jeremy M. Hutson
Presented by Robert C. Bird (Durham University, United Kingdom)

P3: Ultracold Field-Linked Tetratomic Molecules

Shrestha Biswas, Xing-Yan Chen, Sebastian Eppelt, Andreas Schindewolf, Fulin Deng, Tao Shi, Su Yi, Timon A. Hilker, Immanuel Bloch, Xin-Yu Luo
Presented by Shrestha Biswas (Quantum many body physics division, Max Planck Institute of Quantum Optics , Germany)

Dipolar ground-state molecules weakly bound to so-called field-linked tetratomic molecules would represent an exciting new type of particle to study in the context of ultracold many-body physics. Our recent detection of collisional field-linked resonances [1] and predictions for reasonable lifetimes of tetratomic states motivate us to pursue the creation of such novel particles.

In our experiment we manipulate the dipolar interaction between NaK molecules with a blue-detuned near-circular polarized microwave (MW) field. In the first place, this is done to shield the molecules from inelastic short-range collisions and allowed us to cool them to quantum degeneracy [2]. However, at sufficient high Rabi frequency or at elliptical MW polarization a well in the interaction potential can become deep enough to house field-linked bound states.

Previously we detected collisional resonances of these states by making the MW polarization elliptical, which compromises the shielding performance. We now developed a new generation of MW setup, which provides 100 watt MW power with ultralow phase noise. This should allow us to cross the field-linked resonance in a stable parameter regime and paves the way towards efficient conversion of NaK molecules to tetratomic molecules. A novel crossover from a dipolar p-wave superfluid to a BEC of tetratomic molecules might also be achievable.

References:
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P4: Ultra-cold potassium-cesium mixtures in an optical dipole trap

Mateusz Bocheński and Mariusz Semczuk
Presented by Mateusz Bocheński (Faculty of Physics, University of Warsaw, Poland)

We present our recent results on the production of ultracold mixtures of ^{39}K+Cs and ^{41}K+Cs confined in an optical dipole trap. We obtain samples of nearly 5×10^5 atoms of each species at ~10 μK which is a good starting point for studies of collisional properties of the ^{39,41}K+Cs mixture (in particular, search for Feshbach resonances) as well as for photoassociation spectroscopy required for the formation of ground state molecules.

We begin by simultaneous trapping of cesium and one of the potassium isotopes in magneto-optical traps while minimizing losses due to heteronuclear collisions. After the compression of the clouds by increasing the magnetic field gradient and appropriately red-detuning trapping beams, we apply gray molasses cooling techniques to both species. The potassium isotopes are cooled to ~10 μK using gray molasses on the D1 line, while for cesium we use light tuned near the D2 line. The dipole trap loading immediately follows the sub-Doppler cooling stage. Our studies have shown that the experimental sequence optimized for loading the dipole trap with only a single species needs to be slightly modified for the mixture and requires minor timing changes to match the cooling steps for cesium and potassium.
The mixture is trapped in a single-chamber system, where dispensers placed at a distance of about 10 cm from the center of the optical dipole trap are the only source of atoms. By properly balancing the current running through the dispensers and the light-induced atomic desorption timing we obtain a single species lifetime exceeding 10 s, sufficient for most applications, possibly even including reaching simultaneous quantum degeneracy.
In future experiments, we will pursue the search for Feshbach resonances in the ^{41}K+Cs mixture and photoassociation spectroscopy of KCs to identify a suitable pathway for reaching the ground state of the molecules with STIRAP.

P5: Polaron and bipolaron formation in a Bose gas

Ubaldo Cavazos Olivas and Krzysztof Jachymski
Presented by Ubaldo Cavazos Olivas (Institute of Theoretical Physics, 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 transport phenomena in condensed matter. One particular example are hybrid systems of atoms and ions, which are rapidly developing [1]. A distinctive property of these kind of systems at ultralow temperature is the emergence of the so-called polaron. A quantum bath composed of bosonic atoms weakly coupled to an ion can be properly described by means of Bogoliubov theory. Nevertheless, this approach is no longer valid as soon as the strong coupling regime is taken into account, leading to an instability with an infinite number of bosons collapsing into the ion. 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 and circumvent the bosons unstable behavior, based on [3], a variational approach is adopted. Employing a regularized potential that retains the correct long-distance behavior, we study the properties of interest in the formation of ionic Bose polaron and bipolaron, such as their energy, the number of bosons that takes part in the cloud formation, and the induced interactions which are tunable by the potential parameters.

References:
[1] Tomza, M. et al. Cold hybrid ion-atom systems. Rev. Mod. Phys. 91, 035001(2019).
[2] Astrakharchik, G.E., Ardila, L.A.P., Schmidt, R. et al. Ionic polaron in a Bose-Einstein condensate. Commun Phys 4, 94 (2021).
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P6: From polarons to molecules in a Bose-Einstein condensate

Arthur Christianen
Presented by Arthur Christianen (Max Planck Institute of Quantum Optics, Germany)

The creation of Feshbach molecules from a mixture of ultracold atoms is typically viewed as a two-body process in which only the two atoms forming the molecule take part. However, in case the mixture is degenerate this picture breaks down. A good example is the case of an impurity atom immersed in a Bose-Einstein condensate (BEC). Here, the impurity will be dressed by excitations from the BEC to form a Bose polaron, a quasiparticle reminiscent of condensed matter. When the boson-impurity interaction strength is now ramped across a Feshbach resonance, we find two possible scenarios. For most parameters there is a smooth crossover between a polaron state and a molecule-like state, but in case of light impurities and weak interboson repulsion, impurity-mediated interactions originating from the Efimov effect can cause a local collapse of the BEC. Also in the crossover case the Efimov effect is important, because not only dimers can be formed, but also trimers or larger bound states. In fact, the condensate can actually coherently couple these different molecular states! In collaboration with the group of Martin Zwierlein, we have found evidence for the formation of coherent dimer-trimer superpositions in photoassociation experiments in a BEC. I will show how the experimental rf-spectra can be simply understood from a three-level model considering a free impurity, a dimer and trimer state, all coherently coupled by the background condensate.

P7: Loading dynamics of a dual-species magneto-optical trap of cesium and potassium

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

We have measured, for the first time, the process of loading of dual species magneto-optical traps (MOTs) of cesium with three stable isotopes of potassium (^{39}K, ^{40}K and ^{41}K). Based on loading curves measured using fluorescence detection we have derived coefficients of the equations describing the MOT dynamics extracting the loading rate of the traps and losses induced by collisions with both the thermal background gas and co-trapped atoms. Usually these coefficients are extracted by analysis of the steady state of the trap [1,2], but in our approach we have chosen to propagate the equation using 4th order Runge-Kutta algorithm and we have fitted it to experimental results. We have been able to account for additional nonlinear terms in the MOT dynamics equation and our solution is more general - it covers also cases without the analytical solution.

We have studied the influence of light induced atomic desorption (LIAD) on the loading dynamics of both the single species and dual species MOTs. The LIAD increases the partial pressure of atoms of interest by desorbing them from the glass cell walls which leads to the increased loading rate and thus larger MOTs. With our method of analysis we can include the time varying partial pressure directly in the equation and analyze how the LIAD changes the environment inside our experiment chamber.

References:
[1] Torralbo-Campo, L., et al., Sci Rep 5, 14729 (2015)
[2] G. D. Telles, et al., Phys. Rev. A 63, 033406 (2001)

P8: 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 (Faculty of Physics, 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 describe e.g. the decoherence of a qubit in a disordered environment. We propose a method of realizing an ultracold quantum simulator for such a model. The proposed system consists of a single Rydberg atom („central spin") and polar molecules ("environment spins"), coupled via dipole-dipole interactions. By mapping internal particle states to spin states, spin-exchanging interactions can be simulated. The model can be precisely controlled by directly manipulating the placement of environment spins. As an example, we consider a ring-shaped arrangement of environment spins, and show how the system's time evolution is affected by the tilt angle of the ring.

P9: A New Lithium 6 Quantum Gas Microscope : Exploring the Projection of a Many-Body Wavefunction onto Single Atoms

Tim de Jongh, Joris Verstraten, Maxime Dixmerias, Kunlun Dai, Shuwei Jin, Bruno Peaudecerf, Tarik Yefsah
Presented by Tim de Jongh (Laboratoire Kastler Brossel, France)

The quantum gas microscope is a powerful tool that allows probing dilute quantum matter with single atom resolution, and has proven extremely useful for analog quantum simulation of lattice and spin-chain Hamiltonians. Here we report on the realization of a Lithium 6 quantum gas microscope devoted instead to the study of Fermi gases in continuous space and explore the projection dynamics from an initial many-body wavefunction onto individual lattice sites. This new "continuous space quantum gas microscope" offers the perspective to probe strongly interacting Fermi gases and topological quantum matter at an unprecedented length scale.

P10: Generation of entanglement in ultracold collision processes

Yimeng Wang
Presented by Yimeng Wang (Free University of Berlin, Germany)

This project attempts to quantify the entanglement generated in ultracold collisions. We especially focused on the motional degree of freedom for pure states. We discussed the entanglement between the proton and electron in Hydrogen. We pointed out the issue of the plane-wave initial condition and discussed possible ways to avoid it. Finally, we discussed the relation between scattering phase shifts and the motional degree of entanglement in a hard sphere model.

P11: Towards ground state CsYb molecules

T. Franzen, S. Segal, K. Wilson and S.L. Cornish
Presented by Tobias Franzen (Durham University, United Kingdom)

Combinations of alkali-metal and closed-shell atoms are a promising system for the production of 2Σ molecules as well as for the study of a large range of interacting quantum systems. Opportunities for species selective manipulation by magnetic and optical fields and the narrow intercombination line transitions in Yb open new possibilities. On the other hand, magnetic Feshbach resonances, the workhorses of ultracold molecule production from laser cooled atoms, are significantly more sparse and weaker than in bi-alkali systems. We present recent progress on our CsYb experiment, working towards the production of ground-state CsYb molecules.

P12: The low-lying excited states of $LiYb^+$

Marta Gałyńska, Paweł Tecmer, Katharina Boguslawski
Presented by Marta Gałyńska (Nicolaus Copernicus University in Toruń, Poland}

The ytterbium atom is a highly-valuable element because of its closed f-shell and the $4f^{14}6s^2$ ground-state electronic configuration, which makes its electronic structure similar to the group II-atoms. However, ytterbium has 70 electrons and is classified as a heavy element, which is an extraordinary challenge for state-of-the-art quantum chemistry because of nonnegligible spin-orbit coupling effects and the large number of electrons that need to be correlated. However, the spin-orbit coupling effects are often omitted during quantum chemistry investigations of ytterbium compounds because of the higher cost of the calculations. During the current project, we investigate the influence of relativistic effects on the low-lying excited states of $LiYb^+$ using the equation of motion coupled cluster (EOM-CCSD) method. All presented calculations were done with relativistic four-component Hamiltonian implemented in the DIRAC quantum chemistry software.

P13: Interactions and cold collisions of AlF in the ground and excited states with He: implications for buffer gas cooling

Sangami Gaesan Santhi, Matthew Frye, Marcin Gronowski, Michał Tomza
Presented by Sangami Gaesan Santhi (Faculty of Physics, University of Warsaw, Poland)

Aluminium monofluoride is a promising candidate for laser cooling and the production of dense ultracold molecular gases, thanks to its significant chemical stability and diagonal Frank-Condon factors. In this study, we examine the interactions and collisions between AlF in the $X^1\Sigma^+$, $a^3\Pi$, and $A^1\Pi$ electronic states and ground-state He using state-of-the-art \textit{ab initio} quantum chemistry techniques. We construct accurate potential energy surfaces (PESs) employing either the explicitly correlated coupled-cluster CCSD(T)-F12 method augmented by the CCSDT correction or the configuration-interaction method for higher-excited electronic states. Subsequently, we utilize these PESs in coupled-channel calculations to determine the scattering cross-sections for AlF+He collisions. We estimate the uncertainty of the calculated PESs and apply it to assess the uncertainty of the scattering results. Although we find relatively low sensitivity of the cross-sections to the variation of the PESs, the positions of shape resonances remain uncertain.

P14: 1- and 2-Photon Photoassociation Spectroscopy of RbYb near the Yb intercombination line

A. Görlitz, T. Franzen, B. Pollklesener, C. Sillus, A. Kallweit, C. Castor
Presented by Axel Görlitz (Institute of Experimental Physics, Heinrich-Heine-Universität Düsseldorf, Germany)

Ultracold dipolar molecules constitute a promising system for the investigation of topics like ultracold chemistry, novel interactions in quantum gases, precision measurements and quantum information. Here we report on first experiments in our new apparatus for the production of ultracold RbYb molecules. This setup constitutes an improvement of our old apparatus, where the interactions in RbYb and possible routes to molecule production have already been studied extensively [1,2]. In the new setup a major goal is the efficient production of ground state RbYb molecules. We employ optical tweezers to transport individually cooled samples of Rb and Yb from their separate production chambers to a dedicated science chamber. In this new apparatus we have observed 1- and 2-photon photoassociation transitions near the intercombination line of Yb. Thus, we were able to improve previous measurements of the binding energies of weakly bound vibrational levels in the electronic ground state of RbYb by two orders of magnitude [3].

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[2] C. Bruni et al., PRA 94, 022503 (2016)
[3] T. Franzen et al., PRA 107, 023114 (2023)

P15: Collisions in a quantum gas of bosonic $^{23}Na^{39}K$ molecules

J. Heier, M. Meyer zum Alten Borgloh, P. Gersema, K. K. Voges, L. Karpa, S. Ospelkaus-Schwarzer, C. Karam, O. Dulieu
Presented by Jule Heier (IQO / Leibniz Universität Hannover, Germany)

We report about our experiments with quantum gases of polar $^{23}Na^{39}K$ molecules. We discuss molecule-molecule collisions including the origin of loss processes in a cloud of chemically stable $^{23}Na^{39}K$ molecules, as well as atom-molecule collisions between NaK and K in different hyperfine states and magnetic field strengths.
Furthermore, we present a method for suppressing molecular loss using two optical photons at Raman resonance, leading to a potential barrier that protects the colliding molecules from reaching the short range.

P16: Two-photon optical shielding of collisions between ultracold polar molecules

Charbel Karam, Mara Meyer, Romain Vexiau, Maxence Lepers, Silke Ospelkaus, Nadia Bouloufa-Maafa, Leon Karpa and Olivier Dulieu
Presented by Charbel Karam (Paris Saclay University, France)

We propose a method to engineer repulsive long-range interactions between ultracold ground-state molecules using optical fields, thus preventing short-range collisional losses. It maps the microwave coupling recently used for collisional shielding onto a two-photon transition, and takes advantage of optical control techniques. In contrast to one-photon optical shielding [Phys. Rev. Lett. 125, 153202 (2020)], this scheme avoids heating of the molecular gas due to photon scattering. The proposed protocol, exemplified for $^{23}Na^{39}K$, should be applicable to a large class of polar diatomic molecules.

P17: Selection and control of cryogenically-cooled (bio)nanoparticle beams with external fields

Jingxuan He, Lukas Hass, Xuemei Cheng, Muhammed Amin, Lena Worbs, Jannik Lübke, Surya Kiran Peravali, Armando D. Estillore, Amit K. Samanta, Jochen Küpper
Presented by Jingxuan He (CFEL, DESY, Germany)

Unraveling the elementary steps of biological processes and chemical reactions has been a long-time goal. By using x-ray single-particle diffractive imaging, we can investigate the three-dimensional molecular structure of individual nanoparticles at atomic resolution through reconstructing a series of two-dimensional diffraction patterns [1].

However, because of the typically low signal-to-noise ratio, this requires the collection of a large amount of diffraction patterns. Since every intercepted particle is destroyed by the intense x-ray pulse, a new and preferably identical sample particle has to be delivered to every pulse. Here, we present an approach to prepare dense beams of cryo-cooled nanoparticles and macromolecules with buffer-gas cell cooling and aerodynamic focusing techniques [2-3].

Besides, we developed several control mechanisms with external fields at room temperature. For example, realizing a stream of pure, identical particles with electric field [4], and aligning the particles' arbitrary orientation in space by applying optical field (ns-laser induced alignment). Envisioned future experiments plan to make use of our cryogenic nanoparticle cooling setup together with efficient field-control to achieve a very high degree of alignment for shock-frozen proteins and, in turn, subnanometer resolution in single particle x-ray imaging.

References:
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[3] L. Worbs, et al., In preparation, (2022)
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P18: Magic wavelength for a rovibrational transition in molecular hydrogen

Hubert Jóźwiak, Piotr Wcisło
Presented by Hubert Jóźwiak (Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, Poland)

Molecular hydrogen, among other simple calculable atomic and molecular systems, possesses a huge advantage of having a set of ultralong living rovibrational states that make it well suited for studying fundamental physics and testing quantum theory. Frequencies of rovibrational transitions in the ground electronic state of molecular hydrogen are measured with uncertainties reaching a sub-parts-per-billion level.

To maintain the progress in accurate metrology, a cold H_2 sample will have to be trapped in an optical lattice. However, since the isotropic dipole polarizability in the v=0 and v=1 vibrational levels of H_2 differs by almost 10%, enormous light shift will dominate the uncertainty budget for the determination of the transition frequency.

We find a rovibrational transition for which the AC Stark shift is largely compensated by the interplay between the isotropic and anisotropic components of dipole polarizability. The residual AC Stark shift can be completely eliminated by tuning the trapping laser to a specific "magic wavelength" at which the weak quadrupole polarizability cancels the residual dipole polarizability.

P19: Parity violation in laser-coolable chiral molecules

Adam Koza, Michał Tomza
Presented by Adam Koza (Faculty of Physics, University of Warsaw, Poland)

Laser cooling is an excellent method to control molecules for precision measurement, quantum information, many-body physics, and fundamental physics applications. However, asymmetric top molecules (ATMs), due to their complex internal structure, are challenging for experimental manipulation. Although potentially difficult to produce, ultracold ATMs offer many qualitatively unique features useful for a broad range of science. Chiral molecules, from the definition, are classified as ATMs. Precise spectroscopy of such molecules can probe small shifts caused by parity violation effects (PV) in vibrational spectra of right- and left-handed enantiomers. In this study, we investigate the possibility of laser cooling of chiral systems like M-OCHDT, where M is a heavy metal atom, e.g. ytterbium (Yb). For this purpose, we calculate Frank-Condon factors using quantum chemistry methods. Next, we analyze parity violating potential along selected normal modes with Dirac-Coulomb Hamiltonian. Finally, we estimated PV shifts for selected vibrational transitions by solving the vibrational Schrodinger equation. We found out that for chiral isotopologues of symmetric top molecules, one can keep high values of FCFs and perform effective laser-cooling. In that way, the measurement of PV shifts on ultracold chiral molecules seems to be performed soon by experimentalists.

P20: Chemical reactions of ultracold alkaline-earth-metal diatomic molecules

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

We study the energetics of chemical reactions between ultracold ground-state alkaline-earth-metal diatomic molecules. We show that the atom-exchange reactions forming homonuclear dimers are energetically allowed for all heteronuclear alkaline-earth-metal combinations. We perform high- level electronic structure calculations on the potential energy surfaces of all possible homo- and heteronuclear alkaline-earth-metal trimers and show that trimer formation is also energetically possible in collisions of all considered dimers. Interactions between alkaline-earth-metal diatomic molecules lead to the formation of deeply bound reaction complexes stabilized by large non- additive interactions. We check that there are no barriers to the studied chemical reactions. This means that all alkaline-earth-metal diatomic molecules are chemically unstable at ultralow temperature, and optical lattice or shielding schemes may be necessary to segregate the molecules and suppress losses.

P21: Modest electric fields lead to enormously larger sticking times in ultracold molecular collisions.

Marijn Man, Tijs Karman, and Gerrit C. Groenenboom
Presented by Marijn Man (Radboud university, the Netherlands)

Collisions between ultracold molecules provide a way to very precisely study chemical collisions or reactions in the quantum regime. Besides being of fundamental importance, these collisions are also the main loss mechanism in ultracold gases. Currently, these collisions are theoretically described using a simple model based on transition state theory and phase space integrals. Unfortunately, experimental results and theoretical predictions don't always agree, so more detailed descriptions are necessary. For this, we turn to classical trajectories. A challenge in using classical trajectories to describe ultracold collisions is that the classical approximation is only valid in the potential well and not when describing long range interactions. In this work, we describe how we can account for this long range interaction when describing the system using classical trajectories. We then show how the classical trajectories can be used to describe the effects of external electric fields on ultracold collision complexes. We find that relatively modest electric fields (around 10 V/cm) could lead to an enormous increase in the sticking time (according to the phase space results from Chrisitanen et al. for NaK+NaK from 6 microseconds to 100 ms). As a result, collision complexes in these fields could be vulnerable to additional loss mechanisms, which might explain the discrepancy between theory and experiment. Additionally, we also estimate that the effect of blackbody radiation (on both diatom-atom systems and diatom-diatom systems) and hyperfine transitions (on diatom-diatom systems) will be small.

P22: Quantum simulation of extended electron-phonon-coupling models in a hybrid Rydberg atom setup

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

State-of-the-art experiments using Rydberg atoms can now operate with large numbers of trapped particles with tunable geometry and long coherence time. We propose a way to utilize this in a hybrid setup involving neutral ground-state atoms to efficiently simulate condensed-matter models featuring electron-phonon coupling. Such implementation should allow for controlling the coupling strength and range as well as the band structure of both the phonons and atoms, paving the way towards studying both static and dynamic properties of extended Hubbard-Holstein models.

P23: Shielding collisions of ultracold CaF molecules with static electric fields

Bijit Mukherjee, Matthew D. Frye, C. Ruth Le Sueur, Michael R. Tarbutt and Jeremy M. Hutson
Presented by Bijit Mukherjee (Department of Chemistry, Durham University, United Kingdom)

We study collisions of ultracold CaF molecules in strong static electric fields. Such fields allow the creation of long-range barriers in the interaction potential, which prevent the molecules reaching the short-range region where inelastic and other loss processes are likely to occur. We carry out coupled-channel calculations of rate coefficients for elastic scattering and loss. We develop an efficient procedure for including energetically well-separated rotor functions in the basis set via a Van Vleck transformation. We show that shielding is particularly efficient for CaF and allows the rate of 2-body loss processes to be reduced by a factor of 10^7 or more at a field of 23 kV/cm. The loss rates remain low over a substantial range of fields. Electron and nuclear spins cause strong additional loss in some small ranges of field, but have little effect elsewhere. The results pave the way for evaporative cooling of CaF towards quantum degeneracy.

P24: Quantum-logic control of complex molecular ions for applications in molecular and chemical physics

Prerna Paliwal, Mikhail Popov and Stefan Willitsch
Presented by Prerna Paliwal (Department of Chemistry, University of Basel, Switzerland)

Over the past years, the coherent manipulation of single isolated quantum systems such as atoms, ions, superconducting circuits, and quantum dots has advanced greatly and yielded important applications in the fields of quantum metrology, quantum sensing, and quantum computing. Recently, extending and applying quantum technologies to molecules has become one of the prime goals of the quantum physics community. However, their complex internal structure and lack of cycling transitions makes it difficult to cool, control and manipulate them. In our lab, we co-trap a single molecular ion together with an atomic ion which acts as a coolant to cool the molecule translationally as well as a messenger for the internal state identification of the molecule without destroying it. The information of the complex molecular ion is mapped onto an easily addressable atomic ion from where it is read out. Here, we highlight the quantum-non-demolition detection of the rovibrational state of single nitrogen ions which is a crucial step towards their coherent manipulation. We show how this method allows us to go beyond the state-of-the-art and prepare molecular ions in well-defined hyperfine-Zeeman states. We also discuss the extension of our technique to polyatomic ions to lay the foundations for the exploration of their spectroscopy and molecular dynamics.

P25: Exploring Kitaev model with Rydberg Atoms: Probing Exotic Spin States through Dipole-Dipole Interactions

Sakthikumaran Ravichandran, Krzysztof Jachymski
Presented by Sakthikumaran Ravichandran (Faculty of Physics, University of Warsaw, Poland)

The Kitaev model has been a captivating platform in the field of quantum spin systems due to the emergence of exotic spin states. In this work, we propose an approach to realising the Kitaev-type interactions using Rydberg atoms, exploiting their strong dipole-dipole interactions to engineer intriguing quantum spin dynamics. By arranging Rydberg atoms in a honeycomb lattice configuration, we take advantage of their large electric dipole moments and precisely tailored interactions. We leverage these dipole-dipole interactions to design an effective spin Hamiltonian that mirrors the anisotropic couplings of the Kitaev model, allowing us to explore its unique physics in a controllable experimental platform. Through a combination of theoretical analysis and numerical simulations, our study aims to unveil the emergence of exotic spin states facilitated by dipole-dipole interactions. The ability to manipulate the dipole-dipole interactions between Rydberg atoms offers new opportunities for controlling, engineering, and exploring novel quantum phases.

P26: Field-Linked Resonances

Andreas Schindewolf, Xing-Yan Chen, Sebastian Eppelt, Roman Bause, Marcel Duda, Shrestha Biswas, Tijs Karman, Timon Hilker, Immanuel Bloch, and Xin-Yu Luo
Presented by Andreas Schindewolf (MPQ, Germany)

Field-linked resonances were predicted 20 years ago by John Bohn's group [PRL 90, 043006 (2003)]. We now realized them [Nature 614, 59 (2023)] by shaping the long-range intermolecular potential that is induced by a microwave field for microwave shielding [Nature 607, 677 (2022)]. By tuning the parameters of the microwave field (polarization, intensity, and detuning from the rotational transition) we can engineer a potential well that is deep enough to house field-linked bound-states, which give rise to the resonances. The coexistence of large dipole-dipole interaction and tunable contact interaction in the vicinity of the field-linked resonances enables the investigation of novel kinds of dipolar superfluids and supersolids.

P27: Dynamics of complexes of aromatic molecules with alkali-metal and alkalineearth-metal atoms with application to spectroscopy and ultracold studies

Leonid Shirkov
Presented by Leonid Shirkov (Institute of Physics, PAS, Poland)

To generate molecules at temperatures below the millikelvin range, an additional cooling process is necessary. Sympathetic cooling, a method that cools precooled molecules by exposing them to ultracold atomic gas, is a promising approach. We study the spectroscopic and collisional behavior of polyatomic aromatic molecules immersed in ultracold atomic gases. The molecules such as benzene, furan, pyrrole, pyridine, and azulene interacting with alkali-metal and alkaline-earth-metal atoms are considered. Prior studies have reported ab initio potential energy surfaces (PESs) for some of the complexes of our interest, complemented by analytical long-range potentials based on analytical Casimir-Polder integrals [1, 2].

We solve the 3D Schrödinger equation, adapted for the complexes of nonlinear molecules with an atom [3, 4], using the obtained PESs. Subsequently, we analyze the rovibrational energies and study elastic and inelastic collisional processes at millikelvin temperatures and discuss the potential for sympathetically cooling for the considered complexes.

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P28: Rotational quenching of C_2 with ^{3}He and ^{4}He collisions at ultracold temperatures.

Ritika Soni and T. J. Dhilip Kumar
Presented by Ritika Soni (Department of Chemistry, IIT Ropar, India)

Atomic and molecular phenomena at temperatures close to absolute zero have become a frontier area of experimental and theoretical research in Chemical Physics. This is due to the spectacular progress achieved in recent years in cooling and trapping of a large variety of atoms and molecules at temperatures in the micro Kelvin and nano Kelvin regimes. Cooling molecules to ultracold temperatures has produced a new research area of ultracold chemistry, whose applications range from testing fundamental symmetries of nature, quantum simulation of spin-lattice models, and ultracold molecules. There is abundant interest in ultracold molecules due to their applications in controlled chemical reactions and high resolution molecular spectroscopy. There are many studies on ro-vibrational energy transfer collisions at ultracold temperatures which shows that the energy transfer can be extremely efficient at ultracold temperatures and is sensitive to the initial ro-vibrational energy levels.

Closed-coupled scattering calculations are carried out at temperatures ranging from 10^{-8} K to 100 K for studying the rotational transitions of C_2 undergoing collisions with isotopes of Helium (^{3}He and ^{4}He) atoms employing the new C_2-He 2D potential energy surface (PES) computed at the CCSD(T)-F12b/aug-cc-pVQZ level of theory. Among the isotopes of He, heavier isotope (^{4}He) is found to have higher value of rotational quenching cross-sections and suggests that the ^{4}He molecule is a good candidate for ^{4}He buffer gas cooling. Wigner's threshold law is found to be valid in this system where the cross-section increases with decrease in the temperature.

P29: Rotation of a molecule in two-dimensional condensate: angulon properties and spontaneous vortex formation

Michał Suchorowski, Michał Tomza, Mikhail Lemeshko, Artem Volosniev
Presented by Michał Suchorowski (Faculty of Physics, University of Warsaw, Poland)

In this study, we explore the behavior of a rotating molecular impurity in a two-dimensional Bose-Einstein condensate. Using a Gross-Pitaevskii-type equation, we investigate how the impurity-bath interaction and size of the condensate affect the angular momentum distribution, density deformation, and density currents in the system. In line with experimental results and angulon theory, we show that the impurity's effective moment of inertia is modified by its interaction with the quantum solvent, leading to a slowing down of its rotation for low angular momentum states. Additionally, we observe the emergence of collective excitations such as solitons and vortices in the system after rapid rotation of the impurity. Our model provides insight into the behavior of impurities in two-dimensional quantum gases and can be seen as an effective description of a rotating molecule on the surface of a superfluid helium droplet.

P30: Excited electronic states of Sr_2: ab initio predictions and experimental observation of the $2^1\Sigma_u^+$ state

J. Szczepkowski, M. Gronowski, A. Grochola, W. Jastrzebski, M. Tomza and P. Kowalczyk
Presented by Jacek Szczepkowski (Institute of Physics, Polish Academy of Sciences , Poland)

Despite its apparently simple nature with four valence electrons, the strontium dimer constitutes a challenge for modern electronic structure theory. Here we focus on excited electronic states of Sr_2, which we investigate theoretically up to 25000 cm^{-1} above the ground state, to guide and explain new spectroscopic measurements. In particular, we focus on potential energy curves for the $1^1\Sigma_u^+$, $2^1\Sigma_u^+$, $1^1\Pi_u$, $2^1\Pi_u$, and $1^1\Delta_u$ states computed using several variants of *ab initio* coupled-cluster and configuration-interaction methods to benchmark them. In addition, a new experimental study of the excited $2^1\Sigma_u^+$ state using polarisation labelling spectroscopy is presented, which extends knowledge of this state to high vibrational levels, where perturbation by higher electronic states is observed. The available experimental observations are compared with the theoretical predictions and help to assess the accuracy and limitations of employed theoretical models.

P31: Superfluid Bose and Fermi gases and their mixtures

Marek Tylutki
Presented by Marek Tylutki (Faculty of Physics, Warsaw University of Technology, Poland)

We present the research on quantum defects in superfluid atomic Bose and Fermi gases and their mixtures. The Fermi gas is modeled with the Bogoliubov-de Gennes equations in the weakly interacting (BCS) regime and with the Density Functional Theory in the strongly interacting (unitary) regime, while the condensate of bosons is described with the Gross-Pitaevskii equation. The Fermi gas is considered in both spin-polarized and unpolarized configurations. Superfluid nature of these systems is manifested through uniquely quantum effects such as the presence of vortex lines, the Josephson effect, solitonic excitations etc.

P32: Many-body Perturbation Theory formulated in terms of physically motivated parameters for 1D atomic chains

Matej Veis, Jozef Noga
Presented by Matej Veis (Comenius University Bratislava, Slovakia)

Contributions to the correlation energy at MP2 level are examined for a finite chain of. hydrogen atoms. We demonstrate that restricting oneself to a subset of MP2 terms, such as pair-states, either doesn't involve a scaling reduction or vanishes at the thermodynamic limit † . Similarities between the terms do appear, and allow for them to be classified by three effective parameters, i.e. momentum transfer, depth and asymmetry of the corresponding diagram. Formulating the perturbative series with respect to these physically motivated parameters not only gives an insight regarding the magnitude of terms, but also allows for their separation into similar groups. Integrating over such groups leads to a size extensive scheme, with bounds on error, that does involve a scaling reduction. As a proof of concept the method was benchmarked against full MP2 and CCSD with STO-6G and cc-pVDZ.

P33: Charge transfer of polyatomic molecules in ion-atom hybrid traps: Stereodynamics in the millikelvin regime

A. Voute, A. Dörfler, L. Wiesenfeld, O. Dulieu, F. Gatti, D. Peláez and S. Willitsch
Presented by Alexandre Voute (Institut des Sciences Moléculaires d'Orsay, CNRS, Université Paris-Saclay, France)

In the framework of ultra-cold chemistry, where reactions can be studied in well-defined quantum states, collisional phenomena between cations and neu- tral atoms are still not fully understood. Widely used semi-classical capture models, such as the one of Langevin [1], fail in some cases in predicting correctly rate constants associated to the charge transfer between two such species. The discrepancies between these models and experiment usually indicate that the de- tailed shape of the relevant potential energy surfaces (PES) at short ion-atom distance are determining in the reaction dynamics [2]. Ion-atom hybrid trap experiments capable of handling molecular ions and atoms at temperatures in the millikelvin regime allow for measuring charge transfer reaction rate constants with precision. We present here the results for the collision between the prototypical triatomic ion N_2H^+ and Rb which also display a deviation from semi-classical models. The focus of this presentation is the exploration of the PESs involved in the N_2H^+ + Rb reaction, carried out with multiconfigurational ab initio electronic structure methods, through which we identify the main reasons for such a deviation [3]. Namely, the charge transfer is limited to certain configurations of the polyatomic system and it occurs via deformation of N_2H^+.
This work hence reveals the onset of anisotropic and polyatomic effects that were absent in the atomic and diatomic molecular ions studied so far in a similar context [2], highlighting the importance of stereodynamics in cold molecular-ion collisions.

References:
[1] G. Gioumousis and D. P. Stevenson, J. Chem. Phys. 29, 294-299 (1958)
[2] A. Dörfler, P. Eberle, D. Koner, M. Tomza, M. Meuwly and S. Willitsch,
Nat. Comm. 10, 5429 (2019)
[3] A. Voute and A. Dörfler and L. Wiesenfeld and O. Dulieu and F. Gatti and
D. Peláez and S. Willitsch, (2023), [under review]

P34: Quantum resonant control of cold Rb–Sr^+ collisions high above the ultracold regime

Maks Walewski, Matthew Frye, Michał Tomza
Presented by Maks Walewski (Faculty of Physics, University of Warsaw, Poland)

Feshbach resonances play a pivotal role in controlling interactions in ultracold atomic gases and atom-molecule mixtures. It has long been believed that Feshbach resonances in atom-ion collisions can only be observed in the ultracold regime, where only a few lowest partial waves contribute to the collision rates. Such conditions (usually $T \lesssim 1\mu K$) are difficult to reach for most ion-atom systems. Here we show that magnetically tunable Feshbach resonances can be used to control the inelastic collisions between a single trapped Sr^+ ion and Rb atoms in the multiple-partial-wave regime. We use the state-resolved measurements of cold inelastic Rb–Sr^+ collisions investigated experimentally in the group of Prof. Roee Ozeri at the Weizmann Institute of Science to calibrate a comprehensive theoretical model of ion-atom collisions. We show the prediction of magnetic Feshbach resonances in Rb–Sr^+ collisions at millikelvin temperatures, much above the few-partial wave regime.

P35: Mercury Rydberg molecules

Agata Wojciechowska, Matthew Eiles, Michał Tomza
Presented by Agata Wojciechowska (Faculty of Physics, University of Warsaw, Poland)

Due to their unusual energy structure and permanent dipole moments, Rydberg molecules are a topic of recent research interest. In our work, we examine the ultralong-range Rydberg molecules, composed of a Rydberg and a ground-state atom. By far, physicists have mostly focused on molecules built with atoms with one valence electron (like Rb, Cs). Some attempts have been made to calculate Sr and Yb molecules but due to their complexity, the progress has stalled. Here we construct a complete model to describe the ultralong-range Rydberg molecule containing the Hg atom which has got two valence electrons but luckily can be treated as a single-channel element. We pave the path toward more complex species and encourage possible experimental realizations.

P36: Testing deep ultraviolet laser cooling of AlF molecules with cadmium atoms

Sid Wright, Jose Eduardo Padilla-Castillo, Simon Hofsäss, Russell Thomas, Stefan Truppe and Gerard Meijer
Presented by Eduardo Padilla (Fritz Haber Insitute of the Max Planck Society, Germany)

Aluminium monofluoride (AlF) is a promising candidate for laser cooling and trapping at high densities. The primary laser cooling transition at 227.5 nm is extremely strong, highly vibrationally diagonal, and it is feasible to slow a molecular beam from 200 m/s to rest in around 1 cm. This offers the potential to greatly increase the number and density of molecules available for ultracold experiments.

As a useful first step towards a magneto-optical trap (MOT) of AlF, we tested our experimental system on cadmium atoms. The $^1P_1$-$^1S_0$ transition in Cd at 228 nm lies conveniently near the laser cooling transition in AlF, with an almost identical radiative lifetime. However, the simple structure of atomic Cd enables slowing and trapping with a single laser, with far fewer loss channels than for AlF. Moreover, the narrow $^3P_1$-$^1S_0$ intercombination line in Cd permits straightforward velocity resolved measurements at the level of 1 m/s, via Doppler-sensitive laser-induced fluorescence.

We compare various laser slowing methods with a cold atomic beam of Cd, and demonstrate rapid loading of a high density Cd MOT on the $^1P_1$-$^1S_0$ transition. Using the intercombination line, we measure the velocity distribution directly in front of the trap location for Zeeman slowing, chirped frequency slowing and crossed beam slowing configurations. Our experiments illustrate the power of deep ultraviolet laser slowing, providing useful guidance and an optimistic perspective for future experiments on AlF.

P37: A hybrid trap of cold ions and cold neutral molecules for ion-molecule reaction studies

Yanning Yin, Christian Mangeng, Richard Karl, Stefan Willitsch
Presented by Yanning Yin (University of Basel, Switzerland)

Benefited from the advances in ion trapping, molecular deceleration and trapping techniques, a hybrid trap of ions and neutral molecules, which is a combination of ion trap and molecular trap, has been developed as a new platform for carrying out proof-of-principle studies on low-temperature ion-molecule collisions.
Here we present our progress towards a hybrid trap of OH molecules and Ca^+ ions. The OH molecules are firstly cooled via supersonic expansion, then decelerated to 30 m/s via a Stark decelerator, and finally loaded into a magnetic quadrupole trap formed by permanent magnets. Using a new voltage switching scheme for the decelerator, we increased the signal of trapped molecules ~7 fold. The Ca^+ ions are first trapped at one stage of a segmented linear Paul trap, cooled via Doppler cooling, and then shuttled to the OH trap position. Once the two traps are superimposed, the position-dependent Zeeman shifts of Ca^+ ions caused by the strongly inhomogeneous magnetic fields of the OH trap (with a gradient up to 1600 Gauss/mm) will cause the laser cooling of Ca^+ to cease. To address this issue, we employed two cooling lasers with properly tuned wavelengths and polarizations and one repumping laser. Consequently, Ca^+ can still be efficiently cooled to a temperature of millikelvin level, comparable to the case without the magnetic field. With the successful magnetic trapping of OH molecules and laser cooling of trapped Ca^+ ions in the same region, a hybrid trap is now being formed and investigated in our lab.

P38: Progress towards ultracold KCs molecules

K. Zamarski, C. Beulenkamp, D. Zhang, M. Landini, H.-C. Nägerl
Presented by Krysztof Zamarski (University of Innsbruck, Austria)

One of the last bi-alkalis that have not yet been observed in the ultracold regime is the KCs molecule, which has proven difficult to associate due to the lack of convenient magnetic field conditions suitable for double-species evaporation. In our current setup, we have developed an efficient simultaneous cooling scheme for potassium and cesium that allowed us to observe the interspecies Feshbach resonances and test various molecular association techniques. At the same time, we are building an upgraded version of the vacuum setup, which is going to combine a high electric field control capability, necessary for tuning the dipolar interactions, with single-site resolution fluorescence microscopy. Such a well-controlled system will provide an excellent platform for studying lattice spin models and exotic phases of matter.

P39: An Experiment to Measure the Electron's Electric Dipole Moment Using an Ultracold Beam of YbF Molecules

M. Ziemba, F. Collings, R. Jenkins, G. Li, S. Swarbrick, J. Lim, B. E. Sauer and M. R. Tarbutt
Presented by Michael Ziemba (Centre for Cold Matter, Imperial College London, United Kingdom)

The fact that more matter than antimatter has been produced in the early stages of the universe is unexplained and known as the matter-antimatter-asymmetry problem [1]. One precondition is the combined violation of charge conjugation and parity (CP-violation) which is too small in the Standard Model. In almost all theories, CP-violation is also a precondition for the electron to have an electric dipole moment (de). In this respect, a measurement of de can be a test of theories beyond the Standard Model.

The value of de can be determined by measuring the precession rate of the electron spin in a strong electric field. Heavy polarized molecules with their high intra-molecular fields have already set a limit of $|d_e| \sim 4.1\times10^{-30}$ e cm [3]. To improve on this, we create a collimated, bright beam of laser cooled YbF molecules [4] and have built an experiment to measure de using this beam [2]. I will present key aspects of this experiment which we hope can determine de with an uncertainty of 5×10^{-30} e cm in one day of measurement [4].

References:
[1] L. Canetti et al. New J. Phys. 14 095012 (2012).
[2] N J Fitch, J Lim, E A Hinds, B E Sauer, and M R Tarbutt. Quantum Sci. Technol., 6, 014006, (2021).
[3] T. Roussy, et. al. "A new bound on the electron's electric dipole moment". arXiv:2212.11841 (2022).
[4] X. Alauze et al. Quantum Sci. Technol. 6, 044005 (2021).

Notes

Notes

Organisational matters for evening activities:

- **Welcome Dinner**

We are pleased to invite you to pub **"Lolek Grill&Bar"**
The **dinner** starts at **19:00**

Venue adress:
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 16:00.**

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 **"Kameralna"**
The **dinner** starts at **19:30**

Venue adress:
Mikołaja Kopernika 3, Warsaw

Connection from workshop venue:
The most convenient connection to the restaurant is with **tram 7**, **tram 9**, **tram 25**, **bus 128** or **bus 175**.

Warsaw Time GMT+2	September 5th Tuesday	September 6th Wednesday	September 7th Thursday	September 8th Friday
		Session B1	**Session C1**	**Session D1**
09:00 - 09:30		Michael Tarbutt	Silke Ospelkaus-Schwarzer	Gerhard Rempe
09:30 - 10:00		Tim Langen	Stefan Truppe	Loïc Anderegg
10:00 - 10.15		Matthew Frye	Hannah Williams	Piotr Wcisło
10.15 - 10.30		Luke Caldwell	Marcin Gronowski	Ashwin Singh
10:30 - 11:00		Coffee Break	Coffee Break	Coffee Break
		Session B2	**Session C2**	**Session D2**
11:00 - 11:30		Florian Schreck	Christiane Koch	Edvardas Narevicius
11:30 - 12:00		Gabriel Patenotte	Kaden Hazzard	Bas van de Meerakker
12:00 - 12.15		Mikhail Lemeshko	Kai Dieckmann	Roman Bause
12:15 - 12.30			Giacomo Valtolina	Yuly Andrea Chamorro Mena
12:30 - 13.00	Registration & Welcome Coffee	Workshop photo	Lunch Break	Lunch Break
13.00 - 13:30		Lunch Break		
13:30 - 14:00				
	Session A1	**Session B3**	**Session C3**	**Session D3**
14:00 - 14.30	Sebastian Will	Alan Jamison	Discusion panel on future of ultracold molecules	Mateusz Borkowski
14:30 - 15:00	Xin-Yu Luo	Calder Miller		Aleksander Woźniak
15:00 - 15:30	Tijs Karman	Thomas Bilitewski	Coffee Break	Matthew Eiles
15:30 - 16:00	Coffee Break	Coffee Break	Transfer to Old Town by public transport	Coffee Break
	Session A2	**Session B4**	**Social Activities**	
16:00 - 16:30	Maxence Lepers	Simon Cornish	Old Town Sightseeing	
16:30 - 17:00	Timur Tscherbul	Jeremy Hutson		
17:00 - 17:15	Baraa Shammout	Poster sesion		
17:15 - 17.30	Anna Dawid			
17:30 - 18:00	Coffee Break			
18:00 - 18:30				
18:30 - 19:00				
19:00 - 19.30	Welcome Dinner			
19.30 - ...			Workshop Dinner	