

MO 19: Poster 3

Time: Thursday 16:30–18:30

Location: P

MO 19.1 Thu 16:30 P

High resolution spectroscopy of biomolecules in a cryogenic 16-pole wire ion trap — ●ENDRES ERIC¹, GEISTLINGER KATHARINA¹, DAHLMANN FRANZISKA¹, MICHAELSEN TIM¹, ONCAK MILAN¹, MOHANDAS SALVI², and WESTER ROLAND¹ — ¹Institut f. Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria — ²Institute of Science Education and Research, Tirupati, India

Spectroscopy plays an increasingly important role in the study of structural details of complex biological systems and the investigation of UV photodamage of genetic material. In combination with electrospray ionization, ion trap spectroscopy has been successfully used to investigate electronic and vibrational transitions in biomolecules in order to determine geometrical structures or the decay channels following electronic excitation.

In this contribution a recently developed linear cryogenic 16-pole wire ion trap for ion spectroscopy at temperatures below 4 K will be presented. The trap offers a large field-free region in the radial direction, reducing radio-frequency heating and provides large optical access perpendicular to the ion beam direction.[1] The low temperatures enabled multiple tagging of glycine ions, allowing high resolution IR action spectroscopy of the OH stretching vibration. Simulated rotational contours of the absorption band yield a rotational temperature of about 6 K.[2] Furthermore, preliminary results of photodissociation measurement of [dAMP-H]⁻, a monomer of DNA, will be presented.

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

[2]Geistlinger et. al., J. Mol. Spectrosc. 379, 111479 (2021)

MO 19.2 Thu 16:30 P

Numerical Justification for Increased Conductance of Ferrocene Molecule at Room Temperature — ●STEPAN MAREK — Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

The conductance of molecular junctions is numerically challenging problem combining physics of macroscopic electrodes/reservoirs and microscopic molecules. Recent experimental advances help guide the theoretical calculations and provide a good testing case for the numerical methods. Perhaps the most widely used approach to numerical electronic structure calculations is the density functional theory (DFT). This method is used to calculate ground state electronic structure of several electrode-plus-ferrocene molecule geometries. The results are then refined in conductance calculations, and by thermal averaging of the conductance in different geometries, predictions on the thermal dependence of the conductance of the junction are made, which qualitatively agree with the experiment.

MO 19.3 Thu 16:30 P

High resolution photoelectron spectroscopy on deeply cold niobium and tantalum clusters — ●FABIAN BÄR, MORITZ WEIGT, and BERND V. ISSENDORFF — Physikalisches Institut der Albert-Ludwigs-Universität Freiburg

The properties of deeply cold niobium clusters Nb₉⁻ to Nb₃₀⁻ and tantalum clusters Ta₅⁻ to Ta₂₂⁻ at 3.9K have been investigated.

In combination with a time-dependent potential applied to the flight tube, our magnetic bottle time-of-flight photoelectron spectrometer has a current resolution of $\Delta E/E = 0.37\%$ [1]. This is at least a factor five better than a standard magnetic bottle spectrometer and still competitive with a hemispherical energy analyzer whose drawback is a significantly worse collection efficiency. Combining the improved spectrometer with a low-jitter, short-pulse excimer laser operating at 157nm, we gain access to bound states down to 7.9eV at a so far unreached precision in such a setup [2].

In this configuration we recorded more detailed photoelectron spectra for small niobium and tantalum clusters cooled down to their vibrational ground state.

[1] M.Weigt, PhD thesis, Albert-Ludwigs-Universität Freiburg (2021).

[2] O.Kostko, PhD thesis, Albert-Ludwigs-Universität Freiburg (2007).

MO 19.4 Thu 16:30 P

New apparatus for synchrotron-based photoelectron spec-

troscopy of cold, mass-selected and cold ions in the gas phase — ●PHILLIP STÖCKS, FABIAN BÄR, LUKAS WEISE, and BERND V. ISSENDORFF — Physikalisches Institut der Albert-Ludwigs-Universität Freiburg

A novel instrumentation is under development for photoelectron spectroscopy of gas phase ions, aiming for wide exploitation of the potential of synchrotron radiation sources like BESSY II for the study of mass-selected nanoparticles, complexes and molecules.

The setup will make use of the strongly increased ion density in an ion trap for photoelectron spectroscopy of size-selected cluster or molecular ions with synchrotron radiation. Photoelectrons emitted by the ions inside the ion trap will be guided by a tailored magnetic field out of the ion trap, extracted from the magnetic guiding field by custom designed electron optics, and transferred into a hemispherical energy analyser with a position sensitive detector. By employing this method, photoelectron intensities can be obtained that are orders of magnitude higher than by direct irradiation of an ion beam. This worldwide unique setup will make core-levels and the full valence band of free ions routinely accessible for the first time and can be used for a broad range of studies, from the characterisation of the electronic structure of transition metal clusters and organometallic complexes via core-level shifts, to the examination of reactions on the surface of catalytically active nanoparticles; tackling problems of both, fundamental importance and direct technological relevance.

MO 19.5 Thu 16:30 P

Detailed investigation of unexpected photoelectron spectra via angle resolved spectroscopy of Copper clusters — ●LUKAS WEISE and BERND V. ISSENDORFF — Physikalisches Institut der Albert-Ludwigs-Universität Freiburg

Angle resolved spectroscopy provides an important test of the theoretical description of clusters since these spectra carry more information than the bare energy levels. The anisotropy of photoelectron spectra for example depends on the angular momentum state.

The cluster anions are produced in a magnetron sputter source, cooled to 7 K and enter a time-of-flight spectrometer for mass measurement and selection. Afterwards electrons are detached by linear polarised laser light and projected onto a MCP detector in a velocity map imaging setup.

The presented analysis utilises the additional information from angle resolved spectroscopy to gain a better understanding of photoelectron spectra, that have not been predicted by theory so far. For Cu₉₁⁻ an electronic shell closing is expected. Previous experiments [1,2], however, have shown an additional peak associated to the occupation of the next orbital, that would be predicted for Cu₉₂⁻. Based on the angle resolved measurements an f-type character can be assigned to the additional state.

[1] O. Kostko, PhD thesis, Albert-Ludwigs-Universität Freiburg (2007).

[2] M. Knickelbein, Chemical Physics Letters 192, 1 (1992), 129-134.

MO 19.6 Thu 16:30 P

Disentangling the relationship between S_N2 and E2 reactions in ethyl halides — ●THOMAS GSTIR, ATILAY AYASLI, TIM MICHAELSEN, ARNAB KHAN, and ROLAND WESTER — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Innsbruck, Austria

The bimolecular nucleophilic substitution reaction (S_N2) and bimolecular elimination reaction (E2) are two essential reaction types in organic chemistry. As both reactions lead to the same ionic product, it is inherently difficult to distinguish between them solely with experimental approaches. In an attempt to overcome this, we measured the reaction of fluoride with iodoethane (CH₃CH₂I) and its fully β-carbon-fluorinated counterpart (CF₃CH₂I). These lead to the complete suppression of the E2 pathway. Here, we report the results of the reactions in the gas phase at four collision energies between 0.4 and 2 eV. For these measurements, we employed a crossed molecular beam setup combined with a velocity map imaging spectrometer. The obtained energy and angle differential cross sections can reveal a mechanistic understanding of reaction dynamics on an atomic level, especially in cooperation with state-of-the-art theory. In the present experiment we

observe an increased signal in the proton transfer channel and at higher collision energies the formation of CF_2Cl^- . Both reaction pathways originate from an attack on a α -carbon hydrogen. In $\text{CH}_3\text{CH}_2\text{I}$ this would most likely lead to a hydrogen migration along the C-C bond and a subsequent E2 breakup.

MO 19.7 Thu 16:30 P

Experimental setup towards High-Resolution Ion-Molecule Crossed Beam Imaging — ●DASARATH SWARAJ, FLORIAN TRUMMER, TIM MICHAELSEN, ARNAB KHAN, ROBERT WILD, FABIO ZAPPA, and ROLAND WESTER — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, 6020 Innsbruck, Austria

Detailed insight into the dynamics of elementary reactions in the gas phase can be obtained from crossed-beam reactive scattering experiments. Crossed beam combined with velocity map imaging (VMI), angle and energy differential crosssections can be obtained.[1][2] In this contribution, we present the design plan and relevant simulations for an experimental setup to investigate ion molecule reactions with higher precision than previously attainable. The ions will be created by laser ionization so that they are mostly in the vibrational ground state. In addition, according to our simulation, a proper shaping of the ionization volume and a very weak acceleration of the ions play a crucial role in deciding the ion beam energy resolution. The ion beam is overlapped with the beam of neutral molecules and the collision products are collected by the VMI spectrometer. We also plan a coincidence detection of both the ionic and neutral products after the reaction, which will be further implemented by a laser ionization scheme. With our new setup, we plan to study fundamental astrophysically significant reactions such as $\text{H}_2^+ + \text{H}_2 \rightarrow \text{H}_3^+ + \text{H}$.

[1] R. Wester, Mass Spectrometry Reviews, 2021.

[2] R. Wester, Phys. Chem. Chem. Phys., vol. 16, pp.396-405,2014.

MO 19.8 Thu 16:30 P

Observation and manipulation of long-lived electronic coherences in lanthanide complexes at room temperature

— ●MIRALI GHEIBI, JAYANTA GHOSH, CRISTIAN SARPE, BASTIAN ZIELINSKI, TILLMANN KALAS, RAMELA CIOBOTEA, ARNE SENFTLEBEN, THOMAS BAUMERT, and HENDRIKE BRAUN — Institute of Physics and CINSaT, University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

The aim of SMolBits - Scalable Molecular Quantum Bits - is the realization of ideal quantum systems with long-lived levels, isolated from the environment to form quantum bits as key building blocks for advanced quantum technologies. Lanthanides are particularly promising with respect to possible applications in quantum-based information storage and gate operations at the atomic and molecular levels. Their energy levels and electronic states are barely influenced by the environment and their bonds to the ligands attached to the lanthanides. Some of them show a prominent absorption feature around 800 nm. In this research, the electronic coherences excited in lanthanide complexes by interaction with IR femtosecond laser pulses and their lifetimes using phase-locked double pulses and fluorescence detection under a confocal-microscope are investigated. An electronic coherence time of more than 600 fs for two different complexes containing Neodymium is observed. Currently, we study Rabi oscillations in these complexes. As a next step, the influence of spectrally phase-shaped femtosecond laser pulses in the non-perturbative regime onto the electronic excitation and the created coherence for quantum gate implementation is researched.

MO 19.9 Thu 16:30 P

Towards quantum control of Calcium ions for the use in molecular spectroscopy — ●MANIKA BHARDWAJ, JOSSELIN BERNARDOFF, JAN THIEME, DAQING WANG, MARKUS DEBATIN, and KILIAN SINGER — University of Kassel, Kassel, Germany

We present our advances towards establishing a new two-dimensional spectroscopy method that selectively maps the suitable quantum states. For this purpose, the molecular ions to be investigated are sympathetically cooled and trapped in an ion trap with laser-cooled calcium ions [1]. We will use the photon-recoil spectroscopy method to study the molecular ions through studying the photon-recoil imparted on co-trapped calcium ion [2].

[1] Groot-Berning, Kornher, Jacob, Stopp, Dawkins, Kolesov, Wrachtrup, Singer, Schmidt-Kaler, Phys. Rev. Lett. 123, 106802 (2019) [2] Wan, Gebert, Wübbena, Scharnhorst, Amairi, Leroux, Hemmerling, Lörch, Hammerer, Schmidt, Nat Commun 5, 3096 (2014)

MO 19.10 Thu 16:30 P

Towards the production of groundstate RbYb molecules — ●CHRISTIAN SILLUS, BASTIAN POLLKLESENER, CÉLINE CASTOR, and AXEL GÖRLITZ — Heinrich-Heine Universität Düsseldorf

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 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. 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. Here we start to study interspecies interactions of different isotopes by overlapping crossed optical dipole traps. We report of first results of implementing an optical lattice and using photoassociation spectroscopy on the way towards groundstate molecules.

MO 19.11 Thu 16:30 P

Self-bound dipolar droplets and supersolids in molecular Bose-Einstein condensates — ●MATTHIAS SCHMIDT¹, PHILLIP GROSS¹, LUCAS LASSABLIÈRE², GOULVEN QUÉMÈNER², and TIM LANGEN¹ — ¹Physikalisches Institut und Center for Integrated Quantum Science and Technology, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — ²Université Paris-Saclay, CNRS, Laboratoire Aimé Cotton, 91405 Orsay, France

We numerically study the many-body physics of molecular Bose-Einstein condensates with strong dipole-dipole interactions. We observe the formation of self-bound droplets, and explore phase diagrams that feature a variety of exotic supersolid states. In all of these cases, the large and tunable molecular dipole moments enable the study of unexplored regimes and phenomena, including liquid-like density saturation and universal stability scaling laws for droplets, as well as pattern formation and the limits of droplet supersolidity. We discuss a realistic experimental approach to realize both the required collisional stability of the molecular gases and the independent tunability of their contact and dipolar interaction strengths. Our work provides both a blueprint and a benchmark for near-future experiments with bulk molecular Bose-Einstein condensates.

MO 19.12 Thu 16:30 P

Preparing and characterizing ultracold bosonic $^{23}\text{Na}^{39}\text{K}$ spin polarized ground state molecules — ●MARA MEYER ZUM ALTEN BORGLOH¹, PHILIPP GERSEMA¹, KAI KONRAD VOGES¹, TORSTEN HARTMANN¹, LEON KARPA¹, ALESSANDRO ZENESINI², and SILKE OSPELKAUS¹ — ¹Leibniz Universität Hannover, Institut für Quantenoptik — ²INO-CNR BEC Center and Dipartimento di Fisica, Università di Trento

Recently, ultracold polar molecules have become the focus of interest for research in quantum chemistry and metrology. Heteronuclear molecules have a large electric dipole moment, which allows the study of long-range and anisotropic dipole-dipole interactions. Moreover, their large number of degrees of freedom, such as rotation and vibration, opens up new possibilities for quantum simulations. We report the preparation of ground-state bosonic spin-polarized NaK molecules with a large electric dipole moment of 2.7 D. Starting from an ultracold quantum gas mixture of K and Na atoms, we first generate weakly bound molecules near a Feshbach resonance. The Feshbach molecules are then transformed into strongly bound molecules in the absolute molecular ground state by stimulated Raman adiabatic passage (STIRAP). The STIRAP pulse is performed within 12 μs and has an efficiency of about 70%, preparing up to 4200 molecules at a temperature of about 300 nK. Finally, we report the dependence of the energy structure of the vibrational ground state manifold on the electric field and the manipulation of the molecular hyperfine and rotational state.

MO 19.13 Thu 16:30 P

Complex Formation in Three-Body Reactions of Cl^- with H_2 — ●CHRISTINE LOCHMANN, ROBERT WILD, MARKUS NÖTZOLD, and ROLAND WESTER — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Österreich

Dihydrogen halide clusters are the subject of various theoretical and experimental studies [1]. In their anionic state they are weakly bound complexes and can provide insight into dynamical processes in chemi-

cal reactions. Here we report the three-body reaction rate of Cl^- with H_2 forming the $\text{Cl}^-(\text{H}_2)$ complex, as well as the temperature dependence of this reaction in the range of 10 - 26 K [2]. Furthermore, we observe the back-reaction with an unexpected dependence to the third power of the density. Comparisons of the experiment in a 22-pole rod and a newly installed 16-pole wire trap [3] are presented and show that the ions reach lower temperature in the 16-pole trap. We have recently also observed a three-body process in the reaction of C_2^- with two H_2 which leads to the product C_2H^- . In the future we plan on expanding the research of three-body reactions at low temperatures. One focus will be the influence of the nuclear spin state of hydrogen on three-body reaction rates.

- [1] F. Dahlmann, et al., J. Chem. Phys. (in press) (2021);
- [2] R. Wild, et al., J. Phys. Chem. A, 125, 8581 (2021)
- [3] K. Geistlinger, et al., Rev. Sci. Instrum. 92, 023204 (2021)

MO 19.14 Thu 16:30 P

Progress on Zeeman slowing of CaF — ●MARIA STEPANOVA, TIMO POLL, PAUL KAEBERT, SUPENG XU, MIRCO SIERCKE, and SILKE OSPELKAUS — Institut für Quantenoptik, Leibniz Universität Hannover

Recently, great progress has been made in direct laser cooling of molecules to temperatures close to absolute zero. However, experiments are limited by the number of molecules that can be captured from molecular beams using typical laser-based trapping methods. In Petzold et al. 2018, we proposed to transfer Zeeman deceleration to laser-coolable molecules and thus substantially increase the number of molecules that can be captured by e.g. magneto-optical traps. Here, we now present our characterisation of the Zeeman force for CaF molecules, Kaebert et al. 2021. We find excellent agreement of the force with an optical Bloch equation model. This shows that the generated force profile can compress the initial molecular velocity distribution from a standard buffer gas cell to the velocity required for trapping in a magneto-optical trap (MOT). We present the current status of our experiment as well as theoretical work on a novel Bayesian-optimised molecular MOT scheme for CaF molecules.

MO 19.15 Thu 16:30 P

Characterization of an experimental setup to investigate cold molecule-Rydberg-atom interactions — ●MARTIN ZEPPEFELD — MPI für Quantenoptik

Strong interactions between molecules and Rydberg atom extend to distances larger than $1\ \mu\text{m}$, promising exciting applications in quantum science. This includes possibilities for cooling internal and external molecular degrees of freedom, nondestructive molecule detection and state readout, and performing quantum gates.

Towards these goals, I will present an experimental setup for the investigation of cold molecule-Rydberg-atom interactions. Cold molecules are produced via velocity filtering with an electrostatic quadrupole guide. Rydberg atoms are produced via two-photon excitation of ultracold atoms in a rubidium MOT. A key feature of the setup is a set of 24 electrodes, allowing the electric fields experienced by the Rydberg atoms to be precisely controlled. Combined with mm-waves at roughly 400 – 500 GHz to drive Rydberg transitions and state selective field ionization for detection, this allows precise control and read-out of the atomic Rydberg states.

MO 19.16 Thu 16:30 P

Modelling laser cooling and molecular structure in BaF — ●FELIX KOGEL, MARIAN ROCKENHÄUSER, EINIUS PULTINEVICIUS, and TIM LANGEN — Universität Stuttgart, 5. Physikalisches Institut, IQST

Cold molecular gases are promising candidates for studies of cold chem-

istry, precision tests of fundamental symmetries and quantum simulation. Motivated by our experiments on barium monofluoride (BaF), we report here on the simulation of laser cooling for this species, using multi-level rate equations and optical Bloch equations. We present efficient Doppler, sub-Doppler and coherent cooling schemes for both bosonic and fermionic isotopologues of this species. In addition, we discuss the analysis of experimental spectra of the lowest vibrational transitions relevant for laser cooling of BaF.

MO 19.17 Thu 16:30 P

Towards nanoplasma formation from size selected helium droplets using an electrostatic deflector — CRISTIAN MEDINA¹, ●SEBASTIAN TRIPPEL², ROBERT MOSHAMMER³, THOMAS PFEIFER³, JOCHEN KUPPER², FRANK STIENKEMEIER¹, and MARCEL MUDRICH⁴ — ¹University of Freiburg, Freiburg im Breisgau, Germany — ²Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ³Max Planck Institute for Nuclear Physics, Heidelberg, Germany — ⁴Aarhus University, Aarhus, Denmark

It has recently been demonstrated that passing a molecule with a large dipole moment embedded inside a helium nanodroplet across an inhomogeneous electric field allows deflecting the entire droplet depending on its mass [1]. We present the calculations and design for a helium droplet size selector apparatus using CsI molecules as dopants. The doped clusters are deflected transversally by a type-B deflector with an inhomogeneous electric field [2]. In the proposed experiment, a nanoplasma is ignited in the helium droplet by a NIR femtosecond laser, tightly focused by a motorized back-focusing mirror, moving the focus across the diverted beam. The resulting electrons and ions emitted by the nanoplasma are collected by an electron velocity-map imaging and an ion time-of-flight spectrometer. The theoretical calculations of the spatial deflections were done using the CMIfly software developed by the Molecule Imaging group (CMI) at the Centre for Free-Electron Laser Science (CFEL)[2].

- [1]D.J. Merthe et al., j. phys. chem. lett. 7 (2016).
- [2]J-P. Chang et al., comput. phys. commun. 185 (2014).

MO 19.18 Thu 16:30 P

Preparations for experiments with triatomic hydrogen ions at the Cryogenic Storage Ring — ●AIGARS ZNOTINS¹, ANNIKA OETJENS¹, FLORIAN GRUSSIE¹, DAMIAN MULL¹, OLDRICH NOVOTNY¹, FELIX NUSSLIN¹, ANDREAS WOLF¹, ARNAUD DOCHAIN², XAVIER URBAIN², and HOLGER KRECKEL¹ — ¹Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany — ²Institute of Condensed Matter and Nanoscience, Louvain-la-Neuve B-1348, Belgium

The triatomic hydrogen ion H_3^+ is considered a key species in astrochemistry. It serves as a benchmark system for theoretical calculations of small polyatomic molecules and has been identified as one of the main drivers of an active interstellar ion-neutral chemistry network, contributing to the formation of complex molecules in space. Additionally, electron recombination of H_3^+ has received a lot of attention, owing to the influence of its rate coefficient on the ionization balance of interstellar chemistry networks. Here, we report current efforts to understand the cooling behavior of H_3^+ and H_2D^+ inside the Cryogenic Storage Ring, and the preparation of laser diagnostic schemes and dedicated ion sources for future studies. We explore the feasibility of using multi-color action spectroscopy of cold H_3^+ ions to probe excited states in the energy region above $20000\ \text{cm}^{-1}$.

As the use of a rotationally cold ion source is a crucial component of the foreseen studies, we present the design and characteristics of a pulsed supersonic expansion source to produce molecular ion beams with low rotational temperatures.