MO 13: Posters 3: Cold Molecules, Helium Nano Droplets, and Experimental Techniques

Time: Wednesday 16:30–18:30 Location: Spree-Palais

MO 13.1 Wed 16:30 Spree-Palais

Centrifuge deceleration of electrically guided continuous beams of polar molecules — •Thomas Gantner, Sotir Chervenkov, Xing Wu, Josef Bayerl, Andreas Rohlfes, Martin Zeppenfeld, and Gerhard Rempe — Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany

We present experimental results from a novel and versatile decelerator for continuous beams of neutral polar molecules [1]. A beam of polar molecules from an effusive nozzle is injected at the periphery of a rotating disk and electrically guided [2] to the centre along a spiral-shaped electrostatic quadrupole guide. Thus the molecules climb up the centrifugal potential hill and get decelerated as they propagate. The deceleration of continuous beams of neutral CF$_3$H, CH$_3$F, and CF$_3$CCH is demonstrated. The combination of the centrifuge decelerator with a cryogenic buffer-gas cooling source [3] is expected to result in the production of even larger fluxes of slow and moreover internally cold molecules amenable to further cooling [4].

[1] S. Chervenkov et al., Phys. Rev. Lett. (in press), arXiv:1311.7119 (2013)

[2] S.A. Rangwala et al., Phys. Rev. A 67, 043406 (2003)

[3] L.D. van Buuren et al., Phys. Rev. Lett. 102, 033001 (2009)

[4] M. Zeppenfeld et al., Nature 491, 570 (2012)

MO 13.2 Wed 16:30 Spree-Palais

Combining a continuous centrifuge decelerator with a cryogenic buffer-gas source — •Xing Wu, Sotir Chervenkov, Thomas Gantner, Joseph Bayerl, Martin Zeppenfeld, and Gerhard Rempe — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

The production of large samples of slow molecules with high internal-state purity is still a major challenge in the fast-growing research field of cold molecules. We propose a promising solution by combining a recently demonstrated centrifuge decelerator [1] with a cryogenic buffer-gas source [2]. The centrifuge decelerator is based on the centrifugal potential in a rotating frame, enables a continuous deceleration of molecular beams to almost a standstill, and is applicable to a large range of species. The cryogenic source provides high intensities of internally cold molecules. In order to optimize the flux of the electrically guided beams [3], both the supersonic and the effusive regime of the buffer-gas cooling have been explored. The obtained results indicate that the optimum is achieved in the so-called boosted effusive regime. In combination with the centrifuge decelerator, continuous beams at intensities of several $10^9 s^{-1} mm^{-2}$ occupying a minimum number of internal states, and with close-to-zero velocities are conceivable.

[1] S. Chervenkov *et al.*, Phys. Rev. Lett. (in press); arXiv:1311.7119

[2] L.D. van Buuren *et al.*, Phys. Rev. Lett. **102**, 033001 (2009)

[3] S.A. Rangwala *et al.*, Phys. Rev. A **67**, 043406 (2003)

MO 13.3 Wed 16:30 Spree-Palais

Finding pathways for creation of cold molecules by laser spectroscopy — •Ivo Temelkov, Horst Knöckel, and Eberhard Tiemann — QUEST und Inst. f .Quantenoptik, Leibniz Universität Hannover

The diatomic alkali molecules are of serious interest for the cold matter physics. This research is focused on developing a model for efficient transfer of ^{23}Na^{39}K molecules from the Na(3s)+K(4s) asymptote to the lowest levels of the singlet ground state. The experiment is done in an ultrasonic beam apparatus, using a Λ-scheme with fixed pump and scanning dump laser. The signals are observed as dark lines on a constant fluorescence. The intermediate level is strongly perturbed helping to overcome the singlet-triplet transfer prohibition. In the beam NaK is created in its singlet ground state and the transfer is driven to the triplet state, but this scheme can work also in the reversed direction. Precise potential energy curves for singlet and triplet ground state already exist from previous work of our group. We observe highly resolved hyperfine spectra of various rovibrational levels (from v=2 up to the asymptote, for N=4,6,8) of the $a^3\Sigma^+$ state with resolution better than 10MHz. Two different theoretical models are used in parallel to describe the observations. The first one is based on molecular parameters. The other uses potential curves, taking into account all couplings as functions of the internuclear distance and calculating the energy levels for all the quantum numbers in a coupled state model. With these results an efficient pathway for the creation of cold NaK molecules is demonstrated.

MO 13.4 Wed 16:30 Spree-Palais

Development of a versatile ion trap based experimental station for the study of biomolecular ions — •Tim Michaelsen, Sunil Kumar, Thorsten Best, and Roland Wester — Institut f. Ionenphysik und Angewandte Physik, Universität Innsbruck

Intramolecular vibrational relaxation of biomolecules upon UV excitation is the key process determining their stability against radiation damage[1]. However, the details of the mechanism behind this process are still poorly understood.

We are currently developing a versatile ion trap based experimental station which will allow us to examine this process in detail. The biomolecular ions are produced in an electrospray ion source[2] with an ion-funnel interface[3], which has already been implemented and characterized. The ions are then guided by a linear quadrupole and mass selected by a second quadrupole. They will be stored and cooled down to 4K in a unique 16-pole ion trap, which is designed to allow for laser irradiation of ions normal to the trap axis similar to our wire-based octupole ion trap[4]. The ions extracted from the ion trap are then analyzed using a reflectron-based time-of-flight mass spectrometer. To investigate the details of the intermolecular vibrational relaxation of chromophore-based molecules, we will choose the fluorescent protein chromophore anion as a model system.

[1] A.V. Bochenkova , L.H. Andersen , Faraday Discuss.163, 297-319 (2013); [2] Gaskell, S. J. , J. Mass Spectrom. 32, 677-688. (1997); [3] Ryan T Kelly, et al., Mass Spectrom. Rev., 29, 294-312 (2010); [4] J. Deiglmayr, et al., Phys. Rev. A 86, 043438 (2012);

MO 13.5 Wed 16:30 Spree-Palais

Spatial separation of molecular clusters and conformers — •Thomas Kierspel[1,2], Daniel A. Horke[1], Yuan-Pin Chang[1], Sebastian Trippel[1], and Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science, DESY, Hamburg — [2]The Hamburg Center for Ultrafast Imaging — [3]Department of Physics, University of Hamburg

Many complex molecules exhibit multiple structural isomers (conformers) [1], even at the low temperatures in a cold molecular beam [2]. These conformers, as well as molecular clusters, typically differ in their electric dipole moment. The dispersion of a molecular beam using the electric deflector can be exploited for the spatial separation of the different species present in the beam [3]. We present the spatial separation of both, *cis-* and *trans-*, conformers of 3-fluorophenol (3FP) [4], the separation of indole-water dimers from a cluster soup [5], and discuss the prospects for conformer separation of glycine, the smallest amino acid. 3FP is a prototypically large molecule and conformational clean samples enable novel experiments like laser pump-, and ultrafast X-ray or photoelectron diffraction probe, to image conformer-interconversion processes. Molecular clusters like indole-water are bridging the gap between isolated and solvated molecules and are a key to understand the molecule-solvent interaction and the influence of the environment on the molecular function.

[1] Suenram et al., *J. Mol. Spectrosc.* **72** , 372-382 (1978) [2] Rizzo et al., *J. Chem. Phys* **83**, 4819 (1985) [3] Chang et al., *Science* **342**, 98-101 (2013) [4] Kierspel et al., *Chem. Phys. Lett.* **591**, 130-132 (2014) [5] Trippel et al., *Phys. Rev. A* **86**, 033202 (2012)

MO 13.6 Wed 16:30 Spree-Palais

Supersonic molecular beams for high-precision measurements using a traveling-wave decelerator — •sreekanth chirayath mathavan, joost e van den berg, corine meinema, janko nauta, ronnie hoekstra, leo huisman, imko smid, and steven hoekstra — university of groningen, groningen, the netherlands

We are building an experimental setup to perform high-precision experiments to test fundamental physics with cold molecules. We combine supersonic expansion with traveling-wave deceleration and laser cooling to create dense, translationally and internally cold molecular samples in the same quantum state. We started our experiments with the SrF molecule, which we already showed can be decelerated, and is laser coolable, which enhances its sensitivity towards high-precision experiments. On this poster, we present our work on the creation of an intense supersonic beam of SrF.

MO 13.7 Wed 16:30 Spree-Palais

Rotational-dynamics studies of state-selected molecules — •Jens S. Kienitz[1,2], Sebastian Trippel[1], Terence G. Mullins[1], Nele L. M. Müller[1], and Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science, DESY — [2]Center for Ultrafast Imaging, University of Hamburg — [3]Department of Physics, University of Hamburg

State-selected, strongly aligned and oriented molecular ensembles serve as ideal samples to image ultrafast chemistry in the molecular frame, for instance, through molecular-frame photo-electron angular distributions or electron- or x-ray diffraction. We developed advanced techniques to manipulate the motion of molecules in cold supersonic beams at a kHz repetition rate [1]. State-, conformer-, and size-selection of neutral molecules was achieved through the dispersion of the molecular beam in the electric deflector. The state-selected molecules were laser aligned or mixed-field oriented in laser and static electric fields. We demonstrated strong alignment as well as mixed-field orientation for different molecular samples up to a 1 kHz repetition rate. We investigated the effects of widely varying pulse laser durations (50 fs to 500 ps), reaching from the impulsive regime to the adiabatic regime, which allowed us to disentangle previous experimental approaches. So far unobserved details of the intricate rotational dynamics were observed in the intermediate regime, e.g., for laser pulses on the order of the rotational period of the molecules.
[1] S.Trippel et al., Mol. Phys., 111, 1738 (2013)

MO 13.8 Wed 16:30 Spree-Palais

Deceleration and deflection of cold Hydrogen molecules by a Rydberg Stark decelerator — •Johannes Deiglmayr, Pitt Allmendinger, Joseph Agner, and Frédéric Merkt — ETH Zurich, Laboratory of Physical Chemistry, Zurich, Switzerland

In the past years our group developed a miniature decelerator for atoms and molecules in Rydberg-Stark-states [1]. It consists of a two-dimensional array of electrodes on a printed circuit board which creates weak electric fields with large field gradients, making the deceleration of atoms and molecules in Rydberg states with high n possible.

Recently we have realized a bent version of our decelerator which deflects the decelerated beam by 10° from the axis of supersonic expansion. The deflected samples of atoms and molecules have translational temperatures on the order of 100mK, which makes them ideally suited for trapping or collision experiments. We will present these results and the current status of the experiment.

[1] S. D. Hogan et al., PRL 108), 063008 (2012); P. Allmendinger et al., PRA 88, 043433 (2013)

MO 13.9 Wed 16:30 Spree-Palais

Perspectives for translational temperature diagnostics of trapped ions by evaporative losses. — •Olga Lakhmanskaya[1], Thorsten Best[1], Sunil Kumar[1], Eric Endres[1], Daniel Hauser[1], Rico Otto[2], Stephanie Eisenbach[3], Alexander von Zastrow[4], and Roland Wester[1] — [1]Universität Insbruck, A-6020, Innsbruck, Austria — [2]University of California, San Diego, California 92093-0332, United States — [3]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany — [4]Institute for Molecules and Materials IMM, Radboud University Nijmegen, 6525 AJ Nijmegen, The Netherlands

We present a scheme for translational temperature diagnostics of ions in a 22-pole ion trap using data for OH^- and D^- anions. This scheme is based on the strong dependence of the lifetime of the ions on temperature. While examining loss rates as a function of buffer gas temperature we have found a breakdown of thermalisation for trap temperatures lower than 25 K. We have investigated this feature in more detail and have found that it does not depend on either buffer gas or the trapping parameters. We have also investigated two regimes for ion losses, either over one of the two end cap electrodes (axial direction) or over the effective potential (radial direction). We have found that evaporation over the end caps may be suitable for translational thermometry.

MO 13.10 Wed 16:30 Spree-Palais

Quantum simulations with trapped molecules with mircowave field — •Yubing Yang — Departement of Physics, University of Freiburg, Stefan-Meier-Strasse 19, D-79104 Freiburg, Germany

Ultracold quantum gases offer a unique setting for quantum simulation of interacting many-body systems. Systems of trapped molecules can be accurately controlled and manipulated with microwave field, a large variety of interactions can be engineered with high precision and measurements of relevant observables can be obtained with nearly 80% efficiency. Here, the authors discuss prospects for quantum simulations using systems of trapped molecules with microwave field , and review the available set of quantum operations and first proof-of-principle experiments for both analog and digital quantum simulations with trapped molecules with microwave field. Here we review recent advances in technology and discuss progress in a number of areas where experimental results have already been obtained.

MO 13.11 Wed 16:30 Spree-Palais

Laser cooling of heavy diatomic molecules — •Corine Meinema, Joost van den Berg, Sreekanth Mathavan, Janko Nauta, Lorenz Willmann, Klaus Jungmann, and Steven Hoekstra — Rijksuniversiteit Groningen, Groningen, the Netherlands

We will combine our travelling-wave decelerator with laser cooling to obtain a gas of ultra cold polar molecules, all in the same quantum state. After deceleration the gas of SrF molecules has a temperature of 150 mK. Laser cooling will be used to reduce this to 150 μK. Due to the complex rotational and vibrational structure, laser cooling is for most types of molecules not possible. However, SrF has an almost closed rovibrational transition, that we can use to scatter sufficient photons before the molecule will be pumped into a dark state. We will present our experimental approach and the latest results.

MO 13.12 Wed 16:30 Spree-Palais

MEASUREMENT OF THE LIFETIME OF THE FIRST VIBRATIONALLY EXCITED STATE OF MGH+ — •Oscar O. Versolato[1,4], Maria Schwarz[1,4], Anders K. Hansen[2], Alex D. Gingell[2], Alexander Windberger[1], Łukasz Kłosowski[3], Joachim Ullrich[4], Frank Jensen[2], José R. Crespo López-Urrutia[1], and Michael Drewsen[2] — [1]Max-Planck-Institut für Kernphysik, Heidelberg, Germany — [2]Aarhus University, Denmark — [3]Nicolaus Copernicus University, Torun, Poland — [4]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

Diatomic hydrides are a basic class of molecules with dipole-allowed rovibrational transitions, readily observable in the interstellar medium (ISM) both in their neutral and singly ionized states. In general, their abundances in the ISM are derived from mm-wave and deep infrared absorption and emission lines for which precise knowledge of the relevant rovibrational transition strengths is required. We present here a method for obtaining such transition strengths employing a direct laser excitation scheme and exploiting the cryogenic environment of our cryogenic Paul trap CryPTEx, in which blackbody radiation induced rotational dynamics are slowed down and excellent vacuum conditions exist, enabling the measurement of the lifetime of the first vibrationally excited state in MgH+ by means of laser excitation to this state, followed by resonance enhanced two-photon dissociation of the ions that were sympathetically cooling into a Coulomb crystal. The method presented here can readily be extended to other molecules of particular astrophysical relevance.

MO 13.13 Wed 16:30 Spree-Palais

ULTRA-TENUOUS ROTATIONAL BUFFER GAS COOLING OF COULOMB-CRYSTALLIZED MGH+ — Anders K. Hansen[1], •Oscar O. Versolato[2,3], Łukasz Kłosowski[4], Simon B. Kristensen[1], Alex D. Gingell[1], Maria Schwarz[2,3], Alexander Windberger[2], Joachim Ullrich[3], José R. Crespo López-Urrutia[2], and Michael Drewsen[1] — [1]QUANTOP, Department of Physics and Astronomy, Aarhus University, Denmark — [2]Max-Planck-Institut für Kernphysik, Heidelberg, Germany — [3]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [4]Nicolaus Copernicus University, Torun, Poland

The preparation of cold molecules is of particular interest for studies of cold chemistry, astrophysics, as well as for fundamental physics. Recent progress in direct laser cooling methods has shown great promise, but these methods are extremely molecule-specific. Buffer gas cooling in multipole traps, although universally applicable, also has significant drawbacks because of the high densities required. Here, we present for the first time results of tenuous helium buffer gas cooling of the rotational degrees of freedom of MgH+ molecular ions at 4-5 orders of magnitude lower pressure than in typical buffer gas settings. The MgH+ ions were sympathetically laser cooled into a Coulomb crystal after which very efficient buffer gas cooling was performed, reaching a record-low molecular ion internal temperature. Effective tuning of the temperature between 7 and 60K, by changing micromotion amplitudes, was demonstrated. Tenuous buffer gas cooling should also enable studies on cold single, heavy molecules of biological interest.

MO 13.14 Wed 16:30 Spree-Palais

Detecting the Rotational State of Electrically Trapped Polyatomic Molecules — •Rosa Glöckner, Alexander Prehn, Martin Zeppenfeld, and Gerhard Rempe — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching

The determination of the internal state of molecules is a key element for their precise control. However, especially for polyatomic molecules, state sensitive detection can be a considerable challenge due to predissociation and fragmentation when addressing electronic transitions with uv light. We present here an alternative for trapped molecules using depletion.

Our method is based on the difference of signals with and without depletion: driving transitions from selected rotational states to untrapped states. Therefore, the detection of the molecule itself can be state independent and thus a simple method like a quadrupol mass spectrometer (QMS) is sufficient. We demonstrate two variations of the method, infrared depletion and microwave depletion, and discuss the assets and drawbacks.

In addition to rotational J-levels, we can address individual M-sublevels. Using this we can extract the narrow field distribution in our homogeneous-field electric trap[1] by measuring the Stark-broadened line shape of the transition between the $|J=3,K=3,M=3\rangle \rightarrow |J=4,K=3,M=4\rangle$ states of CH_3F. We expect our method to work for a large number of molecular species.

[1] B.G.U. Englert *et al.*, *Phys. Rev. Lett.* **107**, 263003 (2011).

MO 13.15 Wed 16:30 Spree-Palais

Sympathetic cooling of OH$^-$ ions using Rb atoms in a MOT — •Henry Lopez[1], Bastian Höltkemeier[1], Julian Glässel[1], Pascal Weckesser[1], Eric Endres[2], Thorsten Best[2], Roland Wester[2], and Matthias Weidemüller[1] — [1]Physikalisches Institut, Ruprecht-Karls-Universität Heidelberg, Deutschland — [2]Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Österreich

Molecular ions are usually caught in high-order multipole radio frequency traps and cooled sympathetically by He buffer gas. In order to reach lower temperatures for a wider range of molecular ions we investigate replacing He with laser-cooled atoms. In particular, we use a new hybrid ion-atom trap to study the interaction of ultracold Rb atoms with mass-selected OH$^-$-water clusters. While the Rb atoms are stored in a Dark-SPOT trap loaded from a 2D-MOT, the ions are trapped in an octupole radio frequency trap consisting of thin wires, enabling optical access to the trapping region. For efficient cooling a dense cloud of atoms is needed, preferably in the ground state to avoid inelastic collisions. In our setup we trap up to 4×10^8 atoms at peak densities of up to 3×10^{11} atoms/cm^3 with almost all atoms being in the absolute ground state. For these parameters our numerical simulations suggest that cooling the ions by at least one order of magnitude can be achieved. On this poster I report on the status of our experiment, its limitations and possible applications.

MO 13.16 Wed 16:30 Spree-Palais

Stretching the Envelope in Crossed Beam Experiments — •Alexander von Zastrow, Jolijn Onvlee, Sjoerd Vogels, David H. Parker, and Sebastiaan Y. T. van de Meerakker — Radboud Universiteit Nijmegen, Institute for Materials and Molecules, Heyendaalseweg 135, 6525AJ Nijmegen

The fundamental understanding of intermolecular interactions is essential for various fields, such as astrophysics. Highly detailed information about these interactions can be extracted from atomic and molecular collisions in crossed beam experiments.

Combining the Stark deceleration technique with velocity map imaging results in high resolution experiments which give detailed information about intermolecular interactions. This is shown in the observation of diffraction oscillations in the differential cross section of state-to-state inelastic scattering of NO molecules with rare gas atoms. Further advantage of this high resolution will be taken in the future. In particular, our approach is ideally suited to investigate low-energy quantum scattering resonances with unprecedented accuracy. The measurement of such phenomena can make a significant contribution to a better understanding of intermolecular interactions, both experimentally and theoretically.

MO 13.17 Wed 16:30 Spree-Palais

Observation of coherent interference and determination of strengths and signs of an electric- and magnetic-dipole transition moment in OH — •H.C. Schewe[1], D. Zhang[1], X. Wang[1], G. Meijer[1,2], B. Sartakov[3], R. W. Field[4], and N. Vanhaecke[1,5] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft Faradayweg 4-6, 14159 Berlin — [2]Radboud University Nijmegen, Institute for Molecules and Materials, Heijendaalseweg 135, 6525 AJ Nijmegen, the Netherlands. — [3]General Physics Institute RAS, Vavilov Street 38, 119991 Moscow, Russia — [4]Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139 — [5]Laboratoire Aimé Cotton, CNRS, Université Paris-Sud, 91405

Spectroscopic investigations of particles are a fundamental method to investigate its structure and dynamics. Higher order transitions like a magnetic-dipole or electric-quradrupole transition reveal a deeper insight into the quantum system itself. Usually these transitions are many orders of magnitude weeker and, therefore, experimentally challenging to determine.

The magnetic dipole transition in the OH radical has been determined in two different ways: (1) using a static electric field, whereby an electric-dipole transition moment is admixed to a magnetic-dipole transition, and (2) using the method of Stark interference: by applying a static magnetic and static electric field, a coherent interference of the electric- and magnetic transition dipole moment could be observed, and the strength and the sign of the transition momenta was determined.

MO 13.18 Wed 16:30 Spree-Palais

En route to many-body physics with ^{23}Na-^{40}K ground-state polar molecules — •Zhenkai Lu, Nikolaus Buchheim, Tobias Schneider, Immanuel Bloch, and Christoph Gohle — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, 85748 Garching, Germany

Ultra cold quantum gases with long-range dipolar interaction promise exciting new possibilities for quantum simulation of strongly interacting many-body systems.

New classes of many-body phases (like super solids and stripe phases) are on the horizon and ferroelectric phases of highly polarizable systems are expected [1][2].

We have constructed an experimental apparatus aiming to create ultracold chemical stable ground-state ^{23}Na-^{40}K molecules. We will present the design considerations, implementation and performance of the experiment. In addition, we will present our recent results on producing ^{23}Na-^{40}K Feshbach molecules.

[1] G. Pupillo, et al. Condensed Matter Physics with Cold Polar Molecules. arXiv: 0805.1896 (2008).

[2] M. Iskin, et al. Ultracold Heteronuclear Molecules and Ferroelectric Superfluids. Phys. Rev. Lett. 99, 110402 (2007).

MO 13.19 Wed 16:30 Spree-Palais

Imaging photoionization dynamics of doped Helium Nanodroplets and molecular Rydberg states — •Johannes von Vangerow[1], Alexandr Bogomolov[2], Barbara Grüner[1], Alexey Baklanov[2], Frank Stienkemeier[1], and Marcel Mudrich[1] — [1]Physikalisches Institut, Universität Freiburg, Hermann-Herderstr. 3, 79108 Freiburg, Germany — [2]Institute of Chemical Kinetics and Combustion, Institutskaya Str. 3, Novosibirsk 630090, Russia

With temperatures in the cold regime (0.38 K) and only weak interaction, doped Helium Nanodroplets are interesting environments to study pertubations of atoms and molecules induced by many particle interaction. Within this context, we will present results concerning the desorption dynamics of the heavy alkali atoms Rb and Cs from helium droplets. Both dopants are weakly attached to the droplet surface. By resonance enhanced multiphoton-ionization via low lying pseudodiatomic Σ- and Π-states and subsequent ion and electron imaging, we observe dissociation dynamics similar to that of a diatomic molecule and an energy transfer to the droplet during the desorption process, suggesting substantial He-droplet excitation.

The second part of the poster focuses on high-lying *gerade* Rydberg states of molecular iodide within the $[^2\Pi_{1/2}]_c 8s; 0g$ and $[^2\Pi_{1/2}]_c 8s; 1g$ band. In a collaborative[1,2] velocity map imaging study, five different dissociation channels have been observed. One channel indicates predissociation via an ion pair state, the others correspond to predissociation via lower lying covalent Rydberg states.

MO 13.20 Wed 16:30 Spree-Palais

IR and UV spectroscopy of biomolecular ions in liquid helium droplets — •Doo-Sik Ahn, Ana Isabel Gonzalez Florez, and Gert von Helden — Fritz-Haber-Institut, Berlin, Germany

Liquid helium droplets are ideal nano-cryostats for the investigation of molecules because of intrinsic characters of superfluid helium droplets such as isothermality at 0.38 K, the weak interaction between the helium matrix and dopant, and a transparency over a wide spectral range from the far IR to the deep UV. For the application of this technique to the cooling and spectroscopic investigation of biomolecular ions in the gas phase, we have developed an experimental setup where mass/charge selected biomolecular ions picked up by helium droplets. The size-distributions of ion-doped He droplets are analyzed by the measurement of arrival time distributions at different acceleration field. IR and UV Spectroscopy can be performed by irradiating the ion-doped He droplets with a pulsed laser and monitoring ejected ions as a function of wavelength. We will report very recent result of IR spectroscopy of various peptide ions doped in He droplets using FHI(Fritz-Haber-Institut) free electron laser, and UV spectroscopy as well.

MO 13.21 Wed 16:30 Spree-Palais

LIF spectroscopy of laser-ablated atoms in He nanodroplets and dense He gas

— •Sharareh Izadnia, Aaron Laforge, and Frank Stienkemeier — Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str.3, 79104 Freiburg, Germany

Van der Waals forces make extremely weak intermolecular bonds and play a crucial role in physical, chemical, and biological systems. Until recently, helium dimers, with an average interatomic nuclear distance of 52 Å, were the weakest bound experimentally observed system [1]. Now, however, an even weaker system, LiHe dimers, has been found by Tariq et al.[2]. Using laser ablation of lithium in a cryogenically-cooled helium buffer gas, LiHe dimers were formed via a three body recombination process and experimentally observed by laser induced fluorescence (LIF)[2].In our lab, we have recently developed a method to dope helium nanodroplets using a similar laser ablation setup. Surprisingly, it was found that not only were the ablated materials doped to nanodroplets, but they were also seeded in a cold He gas jet. In light of this and the previous work, we plan to perform LIF spectroscopy on laser ablated alkali atoms doped to nanodroplets and seeded in a dense gas. Our experimental approach along with the first results will be shown.

[1] R. E. Grisenti, W. Schölkopf, J. P. Toennies, G. C. Hegerfeldt, T. Köhler, and M. Stoll, Phys. Rev. Lett. 85, 2284 (2000)

[2] N. Tariq, N.Al Taisan, V. Singh, and J. D. Weinstein, Phys. Rev. Lett. 110, 153201 (2013)

MO 13.22 Wed 16:30 Spree-Palais

Mass-resolved pump-probe spectroscopy of alkali-doped He nanodroplets

— •Oliver John[1], Johannes von Vangerow[1], Harald Schmidt[1], Daniel Reich[2], Wojciech Skomorowski[2], Christiane Koch[2], Frank Stienkemeier[1], and Marcel Mudrich[1] — [1]Physikalisches Institut, Universität Freiburg, Hermann-Herderstr. 3, 79108 Freiburg, Germany — [2]Physikalisches Institut, Universität Kassel, Heinrich-Plettstr. 40, 34132 Kassel, Germany

Cold helium nanodroplets (400mK) possess several remarkable properties such as suprafluidity, making them attractive matrices for spectroscopy of a wide range of embedded atoms and molecules.

The first topic of this poster concerns Rb-doped He nanodroplets. The aim of this ongoing investigation is to understand the desorption dynamics of Rb dopants upon excitation and ionization by mass-resolved femtosecond pump probe spectroscopy via the pseudodiatomic $6p\Sigma$ and $6p\Pi$ states. Recent results show a pronounced drop of the ion yield for pump probe delays below one picosecond, suggesting either submersion of Rb ions or a reduced ionization cross section in the vicinity of He droplets.

The second topic focuses on vibrational wave packet dynamics within the A-state of lithiumiodide in the gas phase. From the pump-probe transients we derive properties of the potentials including coupling parameters at avoided curve-crossings by comparing to quantum dynamics simulations. In LiI doped He droplets we observe very fast relaxation dynamics, indicating strong interaction with the He.

MO 13.23 Wed 16:30 Spree-Palais

Allyl Radicals in Helium Nanodroplets

— •Daniel Leicht, Daniel Habig, Gerhard Schwaab, and Martina Havenith — Physical Chemistry 2, Ruhr-University Bochum, Germany

The allyl radical is the simplest π-conjugated hydrocarbon radical having an open-shell electronic structure due to its unpaired electron [1]. It has been firmly established that the allyl radical exhibits C_{2v} symmetry with a $2A_2$ ground electronic state [2]. Like all other C_3-hydrocarbon units allyl radicals are believed to be precursors in the formation of soot and polynuclear aromatic hydrocarbons [3]. Furthermore, the allyl radical is a key intermediate in tropospheric chemistry.

Superfluid helium nanodroplets have been demonstrated to be an effective tool for studying transient species such as radicals. Because of their high reactivity the knowledge of these systems and their interactions is still in its infancy. However, spectroscopy in helium nanodroplets makes it possible to investigate not only the bare allyl radical, but also its reactions and interactions with other molecules (e.g. O_2 or HCl) at 0.37 K.

[1] K. Tonokura and M. Koshi, J. Phys. Chem. A 2000, 104, 8456-8461

[2] J.Han et. al., J. Chem. Phys., Vol. 116, No. 15, 15 April 2002

[3] T. Schultz and I. Fischer, J. Chem. Phys., Vol. 109, No. 14, 8 October 1998

MO 13.24 Wed 16:30 Spree-Palais

NC_{4111} NTf_2 in Helium Nanodroplets

— •Matin Kaufmann, Kenny Hanke, Teemu Salmi, Gerhard Schwaab, and Martina Havenith — Physikalische Chemie II, Ruhr-Universität Bochum, Germany

Room temperature ionic liquids (ILs) are organic salts with a melting point around room temperature. Combinations of different cations and anions lead to a plethora of ILs and therefore provide room for many applications as in cleaning processes, gas storage and batteries. Due to their ionic nature, ILs possess a low vapor pressure, and there exist only few studies on gas phase spectroscopy.

Superfluid helium nanodroplets provide a soft matrix for the infrared spectroscopy of single molecules and small clusters. Vapor pressures of only 10^{-6} $mbar$ are sufficient to incorporate molecules into the droplets. Through evaporative cooling the embedded molecules are then cooled to a temperature of 0.37 K where molecular motion is minimal, yielding clean spectra.

We hereby present IR spectra of buthyltrimethylammonium bis(trifluoromethylsulfonyl)imide (NC_{4111} NTf_2). By analyzing the vibrational bands for complexes with different numbers of ions, we obtain information on the interaction of the ions.

MO 13.25 Wed 16:30 Spree-Palais

Single-particle orbit tracking: A versatile tool for monitoring confined diffusion in nanoporous materials

— •Dominic Raithel[1], Daniel Zalami[1], Dominique Ernst[1], Uwe Gerken[1], Jürgen Köhler[1], and Markus Retsch[2] — [1]Lehrstuhl für Experimentalphysik IV Universität Bayreuth, 95447 Bayreuth, Deutschland — [2]Lehrstuhl für Physikalische Chemie I Universität Bayreuth, 95447 Bayreuth, Deutschland

Diffusion and transport processes play an important role in many fields of natural and material sciences. An example is confined diffusion in nanoporous materials, as they are used in catalytic converters. Diffusion processes were generally studied with fluorescence-correlation spectroscopy (FCS) as well as single-particle tracking (SPT) methods using high sensitive CCD or CMOS cameras. We demonstrate a versatile SPT-technique, lately proposed by J. Enderlein [1], called single-particle orbit tracking (SPOT). With SPOT a single fluorescent particle is traced with the rotating focus of the excitation laser orbiting the particle. SPOT allows to follow a fluorescent polymer bead for several minutes with a temporal resolution of 4 ms and a position accuracy in the range of 10 nm [2]. With SPOT we are able to reconstruct the restricted trajectory of a fluorescent polymer bead within an inverse opal nanostructure, a 3-dimensional porous silica structure with cavities in the range of 100 nm. Due to the high spatial accuracy of the SPOT technique we can map the topology of the sample.

[1] J. Enderlein, Appl. Phys. B (71), 773-777 (2000) [2] D. Ernst et al., JOSA (29), 1277-1287 (2012)

MO 13.26 Wed 16:30 Spree-Palais

Fast, precise, and widely tunable frequency control of a cw optical parametric oscillator

— •Alexander Prehn, Rosa Glöckner, Martin Zeppenfeld, and Gerhard Rempe — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

Frequency combs offer a variety of new possibilities for frequency measurement and control. Here we report on the widely tunable, fast and precise frequency control of a commercially available optical parametric oscillator (OPO) locked to a frequency comb. In addition to stabilization to sub-MHz precision, the approach allows for fast frequency ramps in the whole tuning range of 100 GHz. Frequency ramps over more than 10 GHz performed in less than 10 ms are demonstrated, with the OPO instantly relocked to the frequency comb after the ramp at any desired frequency.

We show two complementary examples for the application of the technique. First, rovibrational transitions of CFH_3 molecules stored in an electric trap [1] can be driven quasi-simultaneously even though the transitions are spaced more than 10 GHz apart. Second, we show the frequency resolution of the system by means of Doppler-free spectra of rovibrational lines of H_2CO.
[1] M. Zeppenfeld *et al.*, *Nature* **491**, 570-573 (2012).

MO 13.27 Wed 16:30 Spree-Palais

Laser-induced acoustic desorption setup for the soft vaporization of large molecules — Wilhelm F. Frisch[1,3], •Zhipeng Huang[1,3], Daniel A. Horke[1], and Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science, DESY, Hamburg — [2]Center for Ultrafast Imaging, University of Hamburg — [3]Department of Physics, University of Hamburg

Laser-induced acoustic desorption (LIAD) is a promising technique for the preparation of dense plumes of intact neutral large molecules. Coupled with ionization and spectroscopic characterization techniques, it is shown to be of great utility for the analysis of a variety of thermally labile analytes.

We present our newly set up laser-induced acoustic desorption (LIAD) source, which is coupled to a time-of-flight (TOF) mass spectrometer (MS). In the LIAD experiment the molecules are deposited onto a thin ($\sim$10 μm) metal foil that is irradiated from the backside by the third harmonic of a Nd:YAG laser (355 nm). The induced shockwave travels through the foil and desorbs the molecules from the frontside of the foil [1]. The gas-phase molecules are subsequently strong-field ionized by a 40 fs Ti:Sapphire laser (800 nm) and mass-selectively detected in a TOF-MS. We discuss the efficiency of the source as well as the detailed characteristics of the created gas-phase sample as a function of experimental parameters, such as laser pulse energy and duration or foil parameters.
[1] B. Linder et al., *Anal. Chem.* **57**, 895 (1985)

MO 13.28 Wed 16:30 Spree-Palais

Characterization of a 6 K Ring-Electrode Ion-Trap used for IR Photodissociation Experiments in a Triple Mass Spectrometer — •Tim Esser[1], Nadja Heine[1], and Knut R. Asmis[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany — [2]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstrasse 2, D-04103 Leipzig, Germany

Mass-selective infrared photodissociation (IR-PD) spectroscopy combined with electronic structure calculations, is currently one of the most generally applicable techniques to determine the structure of gas phase cluster ions. To assure that the clusters are in their vibrational ground state they are typically buffer-gas cooled in a cryogenic ion trap. Here, we focus on the characterization of a linear ring-electrode radio-frequency (rf) ion-trap used in a 6K ion trap triple mass spectrometer. Preliminary results on the partially rotationally-resolved IR-PD spectrum of the singly hydrated ammonium ion, $NH_4^+(H_2O)$, allow to determine the rotational temperature as a function of the rf amplitude, buffer-gas pressure and store time. Apart from thermalization, the trap allows for bunching of the continuous ion beam and the attachment of messenger atoms or molecules. A genetic algorithm was developed, in order to automatically optimize the three sets of voltages, which are applied to the 12 pairs of ring electrodes during filling, storing and extraction. We further discuss the influence of the form of the trapping potential as well as the length of the store time on the size, shape and rotational temperature distribution of the ion packages.

MO 13.29 Wed 16:30 Spree-Palais

Development of an in-situ electrochemical flowcell for soft x-ray absorption and emission spectroscopy — •Christoph Schwanke and Kathrin Aziz-Lange — Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY GmbH, Albert-Einstein-Strasse 15, 12489 Berlin, Germany

The investigation of liquid-solid interfaces with soft x-ray absorption and emission spectroscopy is interesting for dye sensitized solar cells, fuel cells, batteries, water splitting, corrosion and electrodeposition. Adding electrodes to a flowcell gives the possibility to get electronic structure information and the oxidation state of these systems in-situ, meaning while a voltage is applied. Additional to the information gained with x-ray absorption and emission spectroscopy the system can be evaluated with cyclic voltammetry in our three electrode setup. Future experiments will investigate a fully working dye sensitized solar cell based on a Zn-porphyrin dye (YD2-O-C8) and a cobalt polypyridine redox couple. The investigations will cover the interactions between the components of dye sensitized solar cells. In this poster we will present details of this experimental technique and first results of cyclic voltammetry.

MO 13.30 Wed 16:30 Spree-Palais

An optical pipeline for femtosecond diffractive imaging — Rick Kirian[1], •Salah Awel[1,2,3], Niko Eckerskorn[4], Andrei Rode[4], Jochen Küpper[1,2,3], and Henry Chapman[1,2,3] — [1]Center for Free-Electron Laser Science, DESY, Hamburg — [2]Center for Ultrafast Imaging, University of Hamburg — [3]Department of Physics — [4]Australian National University, Canberra, Australia

The availability of brief, intense, and coherent x-ray pulses produced by x-ray free-electron lasers (XFELs) has created the potential for major advancements in macromolecular structure determination. Serial femtosecond crystallography (SFX) is among the most succesful emerging new paradigms. It consists of directing a stream of randomly oriented protein microcrystals or molecules across the focus of the XFEL beam. However, delivering single molecules to a sub-micron x-ray focus remains a considerable challenge. Current sample delivery efficiencies for single-molecule imaging based on aerodynamic lens systems are on the order of 10^{-7} on average, which renders experiments infeasible for samples that cannot be obtained in high abundance. In order to confront this challenge, we are developing techniques for manipulating aerosolized nanoparticles with specially shaped laser illumination. Our experiments are presently aimed at transversely confining streams of particles as they exit an aerosol injector, which produces a 50 μm diameter stream, with a counter-propagating “hollow” quasi-Bessel beam. The experiment exploits radiation pressure and/or thermal forces arising from the interaction of the particles with surrounding gas [1].
[1] *Opt. Exp.* **21**, 30492-30499 (2013)

MO 13.31 Wed 16:30 Spree-Palais

Dynamics of a nano-electromechanical rotor driven by single-electron tunneling — •Alan Celestino, Pablo Carlos López Vázquez, and Alexander Eisfeld — MPIPKS, Dresden, Germany

We discuss a nano-electromechanical rotor driven by single-electron tunneling. A possible realization could be a nanotube with quantum dots attached on its extremities, which can freely rotate about a double-walled nanotube axis. The system is driven using a bias voltage between source and drain contacts. Using a few relevant parameters one can set the rotor's dynamics to either intermittent oscillations/rotations or continuous rotational motion. The connection between the dynamical regimes and the current through the device is established. The effect of tuning initial conditions is also addressed, showing a bistable behaviour in the system's phase space. Among the possible applications of such device stand out the signal amplification, current rectification and viscosity measurements.

[1] A. Croy and A. Eisfeld, EPL (Europhys Lett) 98, 68004

MO 13.32 Wed 16:30 Spree-Palais

Vibronic line-shapes of polymeric *cis*-Indolenine squaraine dyes — •Christoph Brüning[1], Eileen Welz[1], Sebastian F. Völker[2], Christoph Lambert[2], and Volker Engel[1] — [1]Universität Würzburg, Institut für Physikalische und Theoretische Chemie, Emil-Fischer-Str. 42, 97074 Würzburg — [2]Universität Würzburg, Institut für Organische Chemie, Am Hubland, 97074 Würzburg

Using a vibronic coupling model we analyze measured absorption and emission spectra of cyclic polymeric *cis*-Indolenine squaraine dyes. From theory, features in the absorption spectra are identified as vibronic structures. The trimer exhibits unusual emission properties which can be explained taking at least two intra-monomer vibrational modes and a geometry distortion disturbing the symmetry into acount.

MO 13.33 Wed 16:30 Spree-Palais

Discrimination between new and aged ETFE plastic samples using Raman spectroscopy and chemometric analysis — •Alexandru Popa, Rasha Hassanein, Anais Colibaba, and Arnulf Materny — Jacobs University Bremen, Bremen, Germany

Ethylene-tetra-fluoro-ethylene (ETFE) a fluorine based plastic has gained widespread popularity due to its unique properties. ETFE is assumed to be stable against solar degradation, acid and alkali proof, and has a low friction coefficient, which enhances its resistance to atmospheric pollution such as dust or dirt particles. Beside these properties, ETFE is a lightweight transparent material and transmits all wavelengths of the solar spectrum. Therefore, it has been increasingly used in building applications. In our contribution, we present results of our recent work where we have applied Raman spectroscopy and chemometric analysis in order to study both 28 years old and new ETFE samples. The goal was to verify the predicted stability of the material. In this context excitation wavelengths of 514.5 and 785 nm have been used. The investigated ETFE samples were supplied by Vector Foiltec GmbH Bremen. The old samples had been partially in long-term use in roof structures and partially stored as reference samples in archives. Raman spectra of the investigated samples have been statistically treated using principal component analysis (PCA) analysis. A clear separation between the samples of different ages has been obtained for the Raman data obtained with 785 nm excitation. Raman spectra obtained with a 514.5 nm excitation only yielded a smaller separation into two clusters.

MO 13.34 Wed 16:30 Spree-Palais

Ultrafast Charge Migration Induced by Inner-Shell Vacancy in Diiodomethane — •Maximilian Hollstein and Daniela Pfannkuche — Jungiusstraße 9, 20355 Hamburg

The ultrafast charge migration on the sub-femtosecond timescale following the inner-shell ionization of an iodine atom of the diiodomethane molecule is investigated theoretically using a truncated configuration interaction method. A significant charge redistribution induced by the inner-shell ionized iodine atom was found which takes place during the first 100 as. Except for fluctuations, the observed charge redistribution remains stationary on the femtosecond timescale. The importance of two-electron correlations within the charge redistribution process is studied by consideration of two-particle correlation functions.

MO 13.35 Wed 16:30 Spree-Palais

Hierarchy of stochastic pure state wavefunctions for open quantum systems — Daniel Süss[1], Walter T. Strunz[1], and •Alexander Eisfeld[2] — [1]TU Dresden — [2]MPI-PKS

A method is presented to efficiently solve open quantum system problems with an non-Markovian structured environment. The approach is based on the Non-Markovian quantum state diffusion (NMQSD). We derive a hierarchy of stochastic differential equations, which can be solved numerically efficient and which converges rapidly to the exact reduced density matrix. We demonstrate the usefulness of the method by considering the spin-boson problem, electronic excitation transfer in the light-harvesting Fenna-Matthews-Olson (FMO) complex and the calculation of absorption spectra of molecular aggregates.

MO 13.36 Wed 16:30 Spree-Palais

The nature of the chemical bond between Carbon and Fluorine in Perfluorocarbons — •Tim Brandenburg[1], Marcus Agåker[3], Kaan Atak[1,2], Mika Pflüger[1], Kathrin Aziz-Lange[1], Christoph Schwanke[1], Tristan Petit[1], Jan-Erik Rubensson[3], and Emad Flear Aziz[1,2] — [1]Joint Ultrafast Dynamics Lab in Solutions and at Interfaces (JULiq) Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Strasse 15, 12489 Berlin, Germany — [2]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [3]Department of Physics and Astronomy, Uppsala University, Box 516, SE 751 20 Uppsala, Sweden

Perfluorocarbons are a special family of molecules, which rarely exist in nature due to the high energy required to build the carbon-fluorine bond. The strong electronegative effect of fluorine on neighboring atoms is still awaiting a clear electronic structure picture description. The insight to be gained is proposed to be the origin of the unique functionalities of these systems. We have used soft X-ray XAS/XES/RIXS to draw a full electronic picture of the unoccupied and occupied molecular orbitals in solution. The effect of fluorine was observed and fingerprinted on Perfluorodecalin as a model system. The obtained experimental spectra are explained with ab initio calculations using ORCA.

MO 13.37 Wed 16:30 Spree-Palais

Fine structure and fragmentation of n=4 states in H_3 — •Steffen J. Meyer, Peer C. Fechner, and Hanspeter Helm — Albert-Ludwigs-Universität, Freiburg, Germany

Neutral triatomic hydrogen is the most simple polyatomic molecule, and a prototype of molecular degrees of freedom, of molecular interaction and of nonadiabatic couplings in particular.

In this contribution we present our results on the three-body fragmentation of principal quantum number n=4 states in H_3, which are coaxially or perpendicularly excited using a narrowband tunable diode laser in a keV neutral beam.

Precise continious frequency tuning allows us to measure and compare the fine structure splitting of the vibrational ground state and vibrational excited states. The splitting depends on the coupling of electronic spin with the various angular momenta of the molecule.

The excited states decay primarily by predissociation into the continuum of three neutral H atoms. Time- and position-sensitive detectors allow to record in coincidence the three slow (≈ 1 eV) neutral ground state hydrogen atoms which emerge in predissociation.

Coincident detection of the three correlated atoms from a single molecule permits to reconstruct the centre-of-mass momentum vectors of the three hydrogen atoms. This experiment, when repeated for many molecules ($\approx 10^4$) delivers a map of momentum correlation of the three H atoms. The observed distribution is a measure of the phase-space dependent action of nonadiabatic coupling which allows the bound state to exit into the continuum.

MO 13.38 Wed 16:30 Spree-Palais

On the equivalence of spatial wave function and complete characterization of linear fragment momenta after many-body breakup — •Peer C. Fechner and Hanspeter Helm — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg

At the example of triatomic hydrogen, we discuss the equivalence of the spatial and momentum wave functions of a many-body system as they evolve after a fragmentation process (Phys.Chem.Chem.Phys., 2014, 16, 453).

State selected H_3 molecules predissociate into the repulsive ground-state and undergo the 3-body decay $H_3 \rightarrow H(1s) + H(1s) + H(1s)$. The correlated fragment momentum vectors of the hydrogen atoms are recorded in the laboratory frame in triple coincidence. Prudent design of the experiment permits to trace out the nuclear frame alignment in the laboratory (the photofragment angular distribution) to arrive at correlated fragment momentum vectors in the center-of-mass. Accumulation of typically $\sim 10^4$ such observations yields a probability map of final momentum configurations, equivalent to the modulus square of the momentum wave function long after the decay. Comparison with the known initial spatial wave function suggests a close relationship of spatial and momentum wave function, which is predicted by theory in the form of the *imaging theorem*. We conclude that prudent imaging of many-body fragmentation provides a laboratory view of the squared many-body wave function at a spatial scale of molecular dimensions at which fragments exit into the realm of independent free particles.

MO 13.39 Wed 16:30 Spree-Palais

Molecular Frame Photoelectron Angular Distributions in Dissociating CF_3I Molecules — •Felix Brausse, Arnaud Rouzée, and Marc Vrakking — Max-Born-Institut für nichtlineare Optik, Berlin

Over the last decade, the emergence of x-ray free-electron lasers (FELs) and high-order harmonic generation (HHG) XUV-sources has enabled the development of diffractive methods for elucidating time-resolved molecular dynamics. Indeed, one of the main driving forces behind the development of the FEL is the possibility to perform x-ray diffractive imaging in molecules; alternatively, diffractive information can as well be encoded onto photoelectrons that are generated by the ionisation of the molecules with an ultrashort XUV or x-ray pulse. The theory of photoelectron–molecule scattering has been studied thoroughly and a number of successful experiments relying on this concept have already been performed at synchrotrons with ground state molecules.

Here, we theoretically investigate the possibility to probe the dissociation dynamics of CF_3I molecules induced by excitation at 266 nm, using the photoelectrons generated by a time-delayed soft x-ray pulse. As a first step, the photoelectron angular distributions of a fixed in space CF_3I molecule in its ground state are calculated with the aid of the Schwinger variational principle and are compared to the predictions from an intuitive forward scattering model.

MO 13.40 Wed 16:30 Spree-Palais

Laser photothermal emission spectroscopy of gases — •Felix Axtmann and Johannes Herbst — Fraunhofer IPM, Freiburg, Deutschland

Laser spectroscopy is a selective and sensitive tool for spectral analyzing molecules in the gas phase. Powerful quantum cascade lasers (QCL) enable the application of laser photothermal emission spectroscopy (LPTES). We demonstrate this for a stand off detection of a narrowband and broadband absorber in the gas phase. With LPTES the sample gas is heated up by the QCL using the vibrational rotational transition of the fundamental mode. Detection of the emitted radiation can be performed either by broadband single detectors or infrared cameras. For analyzing the spectral emission we use a Fouriertransform-Infrared spectrometer (FTIR). By the excitation of a single rotational line in the v4 vibrational mode of methane (1306 cm-1) a complete vibrational spectrum is obtained. This research and measurement technique is used for the development of a methane leak detection system.