

MO 19: MO Poster 4

Time: Thursday 17:00–19:00

Location: Empore Lichthof

MO 19.1 Thu 17:00 Empore Lichthof

Coherent control of Lanthanides as molecular quantum bits using shaped femtosecond laser pulses — ●MIRALI GHEIBI, JAYANTA GHOSH, CRISTIAN SARPE, BASTIAN ZIELINSKI, TILLMAN KALAS, RAMELA CIOBOTEA, ARNE SENFTLEBEN, HENDRIKE BRAUN, and THOMAS BAUMERT — Universität Kassel, Institute of Physics, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

SMolBits - Scalable Molecular Quantum Bits - is a project in the framework of LOEWE (Hessian Initiative for the Development of Scientific-Economic Excellence). Its aim 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 at the atomic and molecular level. 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, the central wavelength of typical Ti:Sapphire laser systems. We have begun investigations of the electronic coherences excited in lanthanide salts by interaction with IR femtosecond laser pulses and their lifetimes using phase-locked double pulses and fluorescence detection under a confocal microscope. As a next step we will study the influence of spectrally phase shaped femtosecond laser pulses in the non-perturbative regime onto the excitation and the created electronic coherence.

MO 19.2 Thu 17:00 Empore Lichthof

Impact of ab initio data in simulations of coherent control of bond making — ●ARCHANA SHUKLA^{1,3}, DANIEL M. REICH^{1,3}, WOJCIECH SKOMOROWSKI¹, ZOHAR AMITAY², ROBERT MOSZYŃSKI⁴, TATIANA KORONA⁴, and CHRISTIANE P. KOCH^{1,3} — ¹Theoretische Physik, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — ²Schulich Faculty of Chemistry, Technion-Israel Institute of Technology, Haifa 32000, Israel — ³Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — ⁴Faculty of Chemistry, University of Warsaw, L. Pasteura 1, 02093 Warszawa, Poland

Coherent control of photoassociation has been successfully achieved in hot magnesium atoms [L. Levin et al., Phys. Rev. Lett. 114, 233003 (2015)] using strong femtosecond laser pulses. The yield of photoassociated magnesium dimers is detected by measuring the UV emission. We study the emission signature of magnesium dimers by combining ab initio electronic structure and molecular quantum dynamics calculations [S. Amaran et al., J. Chem. Phys. 139, 164124 (2013)]. It is found numerically that the UV emission is highly sensitive to the ab initio. In particular we find that enhancement/suppression of the UV emission when using positively/negatively chirped pulses is heavily influenced by the polarisabilities of the excited electronic states which are insufficiently converged in our current ab initio data sets. We present new results for these polarisabilities obtained with the multireference configuration interaction method (MRCI), with which we hope to obtain a more accurate description of the photoassociation dynamics.

MO 19.3 Thu 17:00 Empore Lichthof

Role of coherence for photoelectron circular dichroism after multi-photon excitation in randomly oriented chiral molecules — ●ALEXANDER BLECH¹, R. ESTEBAN GOETZ¹, TIMUR A. ISAEV², BEHNAMEH NIKOBAKH², ROBERT BERGER², LOREN GREENMAN³, and CHRISTIANE P. KOCH¹ — ¹Universität Kassel, Deutschland — ²Philipps-Universität Marburg, Deutschland — ³Kansas State University, Manhattan KS, USA

Photoelectron circular dichroism (PECD) refers to the forward/backward asymmetry in the photoelectron angular distribution with respect to the propagation axis of circularly polarized light. Our existing model for PECD in resonantly enhanced multi-photon ionisation of randomly oriented chiral molecules is based on perturbation theory for the light-matter interaction and on ab initio calculations for the multi-photon absorption, giving semi-quantitative agreement with experimental data for fenchone and camphor.

Here we present an extended model that explicitly takes into account the coherence between non-resonant multi-photon excitation and one-photon ionisation as well as the chirality of the photoelectron contin-

uum by solving the scattering problem for the photoelectron. Our new theoretical description allows us to distinguish the contributions of intermediate and final states to PECD. This will be a first step towards refining our quantum optimal control approach in order to determine the ultimate strength of the chiral response.

MO 19.4 Thu 17:00 Empore Lichthof

Towards molecular quantum bits — ●MARKUS DEBATIN, JOSEFIN BERNARDOFF, DAQING WANG, SAMUEL T. DAWKINS, and KILIAN T. T. SINGER — Universität Kassel, Germany

Lanthanoides embedded into molecules are expected to show long coherence since transitions within the f-shell are expected to be reasonably unperturbed by the surrounding chemical bonds. Our experimental setup, which allows for implantation of ions [1,2,3], will be used to study optical transitions in molecular ions as well as deposition of the molecular ions onto surfaces. On the poster we present our experimental design and discuss possible roadmaps.

[1] W. Schnitzler et al. Phys. Rev. Lett. 102, 070501 (2009). [2] G. Jacob, et al. Phys. Rev. Lett. 117, 043001 (2016). [3] K. Groot-Berning et al. Phys. Rev.Lett. 123, 106802 (2019)

MO 19.5 Thu 17:00 Empore Lichthof

Far Infrared Spectroscopy of neutral boron clusters using tunable VUV generated by 4-wave mixing — ●SASCHA SCHALLER, ALAN GÜNTHER, GERARD MEIJER, and ANDRÉ FIELICKE — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Previous experiments in combination with calculations [1,2] have shown that Boron cluster are able to form versatile structures like planar, ring-like and cages. To record far-infrared spectra for the neutral clusters, a FIR-VUV two-color ionization scheme can be used [3]. In our first experiments, an F2 excimer laser (157 nm) has been used for the ionization step [4]. As the ionization energy depends on cluster size, there is access to only a limited number of cluster sizes for a given VUV photon energy. To overcome the limitation in photon energy given by the fixed frequency F2 laser (7.9 eV), VUV photons are generated by four-wave mixing in Xenon. In the present configuration, which covers an energy range of 6.5 eV to 8.2 eV, two dye lasers (ω_1 , ω_2) interact in a static gas cell and the resulting ($2\omega_1 - \omega_2$) difference frequency is used for ionization. We verified that after creating 7.9 eV photons in this way, the spectra obtained via FIR-VUV ionization reproduce the results obtained via F2 laser ionization.

[1]L. S. Wang, International Reviews in Physical Chemistry 35, 69 (2016). [2]H. J. Zhai et al., Nature Chemistry 6, 727 (2014). [3]M. Putter, G. von Helden, and G. Meijer, Chem Phys Lett 258, 118 (1996). [4]C. Romanescu, D. J. Harding, A. Fielicke, and L. S. Wang, Journal of Chemical Physics 137 (2012).

MO 19.6 Thu 17:00 Empore Lichthof

Photoelectron spectroscopy of size-selected metal clusters at FLASH 2 — ●FABIAN BÄR¹, NORMAN IWE², KARIMAN ELSHIMI¹, KLARA RASPE², SIMON DOLD¹, FRANKLIN MARTINEZ², JOSEF TIGGESBÄUMKER², KARL-HEINZ MEIWES-BROER², and BERND VON ISSENDORFF¹ — ¹Fakultät für Physik, Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany — ²Institut für Physik, Universität Rostock, Albert-Einstein-Str. 23-24, 18059 Rostock, Germany

A newly designed XUV magnetic bottle photoelectron spectrometer (MBPES) has been tested at the free electron laser FLASH2 in Hamburg in combination with a cluster source and two time-of-flight spectrometers in order to address the core levels of metal clusters. The high photon energy of 47 eV with decent bandwidth allowed us to investigate the *5d* levels of lead and the *4d* band of silver clusters with a unique resolution and short measurement time. In this high intensity regime, multiphoton absorption and therefore up to five different charge states have been observed. The results provide a rather comprehensive characterization of the size dependence of the valence and shallow core states density of lead cluster anions in the size range from $n = 3$ to $n = 50$ and silver cluster anions in the size range from $n = 8$ to $n = 70$.

MO 19.7 Thu 17:00 Empore Lichthof

Software adaptation of a quadrupole mass spectrometer for the investigation of cluster fragmentation — ●REBECCA SCHAF,

DANA BLOSS, ANDREAS HANS, ARNO EHRESMANN, and ANDRÉ KNIE — Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

The exploration of the properties of weakly bound cluster is often hampered by fragmentation as a consequence of ionization or other interactions with light or matter. Therefore, many investigations benefit from a detailed understanding of the cluster fragmentation processes. Here, we present the application of a quadrupole mass spectrometer to analyze the fragmentation in dependency of different ionization parameters. Especially for heterogeneous cluster such investigations are crucial for a reliable distinction of effects occurring in cluster formation or fragmentation.

MO 19.8 Thu 17:00 Empore Lichthof

Experimental evidence for core-level intermolecular Coulombic decay in hydrated pyrimidine — •DANA BLOSS¹, CATMARN KÜSTNER-WETEKAM¹, PHILIPP SCHMIDT¹, SASCHA DEINERT², FLORIAN TRINTER², GREGOR HARTMANN¹, ARNO EHRESMANN¹, LORENZ S. CEDERBAUM³, NIKOLAI V. KRZYŻEWOI³, ANDRÉ KNIE¹, and ANDREAS HANS¹ — ¹Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — ²Deutsches Elektronen-Synchrotron (DESY), Notkestrasse 85, 22607 Hamburg — ³Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 229, 69120 Heidelberg, Germany

We investigated the effect of the presence or absence of an aqueous environment for bio-relevant molecules after their exposure to X-ray irradiation in a photoelectron-ion-ion coincidence experiment performed at the P04 at Petra III. In the decay of carbon inner-shell vacancies of hydrated pyrimidine we found evidence for direct intermolecular Coulombic decay. This process protects the molecule from reaching dicationic states via Auger decay and the inevitable fragmentation. The observations are compared with the results of theoretical calculations for a deeper understanding of the occurring effects.

MO 19.9 Thu 17:00 Empore Lichthof

Multi-electron coincidence study on inner-shell ionized water clusters — •CHRISTINA ZINDEL¹, ANDREAS HANS¹, ARNO EHRESMANN¹, UWE HERGENHAHN², and ANDRÉ KNIE¹ — ¹Institut für Physik und CINSaT, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — ²Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

Since the environment of a single atom or molecule plays an important role regarding its decay behavior, new possible relaxation processes emerge by changing from an isolated system to clusters of weakly bound particles. An example is the Intermolecular or -atomic Coulombic Decay (ICD), a non-local charge distribution process that recently gained attention due to its possible role in radiation damage in biological systems. In water clusters, ICD following inner valence ionization has already been observed experimentally. However, that is not the case for ICD following inner-shell ionization and subsequent Auger decay as theoretically predicted about 20 years ago.

We used a magnetic bottle type time-of-flight spectrometer to reveal different de-excitation pathways and to extract the characteristic electron signal. Three emitted electrons (expected to occur due to 1s-photoionization followed by Auger emission and subsequent Intermolecular Coulombic Decay) were detected in coincidence.

MO 19.10 Thu 17:00 Empore Lichthof

Optical properties of cationic gold clusters — •MARKO FÖRSTEL¹, KAI POLLW¹, KARIM SAROUKH¹, ESTE A. NAJIB¹, ALICE GREEN², STUART MACKENZIE², and OTTO DOPFER¹ — ¹Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany — ²Department of Chemistry, University of Oxford, Oxford, UK

Gold is one of the most important model systems in catalysis research. The catalytic properties are strongly dependent on local structure and electronic properties and may change drastically by changing the number of atoms by only one [1]. Unfortunately, due to intrinsic properties of Au, theoretical calculations are not straight forward and methods still need to be improved.

Our newly enhanced setup allows measuring the optical absorption spectra of small gold clusters in hitherto unprecedented quality [2, 3]. Here we present our latest results on small bare and substituted gold clusters cations. We compare the experimentally obtained optical spectra to TD-DFT calculations to draw conclusions about the structure of the excited states, or, correspondingly, use the known structures to

benchmark theoretical methods.

- [1] S. Lang et al., *Angew. Chem. Int. Ed.* **10**, 2017
- [2] M. Förstel et al., *Rev. Sci. Instr.* **88**, 2017
- [3] M. Förstel et al., *Angew. Chem. Int. Ed.* **131**, 2019

MO 19.11 Thu 17:00 Empore Lichthof

Understanding the Geometric and Optical Properties of Cationic Silicon Carbide Clusters — •ROBERT RADLOFF, LARS DAHLLÖF, KAI POLLW, KARIM AHMED SAROUKH, MARKO FÖRSTEL, and OTTO DOPFER — Technische Universität Berlin, Institut für Optik und Atomare Physik, Germany

Silicon carbide (SiC) possesses a unique set of properties that make it a suitable material for high-temperature electronics applications: a wide bandgap, high thermal stability, chemical inertness and high thermal conductivity [1]. Additionally, small SiC molecules like SiC [2], Si₂C [3], etc. as well as SiC dust grains [4] have been observed in the circumstellar environment of carbon-rich stars.

We present the energetic, geometric, and optical properties of small cationic SiC clusters obtained via photodissociation spectroscopy, mass spectrometry, and quantum chemical calculations. We show the first optical spectrum of a SiC cation and present hitherto unreported fragmentation channels and ground state geometries of some cationic SiC clusters.

- [1] J. B. Casady and R. W. Johnson, *Solid State Electron*, **39** (10), 1409-1422 (1996)
- [2] J. Cernicharo et al., *Astrophys. J. Lett.* **341**, L25 (1989)
- [3] J. Cernicharo et al., *Astrophys. J. Lett.* **806**, L3 (2015)
- [4] R. Treffers and M. Cohen, *Astrophys. J.* **188**, 545-552 (1974)

MO 19.12 Thu 17:00 Empore Lichthof

Angle resolved photoelectron spectra of small copper clusters — •LUKAS WEISE and BERND V. ISSENDORFF — Physikalisches Institut der Albert-Ludwigs-Universität Freiburg

Angle resolved spectra are an important test for the theoretical description of clusters since they 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 and enter a time-of-flight spectrometer for mass measurement and selection. Afterwards electrons are detached by linear polarized laser light and projected onto a MCP detector in a velocity map imaging setup.

Here the results for small copper cluster are presented. Although copper clusters have been studied intensively, there are still undiscovered features of their photoelectron spectra. For example Cu₅ shows a strong vibrational structure, which is in good agreement with DFT calculations.

MO 19.13 Thu 17:00 Empore Lichthof

Quantum-state-controlled Penning collisions between lithium and metastable helium atoms — •ALEXANDRA TSOUKALA, TOBIAS SIXT, JIWIEN GUAN, FRANK STIENKEMEIER, and KATRIN DULITZ — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg im Breisgau, Germany

Our research focuses on understanding the mechanistic details of reactive collisions in order to enable control of their outcome. In our experiment, we study quantum-state-controlled Penning collisions between lithium (Li) and metastable helium (He*) atoms. For this purpose, a supersonic beam source of He* atoms is combined with a target of ultracold lithium (Li) atoms confined in a magneto-optical trap (MOT). The full quantum-state control of the reaction partners is achieved by producing a pure beam of He(2³S₁) via the optical depletion of the He(2¹S₀) state using a novel excitation scheme. Additionally, both Li and He* atoms are optically pumped into selected electronically excited or magnetic substates. By alternating the combination of quantum-states for both He* and Li, we observe strong dependencies of the reactivity on the mutual electron spin and angular momentum orientation.

In this contribution, I will give an overview over the different techniques used to achieve quantum-state control of the reaction partners and I will discuss recent experimental results.

MO 19.14 Thu 17:00 Empore Lichthof

Analysis of the coupled states (2)²Σ⁺ and (1)²Π of LiCa — •JULIA GERSCHMANN^{1,2}, ERIK SCHWANKE^{1,2}, HORST KNÖCKEL^{1,2}, SILKE OSPELKAUS^{1,2}, and EBERHARD TIEMANN^{1,2} — ¹Inst. f. Quantenoptik, Leibniz Universität Hannover — ²Laboratory for Nano- and Quantum Engineering, Leibniz Universität Hannover

Molecules consisting of an alkaline and an alkaline earth atom have permanent electric and magnetic dipole moments. This allows manipulations of their states by external fields. Several ab initio calculations have been published on various combinations of a group IA and a group IIA atom. Experimentally, not so much is known about the molecular electronic states.

In 2011, we reported on spectroscopic work on ${}^7\text{Li}^{40}\text{Ca}$ in a heat pipe. Via high resolution Fourier transform spectroscopy some states were investigated. Potential energy curve for the ground state $(1)^2\Sigma^+$ was described up to $v = 19$. However, the transitions between the states $(1)^2\Sigma^+$ and $(2)^2\Sigma^+$ provided at that time only the description of $v' \leq 1$ and N' up to 92 of the state $(2)^2\Sigma^+$. Now we extend the experiment and analysis to include transitions from $v' \leq 4$ up to $N' = 120$ of this state.

In addition, we see perturbations of $(2)^2\Sigma^+$ rotational levels indicating a coupling to the $(1)^2\Pi$ state, which will give molecular parameters of the $(1)^2\Pi$ state.

We will report on the status of the investigations.

MO 19.15 Thu 17:00 Empore Lichthof

A Buffer Gas Beam Source for Barium Monofluoride and Progress Towards Laser Cooling of the Molecular Beam — ●MARIAN ROCKENHÄUSER, RALF ALBRECHT, MICHAEL SCHARWÄCHTER, and TIM LANGEN — 5. Physikalisches Institut and Center for Integrated Quantum Science and Technology IQST, Universität Stuttgart, Germany

Cold molecular gases are the starting point for a large number of novel and interdisciplinary applications ranging from few- and many-body physics to cold chemistry and precision measurements. Especially heavy polar molecules, such as barium monofluoride, are perfect candidates for tests of fundamental symmetries and studies of complex quantum systems with strong, long-range interactions. However, in comparison to atoms, the preparation of molecular gases in the sub-Kelvin regime is complicated by their complex vibrational and rotational level structure and the lack of closed transitions for optical cycling. Nevertheless, thanks to favorable Franck-Condon factors and selection rules, quasi-cycling transitions can be identified for many molecular species, including barium monofluoride. In this contribution, we will report on our buffer-gas beam source for slow and internally cold barium monofluoride molecules. Moreover, we will present our progress towards one-dimensional Doppler cooling of the molecular beam.

MO 19.16 Thu 17:00 Empore Lichthof

Towards photodissociation of cold OH^+ in a 16-pole wire trap — ●CHRISTINE MARIA LOCHMANN, MARKUS NÖTZOLD, ROBERT WILD, and ROLAND WESTER — Institut für Ionenphysik und Angewandte Physik, Technikerstraße 25/3, 6020 Innsbruck, Austria

The hydroxyl cation OH^+ plays an important role in astrochemistry. Its formation represents one of the first steps in the rich oxygen chemistry in the interstellar media, while its column density in these regions could provide a successful tracer of cosmic ray and X-ray ionization rates. The recently published photodissociation spectrum of OH^+ provides the transition frequencies to probe the system in the UV regime [1]. Here we present our progress to probe the distribution of the rotational states of cold OH^+ with a UV-photodissociation scheme. Analogously state-selective photodetachment spectroscopy on cold OH^- has been done previously in our group [2].

The experiments will be carried out in our new multipole wire trap, which can be cooled down to 6K. The trap consists of 16 wires, which can be individually addressed. Accessibility perpendicular to the trap axis allows for laser spectroscopy measurements.

- [1] Hechtischer U. *et al.*, *J. Chem. Phys.* **151**, 044303 (2019)
 [2] Otto R. *et al.*, *Phys. Chem. Chem. Phys.*, 2013, **15**, 612

MO 19.17 Thu 17:00 Empore Lichthof

Reaction studies of astrophysically relevant anions — ●MARKUS NÖTZOLD, ROBERT WILD, CHRISTINE LOCHMANN, and ROLAND WESTER — Universität Innsbruck, Inst. für Ionenphysik und Angewandte Physik, A-6020 Innsbruck

After the radioastronomical discovery of the first interstellar anions, interest has grown in understanding the formation and destruction pathways of negative ions in the interstellar medium (ISM). The simplest anion, H^- , is expected to be present in the ISM, but its detection is difficult as it possess only a single bound state. The most fundamental reaction of H^- is the proton transfer reaction with H_2 , and occurs via tunneling through the reaction barrier at low temperatures. Starting with D^- , we have studied the reaction $\text{D}^- + \text{H}_2 \rightarrow \text{H}^- +$

HD in a cryogenic 22-pole trap. Furthermore, we present results on the reaction $\text{Cl}^- + \text{H}_2 + \text{H}_2 \rightarrow \text{H}_2\text{Cl} + \text{H}_2$ and $\text{H}^- + \text{C}_2\text{H}_2 \rightarrow \text{C}_2\text{H}^- + \text{H}_2$. The former reaction also serves as a temperature diagnostics for our 22-pole trap and our newly developed multipole wire trap.

MO 19.18 Thu 17:00 Empore Lichthof

High-resolution infrared and millimeter-wave spectroscopy of CNH_n^+ ($n = 0,4,6$) ions — ●PHILIPP C. SCHMID¹, SVEN THORWIRTH¹, OSKAR ASVANY¹, CHARLIE R. MARKUS^{1,2}, JOSÉ L. DOMÉNECH³, THOMAS SALOMON¹, MATTHIAS TÖPFER¹, PHILIPP SCHREIER¹, and STEPHAN SCHLEMMER¹ — ¹I. Physikalisches Institut, Universität zu Köln, Köln, Germany — ²Department of Chemistry, University of Illinois, Urbana, IL, U.S.A. — ³Instituto de Estructura de la Materia (IEM-CSIC), Madrid, Spain

Molecular ions play crucial roles in the astrochemistry associated with star formation and planetary atmospheres. In this project we have studied three fundamental cations CNH_n^+ ($n = 9,4,6$) using action spectroscopic techniques in a 22-pole ion trap at a nominal temperature of 4 K [1]. The fundamental diatomic CN^+ [2] as well as the protonated methylene imine, $\text{H}_2\text{C}=\text{NH}_2^+$, and protonated methyl amine, $\text{H}_3\text{C}-\text{NH}_3^+$, were all studied by their pure rotational spectra in the millimeter-wave region employing the method of rotational state-selective He-attachment [3]. CN^+ and $\text{H}_2\text{C}=\text{NH}_2^+$ were also studied at high spectral resolution in the infrared using Laser Induced Inhibition of Complex Growth (LIICG) [1,4].

- [1] O.Asvany et al., *Appl. Phys. B* 114 (2014) 203.
 [2] S. Thorwirth et al., *Astrophys. J. Lett.* 882 (2019) L6.
 [3] S. Brünken et al., *J. Mol. Spectrosc.* 332 (2017) 67.
 [4] S. Chakrabarty et al., *J. Phys. Chem. Lett.* 4 (2013) 4051.

MO 19.19 Thu 17:00 Empore Lichthof

Improving and understanding a cryogenic buffer-gas cell based on comparing Monte-Carlo simulations and experiments — ●FLORIAN JUNG, THOMAS GANTNER, MANUEL KOLLER, JINDARATSAMEE PHROMPAO, ISABEL RABEY, MARTIN ZEPPENFELD, and GERHARD REMPE — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, 85748 Garching bei München

Unlike atoms, molecules can exhibit a permanent electric dipole moment, which makes them amenable to guiding and trapping via electric fields and allows the study of anisotropic dipolar interactions. In addition, they exhibit a rich internal structure that allows to envision applications of molecules in such diverse fields as cold chemistry, quantum information science and quantum simulation. For all of these applications the prerequisite is that molecules are cold. To produce cold molecules at a temperature of a few Kelvin, buffer-gas cells are now established workhorses, cooling molecules via thermalisation with cold atomic gases independent of the molecule type. However, many aspects of the physics of buffer-gas cells are still to be understood.

We here present a comprehensive study of buffer-gas cells in the low-density regime, employing Monte-Carlo simulations and comparing these to experimental data, finding a good agreement between the simulated and measured data. We formulate design guidelines that we employ in our set-up, reaching a signal increase of at least a factor of 2. Combining the cryogenic buffer-gas source with a centrifuge decelerator and an electrostatic trap, collision studies on cold molecular ensembles are now within reach.

MO 19.20 Thu 17:00 Empore Lichthof

Towards trapping ultracold polar molecules in a dark repulsive dipole trap — ●REN-HAO TAO — Max-PlanckInstitut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

Ultra-cold molecules, by virtue of their rich ro-vibrational states and significant dipolar moments, offer us an exciting platform to study new quantum many-body physics. Ample experiments on molecules reactive and nonreactive alike, however, all point to their short in-trap lifetime (a few seconds) as one of the most immediate challenges before we fully take advantage of them. A recent proposal suggests that the trapping light in these experiments, despite being far-detuned from molecule transitions, is still energetic enough to excite two-molecules complexes in a so-called sticky state to higher energy states, the decays from which might lead to losses. To test this theory, we trap molecules using a far blue-detuned light away from the transition between ground and the first rotational excited state of ${}^{23}\text{Na}^{40}\text{K}$. Such a transition, owing to its small linewidth ($2\pi \times 297\text{Hz}$), allows us to effectively reduce trapping intensity without sacrificing trap depth. This leads to trap depth of $4\text{kB} \cdot \mu\text{K}$ and an intensity as low as $4\text{W}/\text{cm}^2$ seen by most molecules. The molecule lifetime in such a trap is projected to increase

by a factor of 20. If observed, such a reduced trap loss might pave the way for a deeper understanding of molecular collisional dynamics in particular and the feasibility of using molecules as a potentially more interesting alternative in simulating quantum many-body interaction in the long run.

MO 19.21 Thu 17:00 Empore Lichthof

Towards enantiomer-specific spectroscopy and control of cold, chiral molecules — ●JU HYEON LEE, JOHANNES BISCHOFF, A. O. HERNANDEZ-CASTILLO, MARCO DE PAS, GERARD MEIJER, and SANDRA EIBENBERGER-ARIAS — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Chiral molecules are of paramount importance in the activity of biological molecules. Even though chemical and biological functionalities of different enantiomers are significantly different, their energy levels are equal, making detecting and quantifying them challenging. Therefore, there is a need for fast and reliable methods that can differentiate and/or separate enantiomers. Recently, the enantiomer-specific state transfer (ESST) method was developed where three mutually orthogonally polarized, resonant, phase-controlled microwave pulses are used to drive connected rotational transitions, resulting in controlled, enantiomer-specific population transfer [1]. We recently designed, built, and characterized a compact spectroscopy setup. It is capable of performing experiments in the 2-25 GHz regime, making studies of a large variety of molecules possible. Furthermore, our setup is equipped with a time-of-flight (TOF) mass spectrometer, and we implemented a combination of optical methods and microwave spectroscopy. Here we present preliminary results towards ESST of chiral molecules that are relatively rigid and simple, and have an aromatic ring, for example: 1-indanol.

1. S. Eibenberger, J. Doyle, & D. Patterson, Phys. Rev. Lett. 118. 123002 (2017).

MO 19.22 Thu 17:00 Empore Lichthof

Isomer Selected Ion-Molecule Reactions of $C_2H_2^+$ + C_3H_4 — ●PHILIPP C. SCHMID^{1,2}, JAMES GREENBERG¹, MIKHAIL I. MILLER¹, THANH L. NGUYEN³, JAMES H. THORPE³, JOHN F. STANTON³, and HEATHER J. LEWANDOWSKI¹ — ¹JILA and the Department of Physics, University of Colorado, Boulder, Colorado, USA — ²I. Physikalisches

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One of the fundamental questions in molecular reactions is to determine how the structure of molecules governs the reaction and thus leads to different reaction products. Studies of isomer resolved chemical reactions can shed light directly on the foundation of how form leads to function. We present the results of gas-phase reactions between acetylene cations $C_2H_2^+$ with two different isomers of C_3H_4 : propyne (HC_3H_3) and allene ($H_2C_3H_2$). The highly controlled environment of an ion trap allows us to precisely measure the reaction products and branching ratios. The difference in observed reaction products from the two different isomers points directly to the role molecular structure plays in these reactions. Through the synergy of experimental results and quantum chemical potential energy surface calculations, we are able to explicate the different reaction mechanisms for the two isomers.

MO 19.23 Thu 17:00 Empore Lichthof

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

Ultracold molecules provide distinct advantages in research on precision measurements, ultracold chemistry and simulations of solid state physics. Current experiments are, however, severely restricted by the initial flux of slow and cold molecules, which limits the size of the trappable ensembles. Our group has developed a novel slowing scheme capable of improving this flux by orders of magnitude. We have already demonstrated the feasibility of our method in a proof of principle experiment and are now in the process of combining our scheme with an optimized buffer gas source to greatly enhance the flux of slow, cold molecules. We present our results of the proof of principle experiment on 39K D1-line and our buffer gas cell as a source of rotationally cold molecules. We further show our recent results of mapping out the CaF hyperfine structure in magnetic fields up to 500 Gauss, a necessary step towards implementing Zeeman slowing, and give insights into the future of our experiment.