

## MO 19: Posters 4: Novelty in Molecular Physics: Femtosecond Spectroscopy, Molecular Clusters, Cold Molecules and Helium Droplets

Time: Thursday 16:30–19:00

Location: Empore Lichthof

MO 19.1 Thu 16:30 Empore Lichthof

**Time-Dependent Modeling of the Ionization Dynamics in Chiral Molecules** — ●MESSAN AFANDE<sup>1</sup>, BEHNAME NIKOBAKHT<sup>2</sup>, R. ESTEBAN GOETZ<sup>1</sup>, TIMUR ISAEV<sup>2</sup>, ROBERT BERGER<sup>2</sup>, and CHRISTIANE P. KOCH<sup>1</sup> — <sup>1</sup>Theoretische Physik, Universität Kassel, Kassel, Germany — <sup>2</sup>Theoretische Chemie, Phillips-Universität Marburg, Marburg, Germany

Experiments based on femtosecond polarized laser pulse excitation of chiral molecules reveal a circular dichroism in the measured photoelectron signal. The observed dichroism is used to get insight into the dynamics of chiral molecules, in particular, in the characterization of the handedness of such molecules. A combination of *ab initio* calculations with a single center expansion reproduces the experimental results semi-quantitatively. Here, this theoretical framework is extended to a time-dependent approach. This allows the study of dynamical effects, including the dependence on the pulse parameters such as chirps. The time-dependent study aims at a better understanding of the dynamics in the ionization process of chiral molecules. Here, we present the time-dependent modeling approach and first results.

MO 19.2 Thu 16:30 Empore Lichthof

**Pump-Probe Experiments in a Collinear Phase Modulation Scheme Using a Low Repetition Rate Laser System** — ●MARCEL BINZ, LUKAS BRUDER, ULRICH BANGERT, and FRANK STIENKEMEIER — Physikalisches Institut, Universität Freiburg, Germany

Recently various active and passive stabilization methods have been developed to facilitate coherent time-resolved spectroscopy in the visible and ultra violet spectral region. Among these, the phase modulation approach of the Marcus group [1] has proven to be particularly sensitive and very versatile. The drawback of this method is however the need of a high repetition rate laser system ( $\gtrsim 200\text{kHz}$ ) which is not available in many labs. Recently, we have successfully implemented this technique with amplified fs laser pulses at 5kHz repetition rate. Performing electronic wave packet interferometry of dilute atomic vapors we could confirm an excellent SNR. This is surprising since the average laser power in these experiments is factor 800 lower than in previous experiments with 80MHz repetition rate. Moreover, we found that phase-synchronous undersampling can be readily performed with the phase modulation scheme allowing to use even lower repetition rate lasers.

[1] P. F. Tekavec, T. R. Dyke, and A. H. Marcus, *J. Chem. Phys.* **125**, 194303 (2006).

MO 19.3 Thu 16:30 Empore Lichthof

**Heterodyne-detected Sum Frequency Generation Spectroscopy of Polyacrylic Acid at the Air/Water- Interface** — ●PATRICK BALZEROWSKI<sup>2</sup>, KONRAD K. MEISTER<sup>1</sup>, JAN VERSLUIS<sup>1</sup>, and HUIB J. BAKKER<sup>1</sup> — <sup>1</sup>FOM-Institute for Atomic and Molecular Physics AMOLF, Amsterdam, The Netherlands — <sup>2</sup>Institute for Physical Chemistry II, Ruhr-Universität Bochum, Bochum, Germany

Here we present our findings on the conformational and hydration behavior of polyacrylic acid (PAA) at the air/water interface studied by heterodyne-detected vibrational sum frequency generation spectroscopy (HDVSFG). The amount of adsorption at the water/air interface and the influence of PAA on the water structure at the interface are found to be highly dependent on the degree of ionization (acid dissociation) of the carboxylic acid groups. At a low degree of ionization PAA is surface active and the spectral features suggest that PAA remains in a dense packing arrangement with intrachain hydrogen bonds. The HDVSFG spectra clearly show that the interfacial water molecules have a net orientation with their OH groups pointing towards the surface. Increasing the ionization degree of the carboxylic acid groups leads to an increase of the negative charge and to a break-up of the intrachain hydrogen bonds. This increase in negative charge comes along with an increase of the VSFG signal of the interfacial water molecules due to their enhanced orientation. At ionization degrees of  $\alpha > 0.203$  PAA loses its enhanced surface propensity and is well dissolved in the bulk. Changing the ionic strength of the solution by addition of NaCl is observed to lead to a recurrence of PAA to the interface.

MO 19.4 Thu 16:30 Empore Lichthof

**Accurate ultra-broadband prism-based amplitude and phase-shaping in the visible** — ●PHILIPP HILLMANN, ALEXANDER KASTNER, JENS KÖHLER, CRISTIAN SARPE, ARNE SENFTLEBEN, and THOMAS BAUMERT — Universität Kassel, Institut für Physik und CIN-SaT, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany

Femtosecond laser pulse shaping is the key technology in quantum control. So far, we were able to demonstrate pulse shaping with sub-cycle temporal accuracy making use of phase and amplitude modulation of femtosecond laser pulses in the infrared spectral region [1]. The experimental demonstration of molecular strong-field control schemes was achieved [2].

Supercontinua exceeding one octave are a prerequisite to generate few-cycle light pulses in the temporal domain. Combining supercontinuum generation spanning from the ultraviolet to near-infrared spectral region with high-throughput prism based pulse shaping [3] opens up the possibility to temporally steer wavepacket dynamics on the sub-cycle timescale expanding the technique to a broader range of electronic systems.

We present the current status of our setup for ultra-broadband amplitude and phase shaping of femtosecond laser pulses characterized by transient grating frequency resolved optical gating.

[1] J. Köhler *et al.*, *Optics Express* **19** (12), 11638-11653 (2011)

[2] M. Wollenhaupt *et al.*, *JPPA* **180**, 248-255 (2006)

[3] T. Binhammer *et al.*, *IEEE* **41** (12), 1552-1557 (2006)

MO 19.5 Thu 16:30 Empore Lichthof

**Excited state dynamics of dimetallic  $[\text{Ag}_2(\text{dcpm})_2]^{2+}$  in gas- and solution phase** — ●FLORIAN BÄPPLER<sup>1</sup>, SEBASTIAN KRUPPA<sup>2</sup>, CHRISTOPH RIEHN<sup>2</sup>, and ROLF DILLER<sup>1</sup> — <sup>1</sup>Dept. of Physics, — <sup>2</sup>Dept. of Chemistry, Univ. Kaiserslautern, 67663 Germany

$[\text{Ag}_2(\text{dcpm})_2]^{2+}$  (dcpm = bis(dicyclohexylphosphanyl)) is a prototype example for luminescent binuclear Ag(I) complexes exhibiting interesting photophysical and photochemical properties. Due to the absence of ligand-centered UV-chromophores it serves as a good model system for the investigation of argentophilic metal-metal interactions [1]. Here, we investigate the excited state dynamics of  $[\text{Ag}_2(\text{dcpm})_2]^{2+}$  in parallel in gas phase by fs transient photofragmentation [2], and in solution ( $\text{CH}_3\text{CN}$ ) by fs transient absorption [2] at room temperature. Surprisingly, both methods reveal similar deactivation kinetics, characterized by a triple exponential decay (1, 10 and 350 ps) after excitation of the silver-centered  $^1\text{MC}(d\sigma^*-p\sigma)$  state at 260 nm. This suggests similar excited state deactivation processes in gas- and solution phase and consequently little influence of solvent ( $\text{CH}_3\text{CN}$ ) molecules. In particular, fast exciplex formation  $[[\text{Ag}_2(\text{dcpm})_2]^{2+}/\text{CH}_3\text{CN}]^*$  as suggested [3] for an analog  $\text{Au}_2$ -complex can be excluded as essential component of the reaction coordinate, although it could occur concomitantly as a side effect in solution. Consequences for the interplay between photophysics and complex-solvent interaction are discussed.

[1] Schmidbaur *et al.*, *Angew. Chem. Int. Ed.* **2015**, *54*, 746-784.

[2] Imanbaev *et al.*, *Chemical Physics* **2014**, *442*, 53-61.

[3] Ma *et al.*, *Chemistry-A European Journal* **2015**, *21*, 13888-13893.

MO 19.6 Thu 16:30 Empore Lichthof

**Ultrafast studies on luminescent mono- and dinuclear copper(I)-complexes in solid and liquid phase** — ●MERTEN GRUPE<sup>1</sup>, FLORIAN BÄPPLER<sup>1</sup>, FABIAN DIETRICH<sup>2</sup>, DANIEL VOLZ<sup>3</sup>, STEFAN BRÄSE<sup>4</sup>, ROLF DILLER<sup>1</sup>, and MARKUS GERHARDS<sup>2</sup> — <sup>1</sup>Dept. of Physics, TU Kaiserslautern, 67663 Kaiserslautern — <sup>2</sup>Dept. of Chem., TU Kaiserslautern, 67663 Kaiserslautern — <sup>3</sup>Cynora GmbH, 76646 Bruchsal — <sup>4</sup>Dept. of Org. Chem., KIT, 76131 Karlsruhe

The efficiency of luminescence in copper-complexes is controlled by several photoinduced intra- and intermolecular processes, such as molecular flattening, intersystem crossing, solvation etc. For the elucidation of the underlying photophysics we employed femtosecond UV/Vis transient absorption (TA) as well as transient reflectivity (TR) spectroscopy and DFT calculations on luminescent mono-<sup>[1]</sup> and dinuclear<sup>[2]</sup> copper(I)-complexes. The results allow a rigorous comparison of the respective ultrafast dynamics in solution and solid phase, possibly controlled by metal-metal cooperativity. Together with the investigations of [3] fundamental kinetics of homo- and heteroleptic

mononuclear copper(I)-complexes can be contrasted.

[1] L. Bergmann et al. *Chem. Commun.*, 2013, 49 6501

[2] D. Volz et al. *Chem. Mater.*, 2013, 25, 3414-3426

[3] M. Iwamura et al. *Acc. chem. res.*, 2015, 48, 782-791

MO 19.7 Thu 16:30 Empore Lichthof

**Ultrafast Ionization and Fragmentation Dynamics of Chlorinated Silane Derivatives** — ●INA HALFPAP, CLARA ADELE VON RANDOW, EGILL ANTONSSON, CHRISTOPHER RASCHPICHLER, and ECKART RÜHL — Physical Chemistry, Freie Universität Berlin, Takustr. 3, 14195 Berlin

The femtosecond pump-probe technique is known to be a suitable approach to study molecular strong-field ionization processes in the time domain. To follow specific fragmentation pathways, mass spectrometry is the most suitable approach. The fragmentation dynamics of highly excited molecular neutrals and ions can be affected by dynamic resonances, where the wavepacket motion on ionic potential energy surfaces plays a crucial role.

We present recent results on the ionization and fragmentation dynamics of trichloromethylsilane ( $\text{SiCl}_3\text{CH}_3$ ), dichlorodimethylsilane ( $\text{SiCl}_2(\text{CH}_3)_2$ ), and chloro-trimethylsilane ( $\text{SiCl}(\text{CH}_3)_3$ ) investigated by a one-color 804 nm femtosecond pump-probe experiment recording the ion yields of fragment ions. The intense pump pulse ( $250 \mu\text{J}/\text{pulse}$ ) is used to ionize the sample molecules which is followed by a time delayed less intense probe pulse ( $70 \mu\text{J}/\text{pulse}$ ). This leads to additional fragmentation of the parent and fragment ions. The yields of parent and fragment ions show broad dynamic resonances with maxima in a range of  $\Delta t = 0.5$  ps. The experimental findings are explained in terms of dynamic ionic resonances leading to an enhanced dissociation of the parent ions as well as some fragment ions.

MO 19.8 Thu 16:30 Empore Lichthof

**Photophysics and Photochemistry of a Dinuclear Pt-Pt Complex and its Trinuclear Ag-Pt-Pt Derivative Studied by Femtosecond Time-Resolved UV/Vis Spectroscopy in Solution** — ●FABIAN RUPP<sup>1</sup>, LIEDY FLORIAN<sup>1</sup>, SEBASTIAN V. KRUPPA<sup>2</sup>, CHRISTOPH RIEHN<sup>2</sup>, and ROLF DILLER<sup>1</sup> — <sup>1</sup>Dept. of Physics, TU Kaiserslautern — <sup>2</sup>Dept. of Chemistry, TU Kaiserslautern, 67663 Kaiserslautern, Germany

Metal-metal interactions are crucial for the design and application of multinuclear transition metal complexes in new electronic devices or chemical catalysis. In a comparative study we investigated the photophysical and photochemical properties of the model compound tetrakis- $\mu$ -pyrophosphitodiplatinate(II) (PtPOP) and its Ag-derivative (AgPtPOP) in solution by fs time-resolved UV/Vis spectroscopy. Whereas PtPOP possesses a strong absorption band in the electronic ground state at 369 nm, the band is shifted to 398 nm for AgPtPOP, allowing selective photoexcitation. PtPOP excited states dynamics such as vibrational cooling, intersystem crossing, coherent wave packet dynamics [1] and electron detachment [2] have been studied intensively. On these grounds the influence of the added  $\text{Ag}^+$  on the molecular dynamics is deduced in particular via wave packet oscillation period and dephasing time. This also allows to characterize the shapes of the potential energy surfaces of the electronic ground and first excited singlet state, respectively.

[1] R. van der Veen et al., *JACS*, 2011, **133**, 305

[2] S. V. Kruppa et al., *Int. J. Mass. Spec.*, 2015, accepted

MO 19.9 Thu 16:30 Empore Lichthof

**Effect of alkyl chain length on the ultrafast vibrational dynamics of C-H stretching in 1-alkyl-3methylimidazolium ionic liquids** — MEHDI M. KAZEMI, MAHESH NAMBOODIRI, JOHANNES KIEFER, and ●ARNULF MATERNY — Physics and Earth Sciences, Jacobs University Bremen, Campus Ring 1, 28759 Bremen

Femtosecond time-resolved coherent anti-Stokes Raman scattering (fs-CARS) is used to study the ultrafast vibrational dynamics in ionic liquids (ILs). The effect of increasing the alkyl chain length,  $n$ , in 1-alkyl-3methylimidazolium bis-(trifluoromethylsulfonylethyl)imidate ( $\text{CnClImTSEFI}$ ,  $n=6,8,10,12$ ) ionic liquid on the vibrational dynamics of C-H stretching is studied. The high frequency C-H stretching modes  $2800\text{-}3000 \text{ cm}^{-1}$  are excited and probed by the fs-CARS excitation around  $3000 \text{ cm}^{-1}$ . The results show that the vibrational dynamics of the ILs depends more on the viscosity than the hydrogen bonding as the alkyl chain length increases.

MO 19.10 Thu 16:30 Empore Lichthof

**Structural Dynamics of Intercalated Water in Graphene Ox-**

**ide** — ●AMUL SHINDE<sup>1,2</sup>, KATRIN ADAMCZYK<sup>1,2</sup>, ANDREAS ROSSO<sup>2</sup>, R. J. DWAYNE MILLER<sup>2,3</sup>, and NILS HUSE<sup>1,2</sup> — <sup>1</sup>Institut für Nanostruktur- und Festkörperphysik, Universität Hamburg, 20355 Hamburg, Germany — <sup>2</sup>Max Planck Institut für Struktur und Dynamik der Materie, 22761 Hamburg, Germany — <sup>3</sup>Departments of Chemistry and Physics, University of Toronto, Toronto, Ontario, Canada M5S 3H6

The effects of nanoconfinement on the structural dynamics of water is of fundamental scientific importance in both natural and engineered environments. Here we present an experimental investigation of intercalated water in graphene oxide (GO) using ultrafast infrared spectroscopy. The water organization in a fluctuating network of intermolecular hydrogen bonds is different to bulk water due to the decreased symmetry and new interactions with GO functional groups. We discuss the structural response of this network to energy input and address the implications for the mechanical properties of multilayered composite materials like GO.

MO 19.11 Thu 16:30 Empore Lichthof

**IR spectroscopy on anionic and cationic, two- and three-centred, isolated nickel-ethanol clusters** — ●DANIEL BELLAIRE<sup>1</sup>, MARKUS BECHERER<sup>1</sup>, FABIAN DIETRICH<sup>1</sup>, ADAM KUBAS<sup>2</sup>, KARIN FINK<sup>2</sup>, and MARKUS GERHARDS<sup>1</sup> — <sup>1</sup>TU Kaiserslautern, Fachbereich Chemie, Erwin-Schrödinger-Straße 52, 67663 Kaiserslautern — <sup>2</sup>Karlsruhe Institute of Technology, Institute of Nanotechnology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

Clusters containing transition metals and aliphatic ligands provide model systems regarding e.g. catalytical properties, magnetism, reactivity and structure. Thus, the successive variation of size and composition of the metal clusters can give a fundamental insight. The investigated nickel clusters are produced by applying laser ablation to a rotating metal rod and by attaching the ethanol ligand(s) in a supersonic beam. The frequencies and frequency shifts of OH stretching vibrations (between different clusters) are probed by means of IR-photofragmentation spectroscopy. An assignment of structure and spin states is performed by comparing the experimentally observed vibrational frequencies with the calculated values obtained from DFT calculations.

Specifically, anionic and cationic  $\text{Ni}_m(\text{ethanol})_n^{+/-}$  ( $m=2,3$ ;  $n=1-3$ ) clusters are spectroscopically investigated and explored by the aforementioned methods. A strong OH bond activation is observed in the anionic cases. The results give insight both into the structure and reactivity of the nickel aggregates.

MO 19.12 Thu 16:30 Empore Lichthof

**Automated size determination of single clusters from x-ray scattering images** — ●ALEXANDER NELDE<sup>1</sup>, BRUNO LANGBEHN<sup>1</sup>, MARIA MÜLLER<sup>1</sup>, DANIELA RUPP<sup>1</sup>, MARIO SAUPE<sup>1</sup>, ANATOLI ULMER<sup>1</sup>, THOMAS MÖLLER<sup>1</sup>, and NINA ROHRINGER<sup>2</sup> — <sup>1</sup>TU Berlin — <sup>2</sup>Max Planck Institute for the Physics of Complex Systems

Short wavelength Free-electron lasers (FELs) allow imaging of individual nano particles in free flight. In laser-cluster interaction studies, single-cluster imaging can be used to sort the single-shot measurement of reaction products (e.g. ions, electrons) by cluster size. The large data sets require automated analysis, often challenging due to detector geometries and noisy background signal. An automated size determination algorithm based on Mie-fits will be presented and the measured size distribution from large xenon clusters imaged at the FLASH FEL will be discussed.

MO 19.13 Thu 16:30 Empore Lichthof

**Optical properties of thionized diamondoids** — ●TOBIAS ZIMMERMANN<sup>1</sup>, THERESA HÖHNE<sup>1</sup>, ANDRE KNECHT<sup>1</sup>, ROBERT RICHTER<sup>1</sup>, ANDREY A FOKIN<sup>2</sup>, PETER R SCHREINER<sup>2</sup>, THOMAS MÖLLER<sup>1</sup>, and TORBJÖRN RANDE<sup>1</sup> — <sup>1</sup>Institut für Optik und Atomare Physik, Technische Universität Berlin — <sup>2</sup>Institut für Organische Chemie, Justus-Liebig-Universität Giessen

Diamondoids, perfectly size- and shape-selectable  $\text{sp}^3$ -hybridized carbon nanoparticles, exhibit intrinsic UV luminescence. It was shown through size- and shape-dependent studies that pristine diamondoids offer detailed insight into luminescence properties of large molecules [1]. However, so far no gas phase luminescence has been observed for diamondoids functionalized with foreign atoms. Recently, it has been predicted that thionization could alter the optical gaps for such particles to the VIS/IR spectral regime [2]. While adamantane-2-thione, the smallest member of the series, is known to show phosphorescence in so-

lution [3], a broader selection of different sized thionized diamondoids could be successfully synthesized just recently. To probe luminescence in the gas phase and the effect of the particle size as well as thionization order, we investigated the electronic structure of this series in a combined study with synchrotron radiation and an OPO laser system.

[1] R. Richter *et al.*, *Phys. Chem. Chem. Phys.* **17**, 4739 (2015).

[2] M. Vörös *et al.*, *Phys. Rev. Lett.* **108**, 267401 (2012).

[3] K. J. Falk *et al.*, *J. Am. Chem. Soc.* **111**, 6518 (1989).

MO 19.14 Thu 16:30 Empore Lichthof

**A setup for studying correlation effects in poly-anionic metal clusters by photoelectron spectroscopy** — ●MADLEN MÜLLER<sup>1</sup>, FRANKLIN MARTINEZ<sup>2</sup>, GERRIT MARX<sup>1</sup>, PATRICE OELSSNER<sup>2</sup>, SLAWOMIR SKRUSZEWICZ<sup>2</sup>, JOSEF TIGGESBÄUMKER<sup>2</sup>, ROBERT WOLF<sup>3</sup>, KARL-HEINZ MEIWES-BROER<sup>2</sup>, and LUTZ SCHWEIKHARD<sup>1</sup> — <sup>1</sup>Ernst-Moritz-Arndt-Universität, Greifswald, Deutschland — <sup>2</sup>Universität Rostock, Rostock, Deutschland — <sup>3</sup>Max-Planck-Institut für Kernphysik, Heidelberg, Deutschland

Photoelectron spectroscopy experiments provide insight into the electronic structure of atomic clusters. In the case of multiply negatively charged clusters, electron affinities and Coulomb barriers can be probed by varying the photon energy. In addition, poly-anionic metal clusters serve as model systems for electron-correlation phenomena. A setup is presented, which combines a radio-frequency ion trap, used for cluster-size selection, with a velocity-map imaging and a magnetic-bottle time-of-flight electron spectrometer. As a first test, measurements on mono-anionic fullerenes with respect to the first electron affinity, thermionic electron emission and the photoelectron angular distribution of the excess electron are conducted by the use of UV nanosecond pulses. The investigations will be extended to poly-anionic metal clusters, in the future. As higher charge states are only observed for larger cluster sizes, the enhanced requirements on the mass resolving power will be matched by a multi-reflection time-of-flight mass-separator. The project is funded by the Collaborative Research Center (SFB) 652.

MO 19.15 Thu 16:30 Empore Lichthof

**Characterization of pulsed nozzles for production of atomic and molecular clusters** — ●MATTHIAS BOHLEN, JONAS GRZESIAK, AARON LAForge, RUPERT MICHIELS, NICOLAS RENDLER, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg

Pulsed nozzles in general offer many advantages over continuous beams such as higher droplet densities and reduced gas load. We use a home-built pulsed nozzle, developed in cooperation with CRUCS Center at UBC, Vancouver, that produces gas pulses down to 20  $\mu$ s duration at repetition rates up to several hundred Hz. Investigations of power consumption and other properties are presented. A rich variety of applications, that include the production of water and ammonia clusters, is discussed as well as the characterization of the influence of multiple source parameters on the cluster size distribution.

Additionally, we have recently introduced a new method for doping clusters by laser ablation [1]. Here, we present the results from characterization of the laser ablation setup. In particular, it was shown that pulsed nozzles produce beams of both doped and seeded laser ablated material.

[1] R. Katzy, M. Singer, S. Izadnia, A.C. LaForge, F. Stienkemeier; *Rev. Sci. Instrum.*, in press

MO 19.16 Thu 16:30 Empore Lichthof

**Infrared Laser Spectroscopy of Organic Radicals and their Bimolecular Complexes** — ●DANIEL LEICHT, MATIN KAUFMANN, RAFFAEL SCHWAN, DANIEL HABIG, GERHARD SCHWAAB, and MARTINA HAVENITH — Ruhr-Universität Bochum, Bochum, Germany

Organic radicals are known to be important intermediates in many reactions e.g. in combustion, explosives and tropospheric chemistry. Using the technique of helium nanodroplet infrared spectroscopy we study organic radicals including but not limited to the allyl and benzyl radicals. The helium droplet environment enables us to not only study the bare radicals but also their bimolecular complexes with other small molecules (i.e. water, hydrochloric acid, oxygen, nitric oxide). In the case of water and HCl we observe the formation of H-bonds to the radicals'  $\pi$ -systems; these H-bonded complexes can be viewed as the exit channel of the hydrogen abstraction reaction by either Cl atoms or OH radicals from the corresponding organic compound. Open-shell species, such as oxygen and nitric oxide, however, chemically react with

the organic radicals to form e.g. peroxy species. The spectroscopic observation of these organic radicals and their complexes therefore helps us to better understand their formation and reactivity.

MO 19.17 Thu 16:30 Empore Lichthof

**High resolution spectroscopy on LiSr** — ●ERIK SCHWANKE, HORST KNÖCKEL, SILKE OSPELKAUS, and EBERHARD TIEMANN — QUEST and Inst. f. Quantenoptik, Leibniz Universität Hannover

The mixed alkali-alkaline earth molecules have recently attracted the interest of the scientific community due to possible applications in the field of cold and ultracold molecules. The combination of alkaline and alkaline earth atoms leads to molecules which have permanent electric and magnetic dipole moments and thus offer manipulation 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 from which one expects  $2\Sigma^+ - 2\Sigma^+$  transitions in the near infrared. Experimentally, not so much is known about the molecular electronic states. We have successfully recorded the near infrared spectrum of LiSr. The molecules were created in a heatpipe and their thermal emission was recorded via a high resolution Fourier transform spectrometer. The assignment of the dense spectrum was facilitated by tuning a diode laser to a molecular line of the emission spectrum, resulting in the observation of P-R-doublets and a simple vibrational progression. We used the rotational constants from ab initio-calculations for a first guess of the rotational quantum numbers. Then we proceeded to take into account more transition lines from higher rotational and vibrational levels. Perturbations due to couplings between the  $2^2\Sigma^+$  state and the  $1^2\Pi$  state have been observed and will be used to investigate the  $2^2\Sigma_{1/2}^+ - 1^2\Pi_{1/2}$  and  $2^2\Sigma_{1/2}^+ - 1^2\Pi_{3/2}$  couplings.

We will report on the status of the investigations.

MO 19.18 Thu 16:30 Empore Lichthof

**Modeling of superradiance in molecular systems** — ●DAVID W. SCHÖNLEBER and ALEXANDER EISFELD — Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden

We study superradiance in molecular systems in a setup similar to the one used in recent experiments [1]. In molecular systems, an excited electronic state can decay into different vibrational states of the electronic ground state, which are subject to relaxation. We employ a simple three-level model to analyze the effect of vibrational relaxation, as well as effects of aggregate geometry, on the visibility of superradiance.

[1] *Phys. Rev. B* **92**, 121408(R) (2015)

MO 19.19 Thu 16:30 Empore Lichthof

**Thermalization of OH<sup>-</sup> in Multipole RF-Ion Traps with cold He, H<sub>2</sub> and HD as buffer gas** — ●GERHARD EGGER, SEUNGHYUN LEE, OLGA LAKHMANSKAYA, ERIC ENDRES, DANIEL HAUSER, and ROLAND WESTER — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Österreich

High order multipole ion traps are a versatile tool for performing spectroscopy on cold molecular ions and analyzing cold ion-neutral reaction dynamics with astrophysical relevance. In contrast to a Paul trap, the linear 22-pole trap features a large field free region [1]. Cooling is achieved by collisions with neutral buffer gas, thermalizing the kinetic temperature as well as the internal degrees of freedom which works well for many ion species. Furthermore, the temperature can be tuned from several Kelvin to room temperature, which enables temperature dependent measurements of reactions. With rotationally resolved near threshold photodetachment of OH<sup>-</sup> the rotational temperature can be determined [2].

Interestingly, below 20 K the rotational temperature does not decrease linearly any more even though the trap temperature is reduced [2]. This can not easily be explained by the known heating effects. Therefore further measurements at different temperatures have been performed. Clearly seeing the effect in He buffer gas we performed corresponding measurements also in H<sub>2</sub> and HD. These results will be presented.

[1] R. Wester, *J. Phys. B* **42**, 154001 (2009) [2] R. Otto *et al.*, *Phys. Chem. Chem. Phys.* **15**, 612 (2013)

MO 19.20 Thu 16:30 Empore Lichthof

**Cold Penning-Reactions using a Li-MOT** — ●JONAS GRZESIAK, FRANK STIENKEMEIER, and MARCEL MUDRICH — Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg i.Br.

Cold reactive scattering, especially in merged beams, has recently attracted wide attention.[1] Our setup for measuring elastic scattering of cold atoms and molecules originating from a rotating nozzle and atoms trapped in a Li-MOT has been extended for investigating reactive scattering. To this end we use a pulsed supersonic and cryogenic source with different homemade discharge units to provide an intense and cold beam of metastable rare gas atoms. We discuss the optimization of the metastable source as well as first results on cold Penning reactions of the pulsed beam atoms with the ultracold Li-atoms from the MOT. A detailed study of the possible extension of our setup combining the rotating nozzle with the pulsed source in a merged beams experiment is given.

[1] A. B. Henson, S. Gersten, Y. Shagam, J. Narevicius, E. Narevicius, *Science* 338, 234 (2012).

MO 19.21 Thu 16:30 Empore Lichthof  
**Implementation of a Cryogenic Multipole Ion Trap for THz Spectroscopy of Molecular Systems** — ●LENA REMMERS, MORITZ FISCHER, STEFFEN SPIELER, KATHARINA GEISTLINGER, and ROLAND WESTER — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck

Spectroscopy of rovibrational transitions by continuous THz radiation is a promising approach to unravel the structure and dynamics of weakly bound systems. In our group a new setup combining an electro-spray ionization source and a cryogenic multipole ion trap is being built. This approach provides access to intact macromolecules in the gas phase with positive or negative charge. These are focused and guided by means of an ion funnel and a quadrupole ion guide. By use of a quadrupole mass selector the ions are selectively loaded into the 16-pole trap. The cryogenic trap provides a possibility for ground-state preparation of trapped ions via buffergas cooling. This setup will be used to perform rotational spectroscopy of the target molecular ion using a THz radiation source (based on difference frequency mixing of two near infrared diode lasers) and an additional IR-Laser entering the trap perpendicular to the ion path. Here we report on the status and the characteristics of this experiment and on latest results on trapping ions and clusters. First experiments are planned on small  $\text{OH}^-(\text{H}_2\text{O})_n$  and  $\text{H}_3\text{O}^+(\text{H}_2\text{O})_n$  clusters.

MO 19.22 Thu 16:30 Empore Lichthof  
**Towards Highly Sensitive Detection of Cold Formaldehyde via Laser-Induced Fluorescence** — ●ERICH DOBLER, MARTIN IBRÜGGER, ALEXANDER PREHN, ROSA GLÖCKNER, SOTIR CHERVENKOV, MARTIN ZEPPENFELD, and GERHARD REMPE — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

Due to their rich internal structure and the long-range dipole-dipole interaction, cold polar molecules offer many exciting applications ranging from many-body physics to quantum information science. For such experiments, a highly sensitive detection technique to observe even smallest numbers of molecules is essential.

For this purpose, we implement a detection scheme based on laser-induced fluorescence (LIF) for formaldehyde ( $\text{H}_2\text{CO}$ ), the molecule currently under investigation in our optoelectrical cooling experiment [1,2]. Successful detection of  $\text{H}_2\text{CO}$  via LIF has already been shown [3] and, moreover, this technique also allows state-selective measurements. We present the setup and the results from absorption and LIF spectroscopy from the  $\tilde{X}^1A_1$  electronic ground state to the  $4^1$  vibrational manifold of the  $\tilde{A}^1A_2$  excited state of formaldehyde. Those measurements are performed as a first step towards the realization of a LIF-based detection of ultracold molecules.

[1] M. Zeppenfeld *et al.*, *Phys. Rev. A* **80**, 041401 (2009).

[2] M. Zeppenfeld *et al.*, *Nature* **491**, 570-573 (2012).

[3] E. R. Hudson *et al.*, *Phys. Rev. A* **73**, 063404 (2006).

MO 19.23 Thu 16:30 Empore Lichthof  
**Mixed-field orientation of molecules without rotational symmetry: time-dependent analysis** — ●LINDA V. THESING<sup>1</sup>, ROSARIO GONZÁLEZ-FÉREZ<sup>2</sup>, and JOCHEN KÜPPER<sup>1,3,4</sup> — <sup>1</sup>Center for Free-Electron Laser Science, DESY — <sup>2</sup>Instituto Carlos I, Universidad de Granada — <sup>3</sup>The Hamburg Center for Ultrafast Imaging, University of Hamburg — <sup>4</sup>Department of Physics, University of Hamburg

We theoretically investigate the rotational dynamics of molecules without rotational symmetry in combined non-resonant laser fields and static electric fields. It was experimentally demonstrated that asymmetric top molecules with a permanent dipole moment non parallel to

any principal axis of polarizability can be 3D aligned and orientated using elliptically polarized laser pulses in combination with weak dc electric fields [1]. A theoretical analysis assuming adiabatic behavior was not able to explain these findings accurately [1]. Here, we solve the time-dependent Schrödinger equation for different field configurations for 6-chloropyridazine-3-carbonitrile (CPC) as an example molecule in order to study the influence of nonadiabatic phenomena that have previously been shown to play an important role for mixed field orientation dynamics [2].

[1] Hansen *et al.*, *J. Chem. Phys.* **139**, 234313 (2013)

[2] Nielsen *et al.*, *Phys. Rev. Lett.* **108**, 193001 (2012)

MO 19.24 Thu 16:30 Empore Lichthof  
**A Novel Scheme for Slowing Molecules** — ●MAURICE PETZOLD, MIRCO SIERCKE, PAUL KAEBERT, PHILIPP GERSEMA, and SILKE OSPELKAUS — Institut für Quantenoptik, Leibniz Universität Hannover

Current efforts to directly cool molecules to degeneracy are largely limited by the flux of slow molecules available in experiments. While slowing methods for molecules have been available for a long time, they have not been able to achieve efficiencies comparable to methods used for atoms. In this poster, we present our ideas for novel slowing methods of molecules. We propose a novel scheme based on radiative forces to slow down molecules to trappable velocities. The magneto-optical scheme is continuous and provides compression of the 1D-velocity distribution. We give detailed calculations of the forces obtained for the case of SrF and give estimates for the expected flux of cold molecules. To demonstrate the feasibility of our approach, we report on progress on applying our method to a thermal beam of Potassium atoms.

MO 19.25 Thu 16:30 Empore Lichthof  
**Stopping intense beams of internally cold molecules via centrifugal forces** — ●XING WU, THOMAS GANTNER, MARTIN ZEPPENFELD, SOTIR CHERVENKOV, and GERHARD REMPE — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany

Cryogenic buffer-gas cooling produces intense beams of cold molecules [1][2]. It offers a versatile source for studying collision dynamics and reaction pathways in the cold regime, and a variety of other applications. In order to be trapped and further cooled [3], these cold molecular beams still need to be decelerated. Here, we demonstrate that intense and continuous beams of electrically guided molecules produced by a cryogenic buffer-gas cell [2], can be brought to a halt by the centrifugal force in a rotating frame [4]. In addition, our RF-resonant depletion detection shows that up to 90% rotational-state purity can be achieved in the so-produced cold molecular beams. In combination with complete trajectory simulations which resolve the guiding efficiency for different states, it allows us to determine the internal temperature of these buffer-gas cooled molecules.

[1] J. D. Weinstein *et al.*, *Nature* **395**, 148 (1998)

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

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

[4] S. Chervakov *et al.*, *Phys. Rev. Lett.* **112**, 013001 (2014)

MO 19.26 Thu 16:30 Empore Lichthof  
**Infrared spectroscopy of trimethylamine N-oxide in helium droplets** — ●RAFFAEL SCHWAN, MATIN KAUFMANN, DANIEL LEICHT, GERHARD SCHWAAB, and MARTINA HAVENITH — Ruhr-University Bochum, Germany

Helium nanodroplet spectroscopy is a well-established experimental technique to investigate reactive species like radicals or ions as well as weakly bound aggregates. Due to the ambient temperature of 0.37 K of the helium droplets only the ro-vibrational ground state of the investigated species is populated, which simplifies the observed infrared spectrum. Since helium droplets are superfluid, embedded molecules can still rotate freely.

Trimethylamine N-oxide (TMAO) is a naturally occurring osmolyte and plays an important role in the stabilization of proteins. Recent results using THz spectroscopy show the formation of TMAO-water aggregates involving 3-4 water molecules which are bound strongly to TMAO via hydrogen bonding [1].

First infrared spectra of the isolated TMAO molecule in helium droplets were obtained. For a distinct assignment of the spectral features mass-selective measurements were used. Future measurements aim to observe the stepwise formation of TMAO-water aggregates in helium droplets by characterizing the aggregates based on their infrared spectra and corresponding ab initio calculations.

[1] Knake, L., Schwaab, G., Kartaschew, K., Havenith, M. (2015).

The Journal of Physical Chemistry B, 119(43), 13842-13851.

MO 19.27 Thu 16:30 Empore Lichthof  
**Characterization of Microstructured Electric Trap for Optoelectrical Cooling of Polar Molecules** — ●MARTIN IBRÜGGER, ALEXANDER PREHN, ROSA GLÖCKNER, MARTIN ZEPPENFELD, and GERHARD REMPE — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching

Due to their rich internal level structure, polar molecules offer a wide range of exciting applications such as quantum simulation and controlled chemistry. However, many applications rely on long interaction times and localization, thus requiring trapping of the molecules. In our approach the trap consists of a pair of microstructured capacitor plates [1] creating a box-like potential. With this configuration we achieve record-long lifetimes for polar polyatomic molecules and dramatically reduce Stark broadening, therefore providing the optimal environment for optoelectrical Sisyphus cooling.

Here we investigate the properties of our trap with cooled formaldehyde [2]. We find  $1/e$  trap decay times of up to one minute and confirm via Stark spectroscopy [3] the box-like potential. A homogeneous offset field inside the trap allows us to spectroscopically resolve transitions between single  $M$  sublevels of different rotational states. This enables us to control the rotational state and prepare the molecules in single  $M$  sublevels by optical pumping [4].

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

[2] A. Prehn *et al.*, arXiv:1511.09427 (2015).

[3] R. Glöckner *et al.*, *New J. Phys.* **17**, 055022 (2015).

[4] R. Glöckner *et al.*, arXiv:1511.07360 (2015).

MO 19.28 Thu 16:30 Empore Lichthof  
**Micro Solvation of Glycine** — ●MATIN KAUFMANN, RAFFAEL SCHWAN, DANIEL LEICHT, DEVENDRA MANI, GERHARD SCHWAAB, and MARTINA HAVENITH — Lehrstuhl für Physikalische Chemie II, Ruhr-Universität Bochum

Glycine is the smallest amino acid and serves as a model system for the interaction of amino acids and water. In the gas phase, glycine is in its neutral form, while in crystal structure and aqueous solution it occurs as a zwitterion.

Theoretical [1] and experimental [2] studies on the micro solvation of glycine have been carried out, however, no unambiguous statement was made on the number of water molecules needed to transition from hydrogen bonded structures involving the neutral form of glycine to structures involving the zwitterionic form of glycine.

The helium nanodroplet isolation technique is established as a way to stabilize molecular aggregates and reactive species, making them accessible to spectroscopic studies. Infrared spectra of glycine in complexes with an increasing number of water molecules are recorded and the observed transitions are assigned utilizing ab initio calculations for

most of the viable structures.

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[2] R. Ramaekers, *J. Chem. Phys.* 2004, 120, 4182

MO 19.29 Thu 16:30 Empore Lichthof  
**Optimized Stark deflection and mixed-field orientation of OCS molecules** — JENS S. KIENITZ<sup>1,2</sup>, SEBASTIAN TRIPPEL<sup>1</sup>, KAROL DLUGOLECKI<sup>1</sup>, ROSARIO GONZÁLEZ-FÉREZ<sup>2,3</sup>, and ●JOCHEN KÜPPER<sup>1,2,4</sup> — <sup>1</sup>Center for Free-Electron Laser Science, DESY — <sup>2</sup>Center for Ultrafast Imaging, University of Hamburg — <sup>3</sup>Instituto Carlos I, Universidad de Granada — <sup>4</sup>Department of Physics, University of Hamburg

We demonstrate the use of very strong static electric fields to improve the well-known techniques to state-select molecules in the electric deflector and for mixed-field orientation [1]. These are important methods to provide ideal samples for molecular-frame imaging of molecular dynamics in the gas phase [2]. For the state selection we developed a Stark deflector with a two-rod geometry, similar to [3]. Experimental results confirm a stronger deflection and better state separation than previous stark deflectors. In mixed-field orientation a strong static electric field avoids nonadiabatic effects [4]. Therefore, we extended the idea of a two plate velocity map imaging spectrometer [5] to allow for strong electric fields up to 22 kV/cm. We will present its use in alignment and orientation experiments and disentangle the rotational motion of molecules in combined strong electric fields and laser pulses.

[1] Chang *et al.*, *Int. Rev. Phys. Chem.* **34**, 557 (2015)

[2] Holmegaard *et al.*, *Nat. Phys.* **6**, 428 (2010)

[3] Stefanov *et al.*, *Meas. Sci. Technol.* **19**, 055801 (2008)

[4] Nielsen *et al.*, *Phys. Rev. Lett.* **108**, 193001 (2012)

[5] Papadakis and Kitsopoulos, *Rev. Sci. Instr.* **77**, 083101 (2006)

MO 19.30 Thu 16:30 Empore Lichthof  
**Charge Transfer in hetero-molecular organic Van der Waals complexes** — ●ALEXANDER RUF and FRANK STIENKEMEIER — University of Freiburg, Freiburg, Germany

Charge transfer between excitonic states determines the functionality of many technological and biological systems. Despite their great importance and the extensive previous research the details of the complex quantum mechanical dynamics are still not clearly understood and interpretation of experimental data and simulations is not unequivocal. Single isolated hetero-molecular complexes can serve as an ideal model system to isolate specific effects promoting charge and energy transfer. For this purpose helium nano droplets offer unique properties in respect of complex formation, preparation of initial quantum states, control of environmental interactions and applicability of spectroscopic techniques. An outline of the anticipated experimental approaches to study charge transfer dynamics in model systems is given.