

## MO 21: Posters 4: Novelties in Molecular Physics

Time: Thursday 17:00–19:00

Location: C/Foyer

MO 21.1 Thu 17:00 C/Foyer

**Toward spectroscopy with PAH and fullerene ions in a cryogenic trap** — •JÜRGEN GÖCK<sup>1</sup>, KLAUS BLAUM<sup>1</sup>, CHRISTIAN BREITENFELDT<sup>2</sup>, ULRICH GRÖZINGER<sup>3</sup>, THOMAS HENNING<sup>3</sup>, JONAS KARTHEIN<sup>1</sup>, BASTIAN KERN<sup>4</sup>, SUNIL KUMAR S.<sup>1</sup>, CHRISTIAN MEYER<sup>1</sup>, GAËL ROUILLE<sup>3</sup>, DMITRY STRELNIKOV<sup>4</sup>, ANDREAS WOLF<sup>1</sup>, SEBASTIAN GEORGE<sup>1</sup>, and HOLGER KRECKEL<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany — <sup>2</sup>Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, Felix-Hausdorff-Straße 6, 17487 Greifswald, Germany — <sup>3</sup>Max-Planck-Institut für Astronomie, Königstuhl 17, 69117 Heidelberg, Germany — <sup>4</sup>Institut für Physikalische Chemie II, Karlsruher Institut für Technologie, Kaiserstraße 12, 76131 Karlsruhe

Gas phase spectroscopy with large molecular ions is still a challenging subject. We are currently developing a novel technique which is based on sensitive detection of mid-infrared photons. For this we use the Cryogenic Trap for Fast ion beams (CTF) [1], which reflects the ions back and forth between two electrostatic mirrors. Einzel lenses focus the ion beam toward the trap center. The cryogenic temperature of the environment (<15 K) leads to residual-gas densities of 2000 particles/cm<sup>3</sup>, corresponding to a pressure of  $\sim 10^{-13}$  mbar at room temperature, and an almost black-body radiation free background.

We will present the details about the available ion source and the ion optics used for the injection of the ions into the trap. The measurement principle and the experimental program will be discussed.

[1] M. Lange et al., *Rev. Sci. Instrum.* **81** (2010) 055105.

MO 21.2 Thu 17:00 C/Foyer

**Structural rearrangement by an IR excitation in isolated hydroxychromones** — •ANKE STAMM, MARTIN WEILER, KIRSTEN SCHWING, and MARKUS GERHARDS — TU Kaiserslautern, Fachbereich Chemie, Physikalische und Theoretische Chemie, Erwin-Schrödinger-Straße 52, 67663 Kaiserslautern

Photochemical reactions as the excited state proton transfer are of great interest due to their importance in chemical and biological processes. Molecular beam investigations combined with double, triple and quadruple resonance IR/UV spectroscopic techniques are very powerful tools to analyze structures and photochemically induced reactions. In comparison with (TD)-DFT calculations direct structural information on the electronic ground and electronically excited state of isolated molecules and clusters are obtained. Here we present studies on the photochemically reactive 3-hydroxychromone and 3-hydroxyflavone as well as clusters with water. In order to analyze structures and proton transfer reactions of different isomers/species with overlapping UV transitions in different electronic states, the quadruple resonance methods yield unambiguous results. Furthermore in a new approach for neutral isolated clusters IR/IR/UV/UV spectra indicate that the first IR excitation can lead to a rearrangement reaction of a cluster which is analyzed by the second IR excitation in combination with a resonant two photon ionization.

MO 21.3 Thu 17:00 C/Foyer

**Collinear two-dimensional spectroscopy with shot-to-shot phase cycling** — •SEBASTIAN ROEDING<sup>1</sup>, SIMON DRAEGER<sup>1</sup>, ANDREAS STEINBACHER<sup>1</sup>, PATRICK NUERNBERGER<sup>1,2</sup>, and TOBIAS BRIXNER<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — <sup>2</sup>Physikalische Chemie II, Ruhr-Universität Bochum, 44780 Bochum

Experimental setups to perform two-dimensional electronic spectroscopy are typically based on coherently emitted optical signals in the phase-matching direction [1]. In contrast, the detection of incoherent signals allows the investigation of molecules in different environments, e.g. by fluorescence detection in the liquid phase [2] or by photocurrent measurement in the solid state [3]. In order to discriminate the different signal contributions phase-cycling [4] needs to be applied.

We introduce a novel setup which utilizes an AOPDF pulse shaper (Dazzler, Fastlite) to generate multi-pulse sequences in a collinear beam arrangement. The AOPDF allows the variation of the interpulse delays and their relative phases with 1 kHz rate, enabling a rapid scan and shot-to-shot phase cycling. The pulse shaper output can be guided to separate experiments which permits the investigation of molecules in different environments.

[1] Brixner et al, *Nature* **434**, 625 (2005)[2] Tekavec et al., *J. Chem. Phys.* **127**, 214307 (2007)[3] Aeschlimann et al., *Science* **333**, 6050 (2011)[4] Tian et al., *Science* **300**, 1553 (2003)

MO 21.4 Thu 17:00 C/Foyer

**Ultrafast studies on luminescent dinuclear copper(I) complexes in solid and liquid phase** — •FLORIAN BÄPPLER<sup>1</sup>, PATRICK SINGER<sup>1</sup>, FABIAN RUPP<sup>1</sup>, FLORIAN LIEDY<sup>1</sup>, BENEDIKT BURGARD<sup>1</sup>, DANIEL VOLZ<sup>2</sup>, STEFAN BRÄSE<sup>3</sup>, and ROLF DILLER<sup>1</sup> — <sup>1</sup>Dept. of Physics, TU Kaiserslautern, 67663 Kaiserslautern, Germany — <sup>2</sup>cynora GmbH, 76646 Bruchsal, Germany — <sup>3</sup>Inst. of Organic Chemistry, KIT, 76131 Karlsruhe, Germany

Luminescent dinuclear copper complexes are very promising candidates as emitters in organic light-emitting diodes (OLEDs), as they combine high efficiencies, a widely tuneable emission maximum and low cost. However, further investigation of the primary photophysics and photochemistry is needed to fully understand important effects such as quenching mechanisms, especially in solid state. We present the first femtosecond (fs) transient reflectivity measurements on a dinuclear copper(I) complex Cu<sub>2</sub>I<sub>2</sub>MePyrPHOS[1] in solid state, under varied conditions, such as temperature and sample environment (air, vacuum), alongside with fs-transient absorption measurements in solution [2]. A comparison of the results reveals both similarities and differences between the photophysics in solid and liquid state which are critically discussed.

[1] D. Volz, D. M. Zink, T. Bocksrocker, J. Friedrichs, M. Nieger, T. Baumann, U. Lemmer, S. Bräse, *Chem. Mater.* **2013**, *25*, 3414-3426

[2] D. Imanbaev, Y. Nosenko, C. Kerner, K. Chevalier, F. Rupp, C. Riehn, W.R. Thiel, R. Diller, *Chemical Physics* **442** (2014) 53-61

MO 21.5 Thu 17:00 C/Foyer

**Excitonic spectral diffusion investigated by collinear 2D-VIS spectroscopy** — •MERLE OHLSEN, STEFFEN WOLTER, FRANZISKA FENNEL, and STEFAN LOCHBRUNNER — Institut für Physik, Universität Rostock, 18051 Rostock

Large exciton diffusion lengths are desirable for many organic optoelectronic applications like solar cells. However, the migration distance is often limited by trapping of the excitons due to energetic disorder. A model system consisting of a polymer matrix doped with the perylene bisimide dye Perylene Red has proven to be suitable to investigate the influence of energetic disorder on the mobility of the excitons since its system parameters controlling the relevant processes are well understood [1]. It was shown, that the exciton dynamics in these films are determined by dispersive energy migration on the picosecond timescale. The dynamics can be described by a model based on Förster theory that takes inhomogeneous broadening and energetic disorder of the donor and acceptor states into account [1]. To study the influence of the donor energy on the migration steps, we now focus on the dependence of the dynamics on the optical excitation frequency. To this end a newly implemented collinear 2D-VIS spectrometer based on a pulse shaper is applied. This allows for femtosecond absorption measurements with a site-selective excitation within the inhomogeneously broadened energetic distribution of the Perylene Red molecules.

[1] Fennel F., Lochbrunner, S., *Phys. Rev. B*, **85**, 094203 (2012)

MO 21.6 Thu 17:00 C/Foyer

**Channel-Resolved Electron Recollision in Polyatomic Molecules** — •JOCHEN MIKOSCH, SASCHA BIRKNER, FEDERICO FURCH, ALEXANDRIA ANDERSON, CLAUS PETER SCHULZ, and MARC J. J. VRAKING — Max-Born-Institut, Berlin, Germany

The emerging strong laser field driven spectroscopies promise to bring unprecedented time- and spatial resolution to atomic and molecular dynamics studies. It has become clear in recent years that a number of the initial simplifying assumptions, such as the adiabatic and the single-electron approximation, can break down and have to be replaced by a multi-electron picture. In particular the appearance of multiple ionization continua in Strong-Field Ionization and High Harmonic Generation of polyatomic molecules is being increasingly investigated theoretically and experimentally. Employing laser-aligned hydrocarbon molecules in a reaction microscope, we are studying how multiple strong-field ionization continua manifest themselves in electron recol-

lision, driven by the strong laser field. Electron diffraction patterns for different fragments promise to characterize ionization channel resolved continuum electron wavepackets, emerging from different Dyson orbitals. This might evolve into an ultrafast dynamical probe of electronic coherences in molecules.

MO 21.7 Thu 17:00 C/Foyer

**Realization of ultrafast time resolved spectroscopy using a Kretschmann arrangement** — ●ALIREZA MAZAHERI TEHRANI, FAEZEH MOHAGHEGH, and ARNULF MATERNY — Jacobs University, Campus Ring 1, 28759 Bremen, Germany

The interactions of molecules adsorbed on thin metal films with surface plasmon polaritons are of great importance for spectroscopic applications, such as surface enhanced Raman spectroscopy (SERS). So far, experimental SERS investigations have mostly been performed in the frequency domain using continuous wave lasers. This way, although the results are quite interesting concerning applications, they mostly fail to nicely address the underlying physical concepts and mechanism of SERS. Time-resolved experiments, however, would help us to gain a better understanding of the underlying energy transfer mechanisms between electronic systems of metal and adsorbate due to their different time scale characteristics. In order to study the interaction in a reproducible manner, we use a Kretschmann configuration setup, through which surface plasmons were excited with femtosecond laser pulses (Pump) adjusted to the ground state absorption. Dynamic information of the system, could then be probed by another time-delayed femtosecond laser pulse, which could freely be adjusted to other excited states of adsorbates or to the ground state absorption. This experiment provides us with a much deeper insight into the energy transfer mechanisms between SPPs and molecules. In our contribution, we will present and discuss the time-resolved results.

MO 21.8 Thu 17:00 C/Foyer

**Ultrafast Dynamics of Azobenzene-Polymers** — ●ELENA PAVLENKO and MATIAS BARGHEER — Potsdam University, Germany

The general mechanism of excitation and relaxation in Azobenzene molecules has been a great interest for ultrafast dynamics and now is well understood. Although this molecule was mainly investigated in the liquid phase, few experiments in polymers were reported. We investigate the structural dynamics of the Azobenzene-containing polyelectrolyte multilayer structure PAzo/PAH. The samples are prepared by layer-by-layer deposition, which allows a lateral structuring of the polymer with photoactive species on the nanometer lengthscale. Polished quartz discs are used as the substrate which are surface-modified by adsorption of a PEI layer. Multilayers of PAzo and PAH with different structures are investigated. The sample was excited from the polymer side with 400nm light ( $1.4 \text{ mJ/cm}^2$ ), in order to stimulate Azobenzene. Due to the electronic excitation, Azobenzene molecules can switch their isomerization state. This structural motion leads to a pronounced expansion of the layer on an ultrafast timescale. We analyze the hypersound-wave created by this expansion by broadband time-domain Brillouin scattering. The photoexcitation leads to a transient change of the complex refractive index. The transient absorption change due to the electronic excitation gives access to the imaginary part. The transient reflection change allows us to observe an optical contraction of the layer, which can be explained by two contributing effects: physical expansion and an even stronger reduction of the real part of the refractive index.

MO 21.9 Thu 17:00 C/Foyer

**Spectroscopic tracking of the primary visual event** — ●JONG MIN LIM, ALEX S DUARTE, GIOVANNI BASSOLINO, CHRISTOPH SCHNEIDERMANN, TORSTEN WENDE, and PHILIPP KUKURA — Physical & Theoretical Chemistry Laboratory, University of Oxford, South Parks Road, Oxford, OX1 3QZ, United Kingdom

The excited-state properties and kinetics of molecules can be extracted from ultrafast time-resolved electronic absorption or emission spectroscopy. It remains experimentally challenging, however, to obtain detailed information about the underlying structural and electronic changes immediately ( $<50 \text{ fs}$ ) after photon absorption, during which some of the most dramatic changes occur. To address these shortcomings, we have developed an ultra-sensitive transient absorption setup capable of simultaneously producing sub-10 fs pump pulses in the visible and dump pulses in the near-IR spectral region. We illustrate the benefits of such an approach by investigating the 11-cis to all-trans photoisomerization of rhodopsin and its chromophore in solution. We track transient absorption signal changes at long time-delays in the

photoproduct spectral region as a function of pump-dump delay. Such measurements do not suffer from coherent artifact contributions commonly encountered in transient absorption and allow us to obtain critical information about the earliest dynamics of the system.

MO 21.10 Thu 17:00 C/Foyer

**Single Molecule Localisation Microscopy of the Distribution of Chromatin Nanostructures Using Hoechst and Dapi Fluorescent Probes** — ●UDO BIRK<sup>1,2,3</sup>, ALEKSANDER SZCZUREK<sup>1</sup>, KIRTI PRAKASH<sup>1</sup>, HYUN-KEUN LEE<sup>1,3</sup>, DOMINIKA ZUREK-BIESIADA<sup>4</sup>, GERIT BEST<sup>2</sup>, MARTIN HAGMANN<sup>2</sup>, JUREK DOBRUCKI<sup>4</sup>, and CHRISTOPH CREMER<sup>1,2,3</sup> — <sup>1</sup>Institute of Molecular Biology, Mainz, Germany — <sup>2</sup>Heidelberg University, Germany — <sup>3</sup>Institut für Physik, Mainz University, Germany — <sup>4</sup>Jagiellonian University, Kraków, Poland

We present a Single Molecule Localization Microscopy application of specific fluorescent DNA dyes such as DAPI, Hoechst and others, in order to obtain chromatin/nuclear DNA density maps with high optical and structural resolution. The approach adopted here is based on photoconversion to the green-emitting form of these dyes that later may undergo a process of switching under high intensity blue light. In mammalian cell nuclei, this technique yielded a single molecule localization precision in the order of 15 - 30 nm, corresponding to an optical (two-point) resolution of roughly 40 - 70 nm. We investigated various DNA structures and obtained data with a DNA-bound fluorophore density as high as 5000 SM/micrometer<sup>2</sup>, significantly higher than previously reported.

[1] A. Szczurek et al. Nucleus 2014.

MO 21.11 Thu 17:00 C/Foyer

**Ion molecule reaction dynamics of two center hydrocarbons** — EDUARDO CARRASCOSA<sup>1</sup>, ●JENNIFER MEYER<sup>1</sup>, FREDRIK LINDÉN<sup>2</sup>, MARTIN STEI<sup>1</sup>, MARTIN BAWART<sup>1</sup>, FABIO CARELLI<sup>1</sup>, WOLF DIETRICH GEPPERT<sup>2</sup>, and ROLAND WESTER<sup>1</sup> — <sup>1</sup>Institute for Ion Physics and Applied Physics, University of Innsbruck, 6020 Innsbruck, Austria — <sup>2</sup>Department of Physics, Stockholm University, Stockholm, Sweden

We present recent results on the studies of the bimolecular substitution ( $S_N2$ ) reactions of halogenated hydrocarbons. These reactions feature rich dynamics and product distributions [1]. The reaction dynamics were recorded with our crossed beam velocity map imaging (VMI) spectrometer [2]. The studied model systems include the reactions of fluoride anions  $F^-$  with methylchloride  $CH_3Cl$  which allows us to study the effect which the leaving group has on the reaction dynamics and product distribution. Moreover using  $CN^-$  as a nucleophile, we are able to study of isomer selective reaction channels. In the future, the ongoing work on the  $S_N2$  reactions of methylhalides will be extended to ethylhalide molecules. If the carbon chain is extended, the substitution reaction  $S_N2$  will be in competition with the elimination reaction E2. The dynamics and energy dependence of this competition of  $S_N2$  and E2 will be studied.

[1] J. Xie, R. Otto, J. Mikosch, J. Zhang, R. Wester, W. L. Hase, Acc. Chem. Res., 47, 2960 (2014) [2] R. Wester, PCCP, 16, 396 (2014)

MO 21.12 Thu 17:00 C/Foyer

**Signatures of Interatomic-Coulombic-Decay in electron-impact ionization of argon dimers** — ●THOMAS PFLÜGER<sup>1</sup>, XUEGUANG REN<sup>1</sup>, and ALEXANDER DORN<sup>2</sup> — <sup>1</sup>Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig — <sup>2</sup>Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg

After decades of investigation of the ionization dynamics of simple atoms and molecules in electron collision experiments, in recent years significant progress was being made. The investigation of small rare gas clusters presents a unique opportunity in atomic physics. In a sense they can be thought of as bridging the gap between sole constituents and macroscopic matter, while still being simple enough to be understood on a particle level. For example, interesting processes were discovered in dimers such as Interatomic-Coulombic-Decay (ICD), which have been found to occur on very short time scales with a high efficiency compared to other possible pathways.

We find signatures of ICD in the triply-charged final-state of  $Ar_2$ , as well as an interesting structure in the kinetic-energy-release spectrum of the doubly-charged final-state of  $Ar_2$  pointing towards two separate mechanisms: a fast and a delayed one. Furthermore, a significant amount of data for the dissociation of  $Ar_3^+ \rightarrow Ar_2^+ + Ar^+$  could be retrieved.

Electronic as well as ionic energy spectra and angular distributions

will be presented.

MO 21.13 Thu 17:00 C/Foyer

**High resolution spectroscopy on LiSr** — ●ERIK SCHWANKE<sup>1</sup>, ASEN PASHOV<sup>2</sup>, ALEXANDER STEIN<sup>1</sup>, HORST KNÖCKEL<sup>1</sup>, and EBERHARD TIEMANN<sup>1</sup> — <sup>1</sup>QUEST und Inst. f. Quantenoptik, Leibniz Universität Hannover — <sup>2</sup>Department of Physics, Sofia University, Sofia, Bulgaria

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 atomic combinations like LiCa, LiSr or RbSr by various groups, reflecting the high interest by experimentalists. Experimentally, not so much is known about molecular electronic states. Up to now the ground state and two electronically excited states of LiCa and few states of LiBa have been characterised. We have successfully recorded the near infrared spectrum of LiSr. The molecules were created in a three section-heattube with different temperatures, this way accounting for the different vapour pressures. The thermal emission was dispersed by a high resolution Fourier transform spectrometer. The assignment of the dense spectrum was made possible by shining a diode laser tuned to a molecular line into the sample. This approach allowed to find and assign those transitions connected with the laser excitation. A first assignment of lines will allow predictions for further measurements. We will report the status of the investigations.

MO 21.14 Thu 17:00 C/Foyer

**Towards THz + IR action spectroscopy of charged water clusters in a cryogenic multipole ion trap** — ●STEFFEN SPIELER, SUNIL KUMAR, SEUNGHYUN LEE, ERIC ENDRES, DANIEL HAUSER, OLGA LAKHMANSKAYA, TIM MICHAELSEN, and ROLAND WESTER — Institute for Ion Physics and Applied Physics, University of Innsbruck, 6020 Innsbruck, Austria

Driving rovibrational transitions by continuous THz radiation in size selected and cryogenically cooled water clusters or macromolecules is a promising approach to unravel the structure and dynamics of weakly bound systems. It will allow to investigate long range interactions that are of fundamental interest for physics, chemistry and in life science. For experiments on intramolecular vibrational relaxation of biomolecules upon UV excitation or rotational transitions in  $OH^-(H_2O)_n$  and  $H_3O^+(H_2O)_n$  a THz radiation source based on difference frequency mixing of two near infrared diode lasers was set up as well as a versatile ion trap based experiment including an electrospray ion source, which can be used to generate intact macromolecular ions (positive/negative) in gas-phase. Ions generated in the electrospray ion source are focused and guided by means of an ion funnel and a quadrupole ion guide. Further more, the ions are mass selected by a quadrupole mass filter and loaded into a 16-pole radiofrequency ion trap. Benchmark THz action spectroscopy experiments on cold hydroxyl anions were performed, proving the applicability of difference frequency mixing based terahertz spectroscopy in an ion trap.

MO 21.15 Thu 17:00 C/Foyer

**Towards Imaging of cold Penning-Reactions using a Li-MOT** — ●JONAS GRZESIAK, HANNA MAIER, FRANK STIENKEMEIER, and MARCEL MUDRICH — Physikalisches Institut, Uni Freiburg, Hermann-Herder-Str 3, 79104 Freiburg i.Br.

Recent developments in merged beams have shed new light on cold reactive scattering.[1] Our setup for elastic scattering of cold molecular beam atoms originating from a rotating nozzle and Li-atoms in a MOT is extended for reactive scattering. To this end a supersonic and cryogenic pulsed nozzle with a home-made dielectric barrier discharge has been constructed which provides an intense and cold beam of metastable atoms. We show first results on cold penning reactions of the pulsed beam atoms with the rotating nozzle beam atoms, as well as reactions between ultracold Li-atoms originating from the MOT and the pulsed beam atoms. In prospect of imaging the reaction kinematics the use of an ion imaging detector is discussed.

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

MO 21.16 Thu 17:00 C/Foyer

**Fabrication of Microstructures by Optical Lithography for Electric Trapping of Polar Molecules** — ●MARTIN IBRÜGGER,

MARKUS KROTTENMÜLLER, ALEXANDER PREHN, ROSA GLÖCKNER, MARTIN ZEPPENFELD, and GERHARD REMPE — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748

Polar molecules cooled to cold and ultracold temperatures offer a wide range of exciting applications ranging from quantum simulation to controlled chemistry. For such experiments, providing a suitable environment to confine the molecules is often essential. For this purpose, a unique design for an electric trap based on confining molecules between a pair of microstructured capacitor plates [1] has allowed us to achieve record-long trap lifetimes [2] and to cool the molecules' motional and rotational degrees of freedom [3,4].

To further improve the properties of our trap, we are currently investigating the in-house fabrication of the trap microstructures based on well-known optical lithography techniques combined with chemical wet etching. Here, we in particular aim for a good high voltage performance combined with minimal surface charges. We present details of our fabrication method as well as the results from high voltage tests.

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

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

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

[4] R. Glöckner *et al.*, *submitted* (2015).

MO 21.17 Thu 17:00 C/Foyer

**Manipulating the motion of neutral polar molecules with microwave fields** — ●SIMON MERZ<sup>1</sup>, JACK B. GRANEK<sup>1</sup>, NICOLAS VANHAECKE<sup>2</sup>, GERARD MEIJER<sup>2,3</sup>, and MELANIE SCHNELL<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Struktur und Dynamik der Materie am Center for Free-Electron Laser Science, D-22761 Hamburg — <sup>2</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin — <sup>3</sup>Institut für Moleküle und Materialien at the Radboud University Nijmegen, NL-6525 AJ Nijmegen

An important remaining challenge in the field of cold molecules is a widely applicable method to manipulate the motion of neutral polar molecules in high-field-seeking states. This is a crucial step towards control of cold molecules in their ground states and of large and more complex molecules. As an alternative to the already demonstrated but discontinued alternating gradient methods, we use the interaction of polar molecules with cavity-enhanced microwave fields. Cylindrical microwave resonators provide transverse-electric field modes that are ideally suited for deceleration experiments [1-3].

Here, we present the latest results of our microwave deceleration experiments [3], using pre-decelerated packets of ammonia molecules and show first steps towards motion control of a beam of cold 4-aminobenzonitrile molecules.

[1] H. Odashima *et al.*, *Phys. Rev. Lett.* **104**:253001 (2010).

[2] S. Merz, *et al.*, *Phys. Rev. A.* **85**:063411 (2012).

[3] S. Merz, *et al.*, *Mol. Phys.* **111**:1855-1864 (2013).

MO 21.18 Thu 17:00 C/Foyer

**Dynamics of  $H_2^+$  in intense laser fields: Full-dimensional approximate quantum-mechanical description of dissociation and ionization** — ●TOBIAS FIEDLSCHUSTER, JAN HANDT, FRANK GROSSMANN, and RÜDIGER SCHMIDT — Technische Universität Dresden

So far, even for nature's simplest molecule  $H_2^+$ , no exact quantum-mechanical description of the laser-induced dynamics (i. e., simultaneously including vibration, rotation, dissociation and ionization) has been achieved.

In this work, we present a full-dimensional approximate quantum-mechanical treatment. It is based on the extension of a recently developed ab-initio Born-Oppenheimer surface hopping approach (M. Fischer, J. Handt and R. Schmidt, *Phys.Rev. A* **90**, 012525 (2014), *ibid* 012526, *ibid* 012527) to hopping between Floquet surfaces.

The obtained results for dissociation and ionization are in very good agreement with recent experimental data (J. McKenna *et al.*, *Phys. Rev. A* **85**, 023405 (2012)).

The extension of the method to many-electron molecules is discussed.

MO 21.19 Thu 17:00 C/Foyer

**Simulating 3D flexible Rydberg aggregates with surface hopping** — ●KARSTEN LEONHARDT, SEBASTIAN WÜSTER, and JAN MICHAEL ROST — Max Planck Institute for the Physics of Complex Systems

Flexible Rydberg aggregates [1] are assemblies of highly excited light atoms, which are set into directed motion by resonant dipole-dipole

interaction [1-4]. They provide a clean platform to study phenomena such as entanglement transport [2,3] and coherent splitting of excitons [4]. Very useful for the simulation of these systems is the surface hopping algorithm (FSSH) [5]. Nevertheless, to study these aggregates in 3D [TALK: A 270], a modification of the FSSH algorithm is needed, which we present here together with recent results of flexible Rydberg aggregates.

#### References

- [1] C. Ates, A. Eisfeld, J. M. Rost, *New. J. Phys.* **10**, 045030 (2008).
- [2] S. Wüster, C. Ates, A. Eisfeld, J. M. Rost, *Phys. Rev. Lett.* **105**, 195392 (2010).
- [3] S. Möbius, S. Wüster, C. Ates, A. Eisfeld, J. M. Rost, *J. Phys. B.* **44**, 184011 (2011).
- [4] K. Leonhardt, S. Wüster, J. M. Rost, *Phys. Rev. Lett.* **113**, 223001 (2014).
- [5] J. C. Tully, *J. Chem. Phys.* **93**, 1061 (1990).

MO 21.20 Thu 17:00 C/Foyer

**Novel setup for a laser-based terahertz-field-driven extreme ultraviolet streak camera allowing for time resolved measurements of the full angle and kinetic energy distribution of electrons** — ●MARTIN RANKE, FAWAD KARIMI, MARKUS PFAU, THOMAS GEBERT, and ULRIKE FRÜHLING — Institut für Experimentalphysik, Luruper Chaussee 149, 22761 Hamburg, Deutschland

In this work, a novel setup of a terahertz (THz) -field-driven extreme ultraviolet (XUV) streak camera for studying femtosecond dynamics in atoms and molecules is presented. High-harmonic generated XUV-pulses are synchronized and superimposed with intense single-cycle THz pulses in a gas target. The XUV pulses are used to excite and ionize atoms or molecules. The resulting electrons are accelerated by the electric THz field which directly relates the change of the momentum to the THz vector potential. The kinetic energies of the electrons are measured fully angle resolved by a new velocity map imaging (VMI) spectrometer. The intense THz pulses are generated with a tilted pulse front setup of near infrared laser pulses by means of optical rectification in a nonlinear crystal.

MO 21.21 Thu 17:00 C/Foyer

**Optimized focusing injector for single-particle coherent diffractive x-ray imaging** — ●NILS ROTH<sup>1,2</sup>, DANIEL HORKE<sup>1</sup>, and JOCHEN KÜPPER<sup>1,2,3</sup> — <sup>1</sup>Center for Free-Electron Laser Science,

DESY — <sup>2</sup>Department of Physics, University of Hamburg — <sup>3</sup>Center for Ultrafast Imaging, University of Hamburg

Single-particle coherent diffractive imaging requires reproducible particles to build up a 3D molecular image [1]. Current experiments are limited by the inefficient delivery of particles and correspondingly low hit-rates, i.e., poor usage of sample and x-ray photons. We are developing a controllable and efficient vaporization and aerodynamic lens [2] system to provide tightly focused beams of nanoparticles and biological systems, which will efficiently be guided to the interaction point. Here, we present detailed numerical simulations, as well as experimental characterization, of such an aerodynamic lens system. In the future this will be combined with optical manipulation and guiding [3]. The increased hit-rate achieved in such a setup will make "molecular-movie" experiments possible.

- [1]Barty *et al*, *Annu. Rev. Phys. Chem.* **64** 415-435
- [2]Lui *et al*, *Aerosol Sci. Technol.* **22** 293-313
- [3]Eckerskorn *et al*, *Opt. Exp.* **21** 30492-30499

MO 21.22 Thu 17:00 C/Foyer

**Lamb-Dip rotational spectroscopy of OCS in the mm-wave region** — ●OLIVER ZINGSHEIM<sup>1</sup>, JAKOB MASSEN<sup>1</sup>, SVEN THORWIRTH<sup>1</sup>, FRANK LEWEN<sup>1</sup>, MARIE-ALINE MARTIN-DRUMEL<sup>1,2</sup>, and STEPHAN SCHLEMMER<sup>1</sup> — <sup>1</sup>I. Physikalisches Institut, Köln, Germany — <sup>2</sup>Harvard-Smithsonian Center for Astrophysics, Cambridge, USA

Carbonyl sulfide (OCS) is a widespread and important molecule in the interstellar medium (ref [1] and references therein). Because of its astronomical relevance and also its importance as a calibration gas in the laboratory the pure rotational spectrum is comparably well studied in particular that of the parent isotopic species (see, for example, ref [2]). Here, we report on high precision Lamb-Dip measurements of rare isotopic species in the frequency range from 75 to 370 GHz. The measurements were performed in a 5m absorption cell with a roof-top mirror to allow for double pass of the mm wave radiation. Transitions of singly substituted isotopologues were measured (<sup>13</sup>C, <sup>17</sup>O, <sup>18</sup>O, <sup>33</sup>S, <sup>34</sup>S) resulting in new significantly improved sets of molecular parameters. Further Lamb-Dip measurements of transient molecules will be performed in the near future.

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