

MO 4: Cold Molecules & Helium Droplets 1

Time: Monday 14:30–16:00

Location: f142

MO 4.1 Mon 14:30 f142

Optimized-focusing injector for single-particle coherent diffractive x-ray imaging — •NILS ROTH^{1,3}, TIM OSSENBRÜGGEN¹, BERND LIENAU³, DANIEL HORKE^{1,2}, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science, DESY, Hamburg, Germany — ²The Hamburg Center for Ultrafast Imaging, University of Hamburg, Germany — ³Department of Physics, University of Hamburg, Germany

Atomic resolution 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 particle injectors. Using in-vacuum microscopes and light scattering we are able to determine the size of the produced particle beam. The distribution of gas from nozzles and particle injectors is studied quantitatively using plasma-formation imaging. This yields an accurate pressure-distribution map, important for benchmarking simulations. The increased hit-rate achieved in such a setup will make "molecular-movie" experiments more likely.

[1] Barty et al., *Annu. Rev. Phys. Chem.* **64** 415-435 (2013),

[2] Lui et al., *Aerosol Sci. Technol.* **22** 293-313 (1995a)

MO 4.2 Mon 14:45 f142

Diffractive imaging of aligned gas-phase molecules — •THOMAS KIERSPEL^{1,2}, FENGLIN WANG^{1,3}, and JOCHEN KÜPPER^{1,2,4} — ¹Center for Free-Electron Laser Science, DESY, Hamburg, Germany — ²The Hamburg Center for Ultrafast Imaging, University of Hamburg, Germany — ³PULSE Institute, Stanford University, Stanford, California, USA — ⁴Department of Physics, University of Hamburg, Germany

Diffractive imaging of aligned and oriented molecules in the gas phase is a promising tool to unravel ultrafast molecular dynamics [1,2], such as internal rearrangement processes or photofragmentation. We present an experimental approach to strongly align molecules at full repetition rate of free-electron lasers [3]. The molecules were non-adiabatically aligned with a chirped laser pulses (pulse duration 94 ps) provided by the available in-house Ti:Sapphire laser system at the Coherent X-ray Imaging (CXI) beamline at the Linac Coherent Light Source (LCLS). We report on the current status of the photon data analysis and discuss prospects for future experiments. This work was carried out in a collaboration with the spokespersons F. Wang, J. Küpper, P. Bucksbaum, and H. Chapman. The collaboration consists of CFEL, PULSE, LCLS, European XFEL, Aarhus University, Kansas State University, Stanford University, and Uppsala University. Use of the LCLS, SLAC national accelerator laboratory, is supported by the US Department of Energy, Office of Science, and Office of Basic Energy Sciences.

[1] *Phys. Rev. Lett.* **112**(8), 083002 (2014) [2] *Ann. Rev. Phys. Chem.*, **64**(1), 415-435 (2013) [3] *J. Phys. B.* **48**(20), 204002 (2015)

MO 4.3 Mon 15:00 f142

X-ray photophysics of gas-phase molecules and clusters — •THOMAS KIERSPEL^{1,2}, SEBASTIAN TRIPPEL¹, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science, DESY, Hamburg, Germany — ²The Hamburg Center for Ultrafast Imaging, University of Hamburg, Germany — ³Department of Physics, University of Hamburg, Germany

Properties of atoms and molecules strongly dependent on their environment. Hydrogen bonds are of universal importance in chemistry and biochemistry and it is, therefore, highly desirable to bridge the gap between isolated and solvated molecules.

We present photophysics and charge redistribution on indole, the chromophore of the amino acid tryptophan, and separated indole-water₁ clusters [1], i.e., indole 'solvated' by a single water molecule, upon side-specific 1s ionization of indole's N atom. The species were spatially separated by the use of strong inhomogeneously electric fields prior the interaction zone. Photoelectrons and ionic fragments were recorded in coincidence with a double-sided velocity map imaging (VMI) spec-

trometer. Indications for charge and proton or hydrogen transfer were observed. Results will be discussed based on the fragmentation channels of the different species and the 3D reconstruction of the molecule's orientation.

This work was carried out in a collaboration with DESY and Kansas State University. The experiment was conducted at the Variable Polarization XUV Beamline P04 of PETRA III at DESY.

[1] Trippel et al., *Phys. Rev. A.* **86**, 033202 (2012)

MO 4.4 Mon 15:15 f142

Internal-state thermometry of cold polyatomic molecules — •XING WU, THOMAS GANTNER, SOTIR CHERVENKOV, MARTIN ZEPPENFELD, and GERHARD REMPE — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany

We present a new method for internal-state thermometry of guided polyatomic molecules. Bright beams of polar molecules are produced by a cryogenic buffer-gas cell and extracted by electrostatic guiding [1]. Their rotational-state distribution is probed via RF-resonant depletion spectroscopy. With the help of a complete trajectory simulation, resolving the guiding efficiency for all the thermally populated states, we are able to determine the internal temperature in the buffer-gas cell based on the RF depletion spectroscopy. This thermometry method is demonstrated for various regimes of buffer-gas cooling, beam formation, and for molecular species of different sizes, e.g., CH₃F and CF₃CCH. The results provide strong evidence that the collisional relaxation rate for rotational degrees of freedom is larger than for motional ones. In addition, the relaxation rates for states with different *K*-quantum number appear to be different.

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

MO 4.5 Mon 15:30 f142

Direct cooling of polar molecules to sub-millikelvin temperatures — •ALEXANDER PREHN, MARTIN IBRÜGGER, ROSA GLÖCKNER, MARTIN ZEPPENFELD, and GERHARD REMPE — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching

Applications of ultracold ($T < 1$ mK) polar molecules including ultracold chemistry, quantum simulation, and high-precision spectroscopy exploit the rich internal level structure and the electric dipole moment of the molecules. The desired use of chemically diverse species requires development of direct cooling methods. However, a versatile technique to cool molecules to the ultracold regime has been lacking.

Here, we present direct cooling of formaldehyde (H₂CO) to the microkelvin regime [1]. Our approach, optoelectrical Sisyphus cooling, which was first demonstrated with methyl fluoride (CH₃F) [2], provides a simple dissipative cooling method applicable to a variety of electrically trapped dipolar molecules. By reducing the temperature by three orders of magnitude and increasing the phase-space density by a factor of $\sim 10^4$ we generate an ensemble of about $3 \cdot 10^5$ molecules with a temperature of about 420 μ K. In addition to producing a record-large ensemble of ultracold molecules, we have good control over the internal molecular state: the molecules in the prepared ensemble populate a single rotational state with more than 80% purity.

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

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

MO 4.6 Mon 15:45 f142

Feasibility of microwave manipulation and Stark deceleration of polyatomic asymmetric molecules — •JACK B. GRANEK¹, SIMON MERZ¹, DAVID PATTERSON², THOMAS BETZ¹, and MELANIE SCHNELL¹ — ¹Max-Planck-Institut für Struktur und Dynamik der Materie, Luruper Chaussee 149, 22761 Hamburg, Germany — ²Harvard University, Department of Physics, Cambridge, USA

Motion manipulation of large molecules or ground-state molecules requires methods that are compatible with high-field-seeking states. In inhomogeneous fields, molecules in high-field-seeking states experience a force towards the field maxima. However, true 3D field maxima cannot be realized in free space with static fields alone so time-dependent fields are required. In previous experiments, focusing and deceleration of ammonia molecules was achieved [1]. Ammonia was considered, to a good approximation, an isolated two-level system. We have performed numerical calculations to predict and develop microwave manipula-

tion experiments for polyatomic asymmetric molecules. This approach goes beyond the two-level approximation often employed for simpler molecules, e.g. NH_3 and acetonitrile [2], and is more broadly applicable. Trajectory simulations were carried out to predict microwave focusing measurements using a cylindrically symmetric microwave res-

onator. We also explore the potential for the Stark deceleration of specific rotational states of similarly complex systems that are low-field seeking up to a certain electric field strength.

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

[2] S. Spieler *et al.*, Mol. Phys. **111**, 1823–1834 (2013).