

## MO 1: Cold Molecules 1

Time: Monday 10:30–12:30

Location: BEBEL HS213

## Invited Talk

MO 1.1 Mon 10:30 BEBEL HS213

**Strongly driven quantum pendulum of a polar molecule**

— ●SEBASTIAN TRIPPEL<sup>1</sup>, TERENCE G. MULLINS<sup>1</sup>, NELE L.M. MÜLLER<sup>1</sup>, JENS S. KIENITZ<sup>1,2</sup>, ROSARIO GONZÁLEZ-FÉREZ<sup>4</sup>, and JOCHEN KÜPPER<sup>1,2,3</sup> — <sup>1</sup>Center for Free-Electron Laser Science, DESY, Hamburg — <sup>2</sup>Center for Ultrafast Imaging, University of Hamburg — <sup>3</sup>Department of Physics, University of Hamburg — <sup>4</sup>Instituto Carlos I de Física Teórica y Computacional and Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, Spain

The behavior of molecules subject to strong laser fields has been a rapidly growing topic in molecular physics and chemistry during the last years. The anisotropic interaction between an isolated molecule and a nonresonant, linearly polarized laser field creates pendular states, i. e., directional superpositions of field-free rotational states [1]. We disentangled the rotational and pendular state wavepacket dynamics of quantum state selected carbonyl sulfide (OCS) molecules. A strong oscillation on the degree of alignment is observed that resembles the motion of a classical pendulum. Features in the transition from impulsive, non-adiabatic to adiabatic alignment and orientation were disentangled, with implications on the switching behavior of fast molecular switches in non dissipative media. In addition, we demonstrated how the combination of quantum state selection and rotational coherence spectroscopy allows for a complete measurement of magnitude and polarization of angular momenta of molecules in field-free space.

[1] B. Friedrich and D. Herschbach, *Phys. Rev. Lett.* **74**, 4623 (1995)

MO 1.2 Mon 11:00 BEBEL HS213

**Superfluid Helium Solvation Effects on Hydrogen Bonded Molecules**

— ●LUKASZ WALEWSKI, HARALD FORBERT, and DOMINIK MARX — Ruhr-Universität Bochum, Bochum, Deutschland

Atomic nuclei become delocalized at low temperatures as a result of quantum effects. For non-interacting atoms the magnitude of this effect increases upon lowering the temperature according to the thermal de Broglie wavelength of free particles. However, strong interactions due to chemical bonding that set in for atoms bound in molecules, counteract this tendency resulting in the, so called, “interaction induced localization”. This effect turns out to be extremely pronounced at ultra-low temperatures of about 1 K, characteristic to superfluid helium nanodroplets. The most affected are protons shared in hydrogen bonds [1], which are confined to a spatial region that corresponds to about 0.1% of the volume occupied by a non-interacting proton at the same temperature. Moreover, applying our recently developed hybrid *ab initio* MD / bosonic MC path integral method [2] to an HCl/water cluster, HCl(H<sub>2</sub>O)<sub>4</sub>, we find that helium solvation has a significant additional localizing effect. In particular, the solvent-induced excess localization is the stronger the lesser the given nucleus is already localized in the gas phase reference situation [3].

[1] Walewski, L.; Forbert, H.; Marx, D. *Mol. Phys.*, **2013**, *111*, 2555.

[2] Walewski, L.; Forbert, H.; Marx, D. *Comp. Phys. Comm.* (accepted).

[3] Walewski, L.; Forbert, H.; Marx, D. *J. Chem. Phys.* (submitted).

MO 1.3 Mon 11:15 BEBEL HS213

**Electron gun for diffraction experiments of controlled gas-phase molecules**

— ●NELE L. M. MÜLLER<sup>1</sup>, SEBASTIAN TRIPPEL<sup>1</sup>, TERENCE G. MULLINS<sup>1</sup>, JENS S. KIENITZ<sup>1,2</sup>, KAROL DŁUGOLECKI<sup>1</sup>, and JOCHEN KÜPPER<sup>1,2,3</sup> — <sup>1</sup>Center for Free-Electron Laser Science, DESY, Hamburg — <sup>2</sup>The Hamburg Center for Ultrafast Imaging, Hamburg — <sup>3</sup>Department of Physics, University of Hamburg

The aim of the presented work is to investigate the structure and dynamics of molecules in the gas-phase. Time-resolved structural information can be gained through various techniques, for example, by electron diffraction experiments. This contribution presents our newly set-up electron gun that will be combined with an existing controlled-molecules apparatus. The gas-phase molecules are prepared in cold, supersonic beams and can be size, isomer, and quantum state selected by means of electric deflection. These samples are then strongly laser aligned by intense picosecond laser pulses and serve as a well-defined sample for electron diffraction experiments. Controlling the molecules' state and spatial orientation increases the amount of information contained in electron diffraction patterns.

The developed electron gun and first experiments will be presented.

MO 1.4 Mon 11:30 BEBEL HS213

**Optimal Control of Vibrational Cooling**

— ●DANIEL REICH and CHRISTIANE KOCH — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

Laser cooling of a molecule's internal degrees of freedom employing broadband optical pumping involves a timescale separation between laser excitation and spontaneous emission. Current approaches fail if the Franck-Condon map governing the optical transitions is preferential to heating rather than cooling. We show that by using optimal control theory to derive shaped pulses for the optical pumping step this issue can be circumvented entirely. To achieve this we have designed two different cooling schemes and corresponding optimisation functionals [1]. The optimised pulses drive population into those excited state levels that have the largest spontaneous emission rates to the target state while accumulating population in the ground state and keeping the cooling cycle loss-free. Our optimisation functionals are also applicable to the laser cooling of other degrees of freedom provided the cooling cycle consists of coherent excitation and dissipative deexcitation steps whose timescales are separated.

[1] D.M. Reich and C.P. Koch, *New J. Phys.* (to be published)

MO 1.5 Mon 11:45 BEBEL HS213

**Cryogenic buffer-gas cooling: comparison of two different regimes**

— ●XING WU, THOMAS GANTNER, SOTIR CHERVENKOV, MARTIN ZEPPENFELD, and GERHARD REMPE — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany

Cryogenic buffer-gas cooling is a promising method for producing bright beams of cold polar molecules [1] for low-temperature collision experiments, chemical reactions, and precision measurements. In combination with the electrostatic guiding technique [2], high-intensity beams of slow and low-field-seeking molecules can be extracted and delivered to further experiments. To optimize the flux of the guided beam, we investigate the performance of buffer-gas cooling in two different regimes, the effusive and the supersonic one. In the effusive regime, molecules with a low peak velocity and a high flux are obtained after the electric guiding. The velocity spread in this case corresponds to the temperature of the cryogenic cell. In the supersonic regime, molecules move at faster forward velocities, but are further cooled in the co-moving frame because of the adiabatic expansion. The output efficiency of the buffer-gas cell is also increased due to the hydrodynamic enhancement. However, the electric guiding of the supersonic beams has only limited performance, most likely because of collisions happening at the entrance of the electric guide, due to the large densities of both buffer gas and molecules in the forward beam.

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

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

MO 1.6 Mon 12:00 BEBEL HS213

**Deceleration of SrF molecules in a traveling wave Stark decelerator**

— ●JOOST E. VAN DEN BERG<sup>1</sup>, SREEKANTH MATHAVAN<sup>1</sup>, CORINE MEINEMA<sup>1</sup>, JANKO NAUTA<sup>1</sup>, KLAUS JUNGSMANN<sup>1</sup>, HENDRICK L. BETHLEM<sup>2</sup>, and STEVEN HOEKSTRA<sup>1</sup> — <sup>1</sup>University of Groningen, Groningen, The Netherlands — <sup>2</sup>LaserLab, Department of Physics and Astronomy, VU University Amsterdam, The Netherlands

We present the first results on the deceleration of SrF molecules in a traveling wave Stark decelerator. Traditional Stark decelerators suffer from overfocusing, leading to losses. This makes it very inefficient to use such a device for the deceleration of heavy diatomics, such as SrF. A long traveling wave decelerator, which is inherently stable, is therefore built in our lab. Using arbitrary waveform generators and high voltage amplifiers we can create true 3D moving electric traps inside the decelerator. After deceleration, we will laser cool the molecules to prepare them for a parity violation measurement. We report the status of the experiment and the possibilities of using different waveforms to optimize the deceleration process.

MO 1.7 Mon 12:15 BEBEL HS213

**Shedding Far-off Resonant Light on Polar Paramagnetic Molecules**

— ●KETAN SHARMA and BRETISLAV FRIEDRICH — Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin, Germany

Interactions with external electric, magnetic or optical fields provide

the chief means to manipulate the rotational and translational motion of neutral gas-phase molecules. All such methods rely on the ability to create directional states of molecules as only in said states are the molecular body-fixed multipole moments available in the laboratory frame. A far-off resonant optical field hybridizes and aligns the rotational states of an anisotropic molecule. These states occur as tunneling doublets of opposite parity and are quasi-degenerate at high optical field intensities. For polar molecules, these states can be efficiently coupled either by the electric dipole interaction with a superimposed electrostatic field or by the electric dipole-dipole interaction

arising between a pair of polar molecules. Thus, a weak static electric field can orient such molecules projecting up to 90% of the dipole moment on the static field direction. For polar paramagnetic molecules, a superimposed magnetic field causes a further parity-conserving hybridization of the molecule's rotational states, doubling the number of the tunneling doublets by removing the degeneracy arising due to the sign of projection of angular momentum on the collinear field axis. The triple field-combination offers a high efficiency and flexibility in amplifying molecular orientation.