Q 4: Cold Molecules (joint session MO/Q)

Time: Monday 11:00–13:00 Location: F102

Q 4.1 Mon 11:00 F102

A Continuous Source of Aluminium Monofluoride Molecules — •Maximilian Doppelbauer[1], Sidney C. Wright[1], Simon Hofsäss[1], José Eduardo Padilla-Castillo[1], Sebastian Kray[1], Russell Thomas[1], Boris Sartakov[1], Stefan Truppe[1,2], and Gerard Meijer[1] — [1]Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Centre for Cold Matter, Blackett Laboratory, Imperial College London, Prince Consort Road, London SW7 2AZ, United Kingdom

The aluminium monofluoride (AlF) molecule is a unique candidate for laser cooling and trapping experiments. As a starting point, we require a high-density molecular source. In our original setup, we can generate AlF by reaction of laser-ablated aluminium atoms with NF_3 in a pulsed cryogenic buffer gas source with more than 10^{12} molecules per steradian per ablation shot. By exploiting the reaction of AlF_3 and Al in a UHV oven above 600°C, we can generate a continuous thermal AlF beam with a total brightness of about 10^{16} molecules per steradian per second.

In this contribution, we present spectroscopic information on vibrational levels up to $v'' = 4$ and rotational levels to above $J'' = 80$ in the $X^1\Sigma^+$ electronic ground state that we obtained using the oven source as well as first experiments laser cooling AlF.

Q 4.2 Mon 11:15 F102

Cryo-cooled beams of "small" macromolecules — •Jingxuan He[1,2,3], Lena Worbs[1,2], Surya Kiran Peravali[1,4], Armando D. Estillore[1], Amit K. Samanta[1,3], and Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Department of Physics, Universität Hamburg, Germany — [3]Center for Ultrafast Imaging, Universität Hamburg, Germany — [4]Fakultät für Maschinenbau, Helmut-Schmidt-Universität,Germany

We have demonstrated the preparation of cold and controlled dense beams of nanoparticles and macromolecules designed for x-ray single-particle diffractive imaging (SPI). We exploit buffer-gas cell cooling and aerodynamic focusing techniques [1-2]. We are extending the cooling and control techniques developed for SPI to experimental investigations of ultrafast electron dynamics in complex biomolecules. We aim at disentangling charge and energy transfer following electronic excitation, which still has important open questions [3].

Here, we present our approach to prepare appropriate samples of cryogenically-cooled proteins to study these also biologically important elemantary processes, for instance, using photofragmentation mass spectrometry and velocity map imaging.

[1]A. K. Samanta, et al., *Structural dynamics* **7** , 024304 (2020)
[2]L. Worbs, et al., *In preparation*, (2022)
[3]H. Duan, et al., *PNAS* **114** , 8493 (2017)

Q 4.3 Mon 11:30 F102

Zeeman slowing of CaF — •Mariia Stepanova, Timo Poll, Paul Kaebert, Supeng Xu, Mirco Siercke, and Silke Ospelkaus — Institut für Quantenoptik, Leibniz Universität Hannover

Our Zeeman slowing scheme for laser-cooling of molecules with favorable Franck-Condon factors promises a substantial increase in molecular number in the velocity range of under 20 m/s, which is required for loading a Magneto-Optical Trap (MOT). The scheme stands out in its ability to not only lower the initial mean velocity of the molecular beam, but also to compress the velocity distribution in a continuous fashion. In this talk, we will present our most recent status on the experiment to achieve the goal of slowing and cooling CaF molecules generated from a buffer gas cell source, followed by our efforts to implement a dual-frequency MOT without sub-Doppler heating, discussed in [1].

[1] S. Xu, P. Kaebert, M. Stepanova, T. Poll, M. Siercke and S. Ospelkaus, DOI: https://doi.org/10.1103/PhysRevResearch.4.L042036

Q 4.4 Mon 11:45 F102

Ortho ground state preparation of cooled and trapped formaldehyde molecules — •Maximilian Löw, Martin Ibrügger, Martin Zeppenfeld, and Gerhard Rempe — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching

Methods to directly cool polar molecules to ultracold temperatures saw remarkable progress in recent years. One of the most promising techniques in this field is optoelectrical Sisyphus cooling which can provide a large number of electrically trapped molecules at the sub-millikelvin level [1]. However, molecules in their absolute ground state cannot be addressed with this approach.

Cold ground state molecules can still be created by first applying Sisyphus cooling to, e.g., formaldehyde (H_2CO) molecules in the rotational states $|J{=}3,K_a{=}3,K_c{=}0\rangle$ and $|4,3,1\rangle$. Then, we use optical pumping to transfer them via a vibrational transition to their ortho ground state $|1,1,0\rangle$. In a proof-of-principle experiment trapped ground state molecules with a temperature of 65 mK and trapping times of several seconds were obtained. There is no fundamental obstacle to achieving lower temperatures in the future.

As formaldehyde in this state is stable against inelastic two-body collisions this fulfills an important requirement for evaporative or sympathetic cooling of this species in, e.g., a microwave trap which takes one a step closer to the long-term goal of quantum degeneracy.

[1] A. Prehn *et al.*, *Phys. Rev. Lett.* **116**, 063005 (2016).

Q 4.5 Mon 12:00 F102

Towards direct laser cooling of barium monofluoride — •Marian Rockenhäuser, Felix Kogel, Einius Pultinevicius, Tatsam Garg, and Tim Langen — UNI Stuttgart, 5. Physikalisches Insitut, IQST

We report on our progress towards the laser cooling of BaF molecules. This molecular species shows high promise for various types of precision measurement applications. However, due to its high mass, complex hyperfine structure and branching losses through intermediate states, it is also notoriously difficult to cool. In an effort to realize laser cooling, we have performed high-resolution absorption spectroscopy of the lowest rovibrational states to determine an improved set of molecular constants. This has allowed us to identify missing cooling and repumping transitions necessary to realize laser cooling of BaF, as well as to realize near background-free fluorescence imaging of a cold molecular beam

Q 4.6 Mon 12:15 F102

Optical properties of the Si_2O^+ cation — •Emil Mickein, Taarna Studemund, Kai Pollow, Marko Förstel, and Otto Dopfer — Institut für Optik und Atomare Physik, Technische Universität Berlin, Berlin, Germany

The emission of SiO from stars is well-known and proven. Moreover, the existence of different μm-sized silicate grains in interstellar dust is observed, but the formation pathway is unknown and information concerning larger molecules and their ions is missing.
In our project we are looking for transitions of cluster and characterize them via their measured optical spectrum.
In this talk, experimental data and quantum chemical calculations on the absorption and dissociation properties of Si_2O^+ are presented. The spectrum of Si_2O^+, which are created in a laser vaporization source, was obtained by photodissociation of mass-selected Si_2O^+ cations in a tandem mass spectrometer. The experimental results are discussed and compared with theoretical results of TD-DFT calculations.
Significantly, our optical spectrum provides the first spectroscopic information for this simple triatomic cation.

Q 4.7 Mon 12:30 F102

Threshold photodetachment spectroscopic studies of C_2^- — •sruthi purushu melath, christine maria lochmann, markus nötzold, robert wild, and roland wester — Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria

Photodetachment spectroscopy is a powerful spectroscopic technique for determining the internal state distribution of a molecular anion. The dicarbon anion, our current molecule of interest, is a well-studied system due to its stable electronic level structure and potential laser cooling transition [1].

Here we present the photodetachment spectroscopy of C_2^- near threshold in a radiofrequency 16-pole wire trap at 8 K. The main goal of the experiment is to analyze the behavior of the cross section near the threshold, determine the electron affinity more precisely than previously measured [2,3], and if possible, obtain a rotationally resolved photodetachment signal as a function of photon energy. The status of

the project will be presented.

[1]. M. Nötzold *et al.,* Phys. Rev. A 106, 023111 (2022) [2]. K. M. Ervin, *et al.,* J. Phys. Chem. 95, 2244 (1991) [3]. B. A. Laws *et al.,* Nat. Commun. 10, 1(2019)

Q 4.8 Mon 12:45 F102

Theoretical study of photoassociation of ultracold ^{23}Na^{39}K and ^{39}K — •Baraa Shammout[1], Charbel Karam[2], Leon Karpa[1], Eberhard Tiemann[1], Silke Ospelkaus[1], and Olivier Dulieu[2] — [1]Institut für Quantenoptik, Universität Hannover — [2]Université Paris-Saclay, CNRS, Laboratoire Aimé Cotton

Understanding the physics underlying ultracold alkali atom-diatom collisions is essential for full quantum control on ultracold molecules. The long-range photoassociation (PA) process of loosely-bound ultracold trimers from a scattering state of atom-diatom is a possible pathway to investigate their collisional properties. In this work, we present a long-range model for modeling photoassociation of ultracold ^{23}Na^{39}K and ^{39}K close to the molecular resonant excitation NaK($X\,^1\Sigma$) $\rightarrow$ NaK($b^3\Pi$). We have calculated potential energy surfaces (PESs) for the low-lying doublet excited states of NaK_2 up to the NaK($b^3\Pi$)+K(4s) dissociation limit. We extracted the energy of vibrational-rotational levels using the time-independent close-coupling method, restricted to the long-range PESs. Finally, we demonstrate the possibility of experimental observation of trimer photoassociation by estimating trimer PA-rates.