

A 25: Cluster and Experimental Techniques (joint session MO/A)

Time: Thursday 14:30–16:30

Location: F142

A 25.1 Thu 14:30 F142

Characterization of a simple supersonic expansion source for small molecular ions — ●LUKAS BERGER¹, AIGARS ZNOTINS¹, FLORIAN GRUSSIE¹, DAMIAN MÜLL¹, FELIX NUSSLIN¹, ARNAUD DOCHAIN², JOFFREY FRÉREUX², XAVIER URBAIN², and HOLGER KRECKEL¹ — ¹Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany — ²Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Louvain-la-Neuve, B-1348 Belgium

The Cryogenic Storage Ring (CSR) [1] at the MPI for Nuclear Physics allows for the storage of molecular ions of almost arbitrary mass at extreme vacuum (residual gas densities on the order of 1000 cm⁻³) and at low temperature ($T < 5\text{K}$). In this environment, small infrared-active molecular ions will cool to their lowest rotational states within minutes. However, some astrophysically relevant molecular ions lack a permanent dipole moment (e.g.: H_2^+ , H_3^+ , H_3O^+) and have to be produced in cold ion sources prior to injection, as they do not cool on experimentally accessible time scales. Here we present the design of a simple supersonic expansion source based on a commercial pulsed valve and an electric discharge. It allows for the production of intense pulses of small molecular ions. We use high-resolution photodissociation spectroscopy of N_2O^+ , employing the STARGATE setup [2] at the Université Catholique de Louvain, to characterize the internal excitation of the molecular ions and extract their rotational temperature.

[1] Von Hahn et al., Rev. Sci. Instrum. 87, 063115 (2016)

[2] Bejjani et al., Rev. Sci. Instrum. 92, 033307 (2021)

A 25.2 Thu 14:45 F142

OH⁺He as simple example to illustrate fundamental concepts of intermolecular interactions. — ●NIMA-NOAH NAHVI, DAVID MÜLLER, and OTTO DOPFER — Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The OH⁺He dimer is a simple cluster for which many concepts of intermolecular interactions can be demonstrated. Nowadays, OH⁺He can be understood quite well, which makes it an interesting and encompassing example for educational purposes.

OH⁺He_n ($n \leq 6$) clusters are grown inside a cryogenic 22-pole ion trap and detected using a reflectron mass spectrometer. The resulting mass spectra are explained with cluster structures determined by CCSD(T) calculations using CFOUR. We investigate and explain certain features of OH⁺He_n to illustrate concepts like solvation shells, potential energy functions, binding energies and vibrational frequencies, charge- and dipole-induced interactions, dispersion contribution, complete basis set limits and BSSE corrections. The results will be compared to those of H₂O⁺He_n and H₃O⁺He_n [1] to establish the effect of the number of protons on the interaction potential and cluster growth.

[1] Müller and Dopfer, Phys. Chem. Chem. Phys., 2022, 24, 11222-11233. <https://doi.org/10.1039/D2CP01192A>

A 25.3 Thu 15:00 F142

Investigation of the homogeneous line width of organic molecules attached to rare-gas clusters — ●ARNE MORLOK, ULRICH BANGERT, LUKAS BRUDER, YLIN LI, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Two-dimensional spectroscopy (2DES) is a powerful method to study dynamics of atoms and molecules with a high spectro-temporal resolution. In our group, we apply the technique to doped cluster beams, which act as miniature cryostats for different organic molecules [1,2]. Previous 2DES experiments on phthalocyanine (Pc) on neon clusters allowed resolution of the homogeneous linewidth of Pc and distinguished fluorescence from the C12 and C13 isotope [3]. We extended this investigation in varying the species of the spectroscopic matrix, hence the clusters, and the probed organic molecules. First results are presented, which suggest differences in the homogenous linewidth and coherence times depending on the coupling between dopant and cluster environment.

[1] L. Bruder et al., Nat. Commun. 9 4823 (2018).

[2] L. Bruder et al., J. Phys. B: At. Mol. Opt. Phys. 52 183501 (2019).

[3] U. Bangert et al., Nat. Commun. 13 3350 (2022).

A 25.4 Thu 15:15 F142

Experimental cross sections for the uptake of alkyl alcohols by binary HNO₃/H₂O clusters — YIHUI YAN¹, ANDRIY PYSANENKO², KAROLINA FARNIKOVA², EVA PLUHAROVA², MICHAL FARNIK², and ●JOZEF LENGYEL¹ — ¹TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — ²Heyrovsky Institute, Czech Academy of Sciences, Prague, Czech Republic

The uptake of oxidized organic compounds by hydrated acid clusters accounts for a substantial portion of atmospheric aerosol particles. Through joint experimental and computational studies, we investigate the uptake of alkyl alcohols on pre-existing hydrated HNO₃ clusters. In our experiments, the HNO₃/H₂O clusters pass through a chamber filled with a particular gas, the molecules collide with the clusters and can stick to the surface. The efficiency of this process is given by the uptake cross section, which is determined experimentally by a combination of mass spectrometry and velocity measurements in a molecular beam. Our previous experiments have shown that the uptake probabilities for the oxidized molecules are significantly larger than for the corresponding volatile organic compounds (VOCs). This increase is attributed to hydrogen bonds between the molecules and clusters, whereas the interactions of the parent VOCs are weaker and nonspecific. In this study, we examine the effect of different O-H bond positions in the oxidized molecule and different carbon chain length on the pickup probability. To learn the details of the pickup process, all experimental measurements are supplemented by MD simulations.

A 25.5 Thu 15:30 F142

Femtosecond pump-probe spectroscopy of tetracene in the gas phase and in helium nanodroplets — AUDREY SCOGNAMIGLIO, NICOLAS RENDLER, ●SEBASTIAN HARTWEG, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Germany

Acenes, specifically tetracene and pentacene, are promising candidates for applications in organic photovoltaics since ensembles of these molecules can undergo singlet fission to produce two triplet excitations from a single singlet excitation. This process may thus allow to produce multiple charge carriers from a single absorbed photon. The potential applications motivate the fundamental study of the ultrafast excitation dynamics of these molecules and their aggregates to provide a fundamental understanding of the underlying processes and energetics. We will present a study of femtosecond pump-probe photoelectron spectroscopy and mass spectrometry of the excited state dynamics of tetracene excited to its brightest singlet state using UV photons. We will compare results for effusive tetracene with preliminary data for tetracene and its clusters in superfluid helium nanodroplets. The doping of organic molecules into superfluid helium nanodroplets offers a promising path to extend the study from isolated molecules to clusters of acenes, but also imposes additional challenges.

A 25.6 Thu 15:45 F142

Plasmon quenching of a single gold nanoparticle in the gas phase — ●BJÖRN BASTIAN, BENJAMIN HOFFMANN, SOPHIA LEIPPE, and KNUT R. ASMIS — Universität Leipzig, Wilhelm-Ostwald-Institut, Linnéstraße 2, D-04103 Leipzig

A split-ring electrode trap design has been optimized to quasi-continuously monitor the mass of single nanoparticles for action spectroscopy, fluorescence spectroscopy and temperature-programmed desorption experiments. The aim is to investigate inherent properties of individual particles and their relation to parameters such as size, shape, temperature, charge state or surface functionalization. One example is a collective electron oscillation of metallic nanoparticles called *localized surface plasmon resonance*. New results are presented that show electronic action spectra of the plasmon resonance of a single 50 nm diameter gold particle and its stepwise quenching by radiative heating.

The particle mass is proportional to its secular frequency in the trap, which is typically monitored by resonant excitation. The resonance frequency is observed as a dip in the intensity of light scattered from the particle when sweeping an excitation frequency. Cryogenic cooling allows to control the adsorption of a messenger gas. Action spectra are obtained by observing the mass loss from desorption of the

messenger due to absorption of light in the visible or infrared range.

We present results on plasmon quenching and current progress in implementing infrared action spectroscopy and to better characterize the particle temperature, adsorption and desorption dynamics.

A 25.7 Thu 16:00 F142

Setup Of A Spectrometer To Detect Raman Optical Activity
— •KLAUS HOFMANN and INGO FISCHER — Universität Würzburg, 97074 Würzburg, Germany

Raman Optical Activity (ROA) is a type of vibrational circular dichroism: chiral samples show different Raman intensities when utilizing circular polarized light. The ROA signal is very sensitive to the molecular geometry and environment of the sample, which can be analyzed by comparing the spectrum with quantum chemical calculations. ROA spectra exhibit high levels of noise and are prone to false signals, since the intensity difference is roughly 0.1% of the corresponding Raman peak.[1]

For this project, a Raman spectrometer was custom-built and modified to detect ROA. A modulation scheme repeatedly converts linear to right and left circular polarized light for excitation. Python was used to automate the experiment, data acquisition and post-processing. The beampath of the spectrometer and its implemented error reduction schemes[2] are shown. Post-processing is used to evaluate the signal. Literature known samples were measured to validate the spectrometer.

[1] V. Parchaňský, J. Kapitán, P. Bouř, RSC Adv. 2014, 4, 57125.

[2] W. Hug, Appl. Spectrosc. 2003, 57, 1.

A 25.8 Thu 16:15 F142

Salt effects on the translocation dynamics of polycationic peptide nucleic acids through a protein nanopore — •IOANA CEZARA BUCATARU¹, ALINA ASANDEI², LOREDANA MEREUTA¹, and TUDOR LUCHIAN¹ — ¹Department of Physics, *Alexandru I. Cuza* University, Iasi, Romania. — ²Sciences Department, Interdisciplinary Research Institute, *Alexandru I. Cuza* University, Iasi, Romania

Peptide nucleic acids (PNAs) are synthetic molecular constructs that mimic DNA in structure, but with an uncharged pseudopeptide backbone made of N-(2-aminoethyl)-glycine, having the ability to form Watson-Crick complementary duplexes with regular DNA. Due to its distinctive properties, PNAs displayed considerable potential for application in molecular diagnostics and antisense therapies. The addition of different charged sidechains to the neutral PNA structure plays an essential part in addressing solubility-related issues that are linked with the use of these molecules. The single-molecule investigations used here focus on the interactions of different length polyarginine-conjugated PNAs (poly(Arg)-PNAs) with the α -hemolysin (α -HL) nanopore, under an applied transmembrane voltage. The effect of ionic strength on the translocation kinetics is demonstrated by using different salt concentrations in the recording buffer. Our results indicate that low ionic strength increases the electrophoretic mobility of poly(Arg)-PNA probes as they pass through the nanopore and reduces their volume. The current findings highlight the intricate interplay between conformation and ion environment that influences the inherent flexibility and function of poly(Arg)-functionalized PNAs.