

## MO 26: Cluster

Time: Friday 14:30–16:00

Location: HS 3042

MO 26.1 Fri 14:30 HS 3042

**Setup for time- and energy-resolved fluorescence measurements of collective effects in polyacene aggregates attached to rare gas clusters** — ●ALEKSANDR DEMIANENKO, MORITZ MICHELBACH, SEBASTIAN HARTWEG, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Germany

Collective effects in organic semiconductors affect excited state lifetimes, important for organic optoelectronic and photovoltaic applications. A complete understanding of the energy level structure, and decay mechanisms require high spectral and temporal resolution. We present a setup combining conventional laser-induced fluorescence (LIF) spectroscopy with time-correlated single photon counting (TC-SPC) and discuss advantages and implementation challenges. Using wavelength-tunable nanosecond dye laser pulses allows us to measure high-resolution LIF spectra of transitions to highly excited states of tetracene embedded in superfluid helium nanodroplets, or deposited on solid rare-gas clusters. The newly implemented TCSPC detection in combination with a femtosecond laser system is aimed at studying radiative and non-radiative decay mechanisms connected to collective effects in aggregates of polyacenes. This technique allows us to cover the sub-ns lifetime region not previously reachable in our fluorescence measurements.

MO 26.2 Fri 14:45 HS 3042

**Investigation of the homogeneous linewidth of organic molecules on solid rare-gas clusters** — ●ARNE MORLOK, ULRICH BANGERT, YILIN LI, FELIX RIEDEL, LEONIE WERNER, LUKAS BRUDER, and FRANK STIENKEMEIER — University of Freiburg, Institute of Physics, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Doped rare-gas clusters are a well-established model system to study molecular systems. In order to harness the full potential of such cluster isolation techniques, it is crucial to understand the residual system-bath interaction between cluster and dopant. We employ two-dimensional electronic spectroscopy (2DES) to study the interaction of organic molecules with solid rare-gas clusters, which allows us to resolve the ensemble inhomogeneity and retrieve information about the molecule-cluster binding configurations [1]. Previously, this approach was applied to resolve the homogeneous linewidth of phthalocyanine molecules attached to neon clusters and ultimately provided a deeper understanding of the structural configurations in a nanoconfined system [2].

We extended this investigation in varying the cluster species and improving the data acquisition scheme, since the previous measurements were limited by long acquisition times. First results are presented, which suggest differences in the homogeneous linewidth and dynamics depending on the cluster species.

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

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

MO 26.3 Fri 15:00 HS 3042

**Collision dynamics and uptake of alcohol molecules by hydrated nitric acid clusters** — YIHUI YAN<sup>1</sup>, KAROLÍNA FÁRNÍKOVÁ<sup>2</sup>, ANDRIY PYSANENKO<sup>2</sup>, EVA PLUHAŘOVÁ<sup>2</sup>, MICHAL FÁRNÍK<sup>2</sup>, and ●JOZEF LENGYEL<sup>1</sup> — <sup>1</sup>TU München, Garching, Germany — <sup>2</sup>Czech Academy of Sciences, Prague, Czechia

Aerosol particles represent one of the most important, yet perhaps the least understood, components of our atmosphere. Due to their influence on global climate, there is a need for detailed kinetic data to be used in climate prediction models. We have therefore developed a novel method for quantifying the uptake process of various molecules by hydrated HNO<sub>3</sub> clusters using a pickup technique. Our experiment combines mass spectrometry of the clusters with velocity measurements. However, the evaluation of the uptake cross sections from the experimental data is based on simplifying assumptions about the molecule-cluster collisions. We validate these assumptions through extensive MD simulations. These calculations allow evaluation of the scattering and uptake processes in the collisions, and subsequently the uptake cross sections can be derived and compared to the experimental values. Herein, we examine the uptake of different alcohol molecules by hydrated HNO<sub>3</sub> clusters. We discuss the dependence of uptake on the length of the carbon chain (i.e., size, mass, and hydrophobicity)

and on steric effects. The combination of experimental data with simulations provides insight into the dynamics involved in molecule-cluster collisions, which is essential for validating our experimental approach.

MO 26.4 Fri 15:15 HS 3042

**Mass Spectrometry Analysis of Binary Formic Acid-Water Clusters upon Collision with Electrons** — ●KEVIN LI<sup>1</sup>, JOZEF ĎURANA<sup>2</sup>, MICHAL FÁRNÍK<sup>2</sup>, and JOZEF LENGYEL<sup>1</sup> — <sup>1</sup>TU München, Garching, Germany — <sup>2</sup>Czech Academy of Sciences, Prague, Czechia

A significant portion of atmospheric particles is formed through the nucleation and condensation of precursor gases in a process known as new particle formation (NPF), where organic acids play a crucial role as key precursor gases that enhance nucleation rates. It is, therefore, essential to understand the collisions of gas-phase molecules with clusters and to establish protocols for analyzing these particles using mass spectrometry. This is particularly important for hydrogen-bonded particles, as they frequently undergo extensive fragmentation upon ionization. In our experiments, mixed clusters of formic acid and water were produced in supersonic expansion and subsequently investigated by mass spectrometry using different ionization methods, namely (i) the electron ionization at 70 eV (EI) and (ii) the low energy electron attachment (EA). While for positive ionization mainly protonated clusters (H<sub>2</sub>O)<sub>n</sub>/(HCOOH)<sub>m</sub>/H<sup>+</sup> were detected, negative mass spectroscopy revealed two species, (H<sub>2</sub>O)<sub>n</sub>/(HCOOH)<sub>m</sub> and (H<sub>2</sub>O)<sub>n</sub>/(HCOOH)<sub>m-1</sub>/HCOO<sup>-</sup>. Both techniques indicate that higher water content in the solution results in clusters with a high degree of hydration and fewer formic acid molecules. Additionally, the fraction of the two anionic species is influenced by cluster size, level of hydration, and electron energy. The detailed behavior of ionization will be discussed in the presentation.

MO 26.5 Fri 15:30 HS 3042

**Electron scattering in neutral water clusters** — ●KATINKA HORN<sup>1</sup>, SVETLANA TSIZIN<sup>1</sup>, LOREN BAN<sup>1</sup>, SEBASTIAN HARTWEG<sup>2</sup>, PETRA HOFFMANN<sup>1</sup>, EGOR CHASOVSKIKH<sup>1</sup>, BRUCE L. YODER<sup>1</sup>, and RUTH SIGNORELL<sup>1</sup> — <sup>1</sup>ETHZ, Laboratory of Physical Chemistry, Switzerland — <sup>2</sup>University of Freiburg, Institute of Physics, Germany

A detailed understanding of low-energy electron scattering in water (with kinetic energies below 100 eV) is crucial to modeling and controlling many processes occurring in nature, ranging from atmospheric chemistry to radiation biology. While condensed and gas phase electron scattering cross sections are known for water, analogous data for scattering in water clusters is still missing. This is the case even though clusters, often exhibiting unique/tunable properties, are of great interest for bridging the gap between the gas and condensed phases. The presented work is an extension and refinement of previous studies, providing more detailed information on electron scattering in neutral water clusters of various sizes ionized with photon energies up to ~50 eV. Electron transport scattering in water clusters was investigated by angle-resolved photoelectron spectroscopy. The scattering cross sections for the model were retrieved from cluster-size and energy resolved data contained in the photoelectron anisotropy parameter  $\beta$ . We found larger electron scattering cross sections for clusters than for the condensed phase, likely due to reduced dielectric screening in clusters. Good agreement to experiment is achieved with a condensed phase scattering model, using a kinetic energy and scattering channel dependent scaling of bulk cross sections.

MO 26.6 Fri 15:45 HS 3042

**Electron transfer processes and the formation of solvated di-electrons by UV excitation in sodium-ammonia clusters** — ●SEBASTIAN HARTWEG<sup>1,2</sup>, JONATHAN BARNES<sup>3</sup>, BRUCE L. YODER<sup>3</sup>, GUSTAVO A. GARCIA<sup>2</sup>, LAURENT NAHON<sup>2</sup>, EVANGELOS MILIORDOS<sup>4</sup>, and RUTH SIGNORELL<sup>3</sup> — <sup>1</sup>Institute of Physics, University of Freiburg, Germany — <sup>2</sup>Synchrotron Soleil, St. Aubin, France — <sup>3</sup>DCHAB, ETH Zürich, Switzerland — <sup>4</sup>Auburn University, Alabama, USA

Solvated electrons play important roles in the origin and formation of radiation damage in biological tissue as well as for large-scale chemical synthesis. Electron solvation has first been observed in alkali ammonia solutions. These systems with their many peculiar concentration dependent properties[1-3] including the formation of stable solvated di-electrons and a transition to a metallic phase, are not well understood

on a molecular level, despite the many studies conducted on them.

I will present our recent photoelectron/photoion coincidence study with support from quantum chemical calculations[4], in which we could identify different electron transfer processes occurring in sodium ammonia clusters upon interaction with UV and VUV radiation. Among these processes, the formation of transient solvated dielectrons and

their subsequent decay via an electron-transfer mediated decay process constitutes the first direct observation of solvated dielectrons.

- 1.Zurek, E., et al. *Angew. Chem. Int. Ed.*, 2009. 48(44)
- 2.Buttersack, T., et al. *Science*, 2020. 368(6495)
- 3.Hartweg, S., et al. *Angew. Chem. Int. Ed.*, 2016. 55(40)
- 4.Hartweg, S., et al. *Science*, 2023. 380(6650)