A 28: Cluster and Nanoparticles I (joint session MO/A)

Time: Thursday 11:00–13:15 Location: HS XV

Invited Talk A 28.1 Thu 11:00 HS XV

Pickup and reactions of molecules on clusters relevant for atmospheric processes — •Jozef Lengyel — Technical University of Munich, Garching, Germany

The uptake of molecules by preexisting clusters in molecular beams is demonstrated using two distinct experiments. In the first one, the doping of hydrated acid clusters with various molecules is investigated. Sticking efficiencies, including uptake cross sections, are determined using the combination of cluster mass spectrometry and velocity measurements. The combined experimental and computational approach provides insights into molecule-cluster collision dynamics, illustrated by a series of measurements involving diverse molecular interactions and steric effects. The second one focuses on the dissociation of nitric acid on large water clusters. While dissociation is often reported for clusters containing as few as five water molecules, it is shown that on nanometer-sized ice nanoparticles, dissociation occurs only to a limited extent, with the majority of nitric acid remaining undissociated on the ice surface.

A 28.2 Thu 11:30 HS XV

Imaging single sea salt aerosol nanoparticles — •Changji Pan for the Sea Salt Nanoparticle-Collaboration — Department of Physics, ETH Zurich, 8093, Zurich Switzerland

The influence of sea salt aerosol particles on atmospheric processes highly depends on their hygroscopicity and capacity as cloud condensation nuclei. These properties are highly related to the particle morphology and the distribution of chemical species inside these nanoparticles. Many studies, however, suffer from the averaging effect in ensemble measurements and the substrate interaction in deposited particles. We performed a direct measurement on in-flight individual sea salt aerosol nanoparticles by single-shot X-ray diffraction imaging at EuXFEL, to retrieve their inner structure and overall morphology as a function of particle size, chemical composition, and humidity.

A 28.3 Thu 11:45 HS XV

Optimized sample-delivery system for coherent-diffractive-imaging of proteins — •Stefanie Lenzen[1,2], Lukas V. Haas[1,3,4], Kevin Janson[1], Amit K. Samanta[1,3,4], and Jochen Küpper[1,2,3,4] — [1]Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron DESY, Hamburg — [2]Department of Chemistry, Universität Hamburg — [3]Department of Physics, Universität Hamburg — [4]Center for Ultrafast Imaging, Hamburg

Determining the structure and dynamics of single native bio-nanoparticles, such as proteins, is still challenging. Several methods, including protein-crystallography and cryo-EM, focus on this challenge, but the biomolecule needs to be fixed, which might lead to structural disentegration, and the temporal resolution of these methods are limited. X-ray free-electron lasers (XFELs) provide ultrashort pulses, enabling diffraction before destruction, and a large number of photons, promising the observation of diffraction patterns *off* single nanoparticles. Aerodynamic-lens stacks were used to deliver collimated and focused particle beams for such experiments on large nanoparticles [1]. We optimized the sample injection and extended the use of particle beams toward smaller nanoparticles and protein complexes like apoferritin. This highlights the use of improved aerosolization methods together with optimized ALS injectors for small bio-nanoparticles. In addition, we present techniques for improved optical-scattering-based detection of proteins.

[1] Lena Worbs, Toward cryogenic beams of nanoparticles and proteins, *Dissertation*, Universität Hamburg (2022)

A 28.4 Thu 12:00 HS XV

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 (CFEL), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Department of Physics, Universität Hamburg, Germany — [3]Center for Ultrafast Imaging (CUI), Universität Hamburg, Germany — [4]Fakultät für Maschinenbau, Helmut-Schmidt-Universität,Germany

We demonstrated the preparation of cold and controlled beams of nanoparticles and macromolecules that are desired for x-ray single-particle-diffractive imaging (SPI) using the buffer-gas-cell (BGC) cooling and aerodynamic focusing techniques [1,2]. The cooling and control techniques we developed for SPI can be extended to experiments to study the electron dynamics in complex biomolecules on the few-femtosecond timescale [3]. Such ultrafast charge- and energy-transfer dynamics following electronic excitation were not revealed so far [4].

We present an approach toward investigating the time-resolved ultrafast dynamics in cryo-cooled proteins [1] induced by ultrashort UV/VIS pulses and advanced detection method including velocity-map-imaging using Timepix3 cameras [5].

[1] A.K. Samanta, *et al.*, *Struct. Dyn.* **7**, 024304 (2020)
[2] S.K. Peravali, *et al.*, *Comput. Fluids* **279**, 106346 (2024)
[3] M. Hervé, *et al.*, *Commun. Chem.* **4**, 124, (2021)
[4] H. Duan, *et al.*, *PNAS* **114**, 8493 (2017)
[5] H. Bromberger, *et al.*, *J. Phys. B* **55**, 144001 (2022)

A 28.5 Thu 12:15 HS XV

Temperature and adsorption dynamics of single nanoparticles in a cryogenic ion trap — •Björn Bastian, Sophia C. Leippe, Kleopatra Papagrigoriou, and Knut R. Asmis — Wilhelm Ostwald Institute, Leipzig University, Linnéstraße 2, D-04103 Leipzig

Characterization of nanoparticles without inhomogeneous broadening and interactions with the environment requires single particle techniques in the gas phase. Our group has shown the feasibility of single nanoparticle action spectroscopy (SNAS) in a cryogenic Paul-type ion trap [1], based on the adsorption of messenger atoms or molecules on the nanoparticle surface and their desorption driven by laser heating with rates that are proportional to the absorption cross section [2].

A quantitative understanding of the sorption dependent SNAS technique and temperature programmed desorption schemes to characterize surface interactions strongly depend on the surface temperature which is difficult to measure or estimate in such experiments. In a collaborative work, we could achieve a first *in situ* measurement using the temperature-dependent emission spectrum of core/shell CdSe/CdS quantum dots and capture the essential heating and cooling processes in a model [3]. The latter helps to estimate surface temperatures for different particles and experimental conditions which is used here to interpret the adsorption dynamics of oxygen on silica nanoparticles.

[1] B. Hoffmann et al., Mol. Phys. 122, e2210454 (2023). [2] B. Hoffmann et al., J. Phys. Chem. Lett. 11, 6051 (2020). [3] S. C. Leippe et al., J. Phys. Chem. C (accepted).

A 28.6 Thu 12:30 HS XV

Cluster beam technologies for matter-wave interferometry — •Severin Sindelar, Bruno Ramirez-Galindo, Sebastian Pedalino, Stefan Gerlich, and Markus Arndt — University of Vienna, Faculty of Physics, Boltzmanngasse 5, 1090 Vienna

Metal nanoparticles are promising candidates for interferometric tests of the quantum superposition principle in the 1 MDa mass range. Cluster interferometry shall allow us to push the limit on quantum macroscopicity well beyond the state of the art and it shall open a window for quantum-enhanced measurements of properties of nanoscale materials.

The cluster beam shall last for a day, have a high brilliance of slow and neutral metal nanoparticles with masses up to 1 MDa and velocities below 30 m/s. The materials must have a work function compatible with single photon ionization using deep ultraviolet (DUV) laser light, ideally high polarizability and low magnetic susceptibility. Here we present our approach to such a cluster source: It is based on metal evaporation and cluster aggregation in an 80 K cold chamber, followed by an aerodynamic lens array.

While interference experiments shall work with neutral clusters, their identification and detection require singly charged particles, which we can select in a quadrupole mass spectrometer with subsequent Daly detection. We present the formation, ionization and spectroscopy of metal clusters, which have a low work function, high absorption cross section and high polarizability. We study their photo physics as a function of size, DUV laser wavelength and laser power to extract the properties that will be needed for interference experiments.

A 28.7 Thu 12:45 HS XV

Laser-induced alignment of macromolecules and nanoparticles — •Lukas Vincent Haas[1,2,3], Xuemei Cheng[1], Muhamed Amin[1], Stefanie Lenzen[1,3], Amit Kumar Samanta[1,2,3], and

Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Department of Physics, Universität Hamburg, Germany — [3]Center for Ultrafast Imaging (CUI), Universität Hamburg, Germany

X-ray free-electron lasers (XFELs) promise to enable the diffractive imaging of single molecules and nanoparticles, but image reconstruction remains a major bottleneck in achieving atomic spatial resolution[1]. Laser-induced alignment of nanoparticles and macromolecules during the diffractive imaging process has the potential to push resolution toward the atomic scale [2]. We present the quantitative computational modeling of nanoparticle alignment using classical mechanics and electrodynamics [3] along with the first experimental evidence of laser-induced alignment of tobacco mosaic virus (TMV) in an XFEL-compatible setup. The alignment was probed through optical scattering. A recently conducted XFEL experiment provides initial results on diffractive imaging of laser-aligned TMV. Comparing computational and experimental results, we conclude that a high degree of alignment is achieved for TMV in our experiments.

[1] K. Ayyer, et al., Optica 8(1) (2021)
[2] J. C. H. Spence, et al., Phys. Rev. lett. 92, 198102 (2004)
[3] M. Amin, et al., arXiv:2306.05870 [physics], (2023)

A 28.8 Thu 13:00 HS XV

Rotational Waver Packet Dynamics of Size-selected Neutral Clusters — •Jiaye Jin, Max Grellmann, Marcel Jorewitz, and Knut R. Asmis — Wilhelm-Ostwald-Institut für Physikalische und Theoretisch Chemie, Universität Leipzig, Leipzig, Germany

We report our results on rotational wave-packet dynamics for the mass-selected neutral clusters in a cryogenic ion trap probed by two-colors femtosecond pump-probe spectroscopy involving the negative-neutral-positive excitation scheme. To achieve this, a rotational wave packet is prepared via photodetachment of mass-selected cold anion using a first linearly polarized laser pulse. The rotation coherence is then probed using a second linearly polarized laser pulse, set either parallel or perpendicular to the polarization of the first pulse, ionizing the neutral molecule. The rotational anisotropy β is then calculated from the cation transients probed at different polarization angles.

Neutral boron cluster B_6 is chosen as the first experimental candidate. So obtained time-dependence of B_6^+ cation measured at parallel probing polarization shows typical J-type recurrences of the initial rotational wave packet at 68 ps, 135 ps, 210 ps and 275 ps. The rotational coherence is confirmed by following measurements using perpendicular polarization, where the recurrent cations signal show opposite intensity compared to the parallel probing. An effect rotational constants is thus obtained by 0.25 cm^{-1}, agreeing well with calculations. These results demonstrate the application in the coherent control for the orientation of mass-selected neutral molecules in a cryogenic ion trap.