MO 25: Novel Experimental Approaches

Time: Friday 11:00–12:45 Location: HS 3044

MO 25.1 Fri 11:00 HS 3044

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 have 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, such as charge and energy transfer following electronic excitation, where the details have not been revealed so far [3]. We present an approach towards investigating the time-resolved ultrafast dynamics in proteins with UV/VIS ultrashort-pulse lasers. The photoexcitation-induced energy transfer, for instance, can be studied by photofragmentation of cryogenically-cooled proteins with time-of-light mass spectrometry and velocity-map-imaging.

[1] A. K. Samanta, et al., *Structural dynamics* **7**, 024304 (2020)
[2] L. Worbs, et al., *In preparation*, (2024)
[3] H. Duan, et al., *PNAS* **114**, 8493 (2017)

MO 25.2 Fri 11:15 HS 3044

Characterizing temperature, charging and adsorption dynamics of single nanoparticles — •Björn Bastian, Sophia Leippe, Kleopatra Papagrigoriou, and Knut Asmis — Wilhelm-Ostwald-Institut, Linnéstraße 2, D-04103 Leipzig

Single nanoparticle (NP) techniques allow to probe intrinsic properties of nanoparticles, but typically rely on surface deposition. Instead, we develop the analysis of single NPs in the gas phase using a cryogenic radio-frequency ion trap and UV/Vis or IR action spectroscopy. Absorption is indirectly monitored using NP mass spectrometry (NPMS): the produced heat causes the loss of messenger atoms or molecules that are adsorbed to the particle surface. Here, we present current progress on controlling and characterizing the charge state, temperature and surface coverage of single trapped NPs that will ease the implementation and quantitative analysis of future experiments.

Inducing charge changes is crucial for absolute mass determination and facilitates control in long experiments (∼ days). Using a filament to emit electrons for electron attachment or charge transfer — mediated by different collision gases at different pressures — we demonstrate full control of the charge state of positively charged silica NPs.

Characterizing binding sites and energies is an important goal for NP characterization and essential for quantitative action spectroscopy. Extensive adsorption measurements on silica NPs are presented and we demonstrate *in situ* fluorescence thermometry for semiconductor quantum dots. We will report on the latest progress to simultaneously measure temperature and adsorption on single fluorescent nanoplatelets.

MO 25.3 Fri 11:30 HS 3044

Laser-induced alignment of macromolecules and nanoparticles — •Lukas Vincent Haas[1,2,3], Xuemei Cheng[1], Muhamed Amin[1], 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, while image reconstruction remains a major bottleneck in achieving atomic spatial resolution [1]. Laser-induced alignment of nanoparticles and macromolecules has the potential to improve the achievable resolution by reducing the complexity of the diffraction volume search space and push it toward the atomic scale [2]. Here, we will present quantitative computational modeling of nanoparticle alignment using classical mechanics and electrodynamics [3] and first experimental evidence of laser-induced alignment of tobacco mosaic virus (TMV) in a setup that is applicable to XFEL experiments [4]. Furthermore, a recently conducted XFEL experiment provides first results on diffractive imaging of laser-aligned TMV. Comparing computational and experimental results, we can 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)

MO 25.4 Fri 11:45 HS 3044

Charge density model for the interaction of molecules with vortex beams — Mikhail Maslov[1], Georgios M. Koutentakis[1], •Mateja Hrast[1], Oliver H. Heckl[2], and Mikhail Lemeshko[1] — [1]Institute of Science and Technology Austria (ISTA), Klosterneuburg, Austria — [2]Christian Doppler Laboratory for Mid-IR Spectroscopy and Semiconductor Optics, Faculty Center for Nano Structure Research, Faculty of Physics, University of Vienna, Austria

We present a new model for the interaction of molecules with the orbital angular momentum of light, which has long been argued to benefit structural studies and quantum control of molecular ensembles. We derive a general description of the light-matter interaction in terms of the coupling between spherical gradients of the electric field and an effective molecular charge density that exactly reproduces molecular multipole moments. Our model can accommodate for an arbitrary complexity of the molecular structure and is applicable to any electric field, with the exception of tightly focused beams. Within this framework, we derive the general mechanism of angular momentum exchange between the spin and orbital angular momenta of light, molecular rotation and its center-of-mass motion. We demonstrate that vortex beams strongly enhance certain ro-vibrational transitions that are considered forbidden in the case of a non-helical light.

MO 25.5 Fri 12:00 HS 3044

Investigation on the dynamics of single atom catalysis in superfluid helium nanodroplets — •Wentao Chen, Brendan Wouterlood, and Frank Stienkemeier — Institute of Physics, University of Freiburg, 79104 Freiburg

We introduce a new experimental approach on the dynamics of single atom catalysis in superfluid helium nanodroplets. Single-atom catalysts have recently emerged as a new type of catalysts which are comprised of one metal atom and has different catalytic properties compared to bulk-particle catalysts. The common way to form single-atom catalysts is to isolate a single metal atom on a supporting surface, which makes it difficult to characterize the catalytic activity of the single atom and separate the influence of the surface. Superfluid helium nanodroplets can be an ideal tool to form the isolated molecule-metal atom complexes by doping the reactant molecule and the metal atom successively. Specifically, we were able to form 1,8-octanediol- Aun(n=0-2) complexes without a supporting surface by sequentially doping octanediol and a gold atom in helium droplets. After ionizing the complexes by electron impact and comparing the fragment, it has been found that the complexes with Au atoms prominently produce C2H4+ in this dissociative reaction, while the complexes without Au atoms have more diverse fragments: C2H4+, HCO+ and CH2OH+. We plan to use femtosecond pump-probe spectroscopy and photoelectron-photoion coincidence methods to study the real-time dynamics of the octanediol- Aun complex during the reaction.

MO 25.6 Fri 12:15 HS 3044

Nanophotonics for precise mid-infrared molecular spectroscopy — •Jérémie Pilat[1], Lucas Deniel[1], Melissa A. Guidry[2], Daniil M. Lukin[2], Bingxin Xu[1], Kiyoul Yang[2], Joshua Yang[2], Jelena Vučković[2], Theodor W. Hänsch[1,3], and Nathalie Picqué[1,4] — [1]Max-Planck Institute of Quantum Optics, Garching, Germany — [2]E. L. Ginzton Laboratory, Stanford University, Stanford, California, USA — [3]Ludwig-Maximilian University of Munich, Faculty of Physics, München, Germany — [4]Max Born Institute, Berlin, Germany

A nanophotonic silicon-carbide waveguide on a 5x5 mm^2 chip dramatically simplifies comb-assisted mid-infrared spectroscopy. The emerging 4H silicon carbide (SiC) on insulator platform provides a high refractive index, strong second- and third-order optical nonlinearity, low losses, and a broad transparency range. Here, a mode-locked laser at

1560 nm excites a dispersion-engineered SiC waveguide. This simultaneously enables frequency-comb self-referencing with an integrated f-2f interferometer and mid-infrared dispersive-wave frequency-comb generation at low 120-pJ pulse energies. By stabilizing the carrier-envelope offset frequency beatnote f_{ceo} provided by the integrated f-2f interferometer and the repetition rate of the mode-locked laser, accurate tunable-laser molecular spectroscopy of methane is demonstrated at 3.6 μm. Our new tool opens up new opportunities for precision measurements in the mid-infrared molecular fingerprint region, where most molecules exhibit characteristic intense rovibrational transitions, of interest to fundamental research and environmental sensing.

MO 25.7 Fri 12:30 HS 3044

Azobenzene based lipids as a tool to manipulate physiochemical properties of membrane mimetic systems via light — •Justin Hornbogen[1], Ritu Rajender[2], Stefan Kins[2], Annette Meister[3], David Glück[4], Sandro Keller[4], and Rolf Diller[1] — [1]Phys. Dept., RPTU, 67663 Kaiserslautern, GER. — [2]Human Biol. Dept., RPTU, 67663 Kaiserslautern, GER. — [3]Inst. Biochem. and Biotech., MLU, 06120 Halle, GER. — [4]Inst. Molecular Bioscience (IMB), Univ. of Graz, 8010 Graz, AUT.

Regulation of physiological membrane properties is an auspicious approach towards the treatment of various illnesses, e.g. Alzheimer disease (AD). Azobenzene (AB) decorated lipids are used to manipulate membranes by photoinduced AB trans(E)/cis(Z)-isomerization. We present the photophysical switching behaviour of 18:0-azo-phosphatidylcholin incorporated into unilamellar phosphatidylcholine (POPC or DMPC) LUV's and glycodiisobutylene/maleic acid lipid particles (POPC- or DMPC-nanodiscs). In addition, we explore the physicochemical impact of AB isomerization by means of methods like (transient) UV/Vis spectroscopy, TEM, DLS and others. The self-assembling nanoparticles can serve as a model system to investigate biochemical functionality of membrane proteins in native-like biomembranes while altering membrane properties such as structure, thickness, lateral pressure, permeability etc. through a light stimulus. Ongoing purification and incorporation of APP and γ-secretase may reveal an influence of AB isomerization on the generation of pathogenic amyloid plaques and γ-secretase activity related to AD.