MO 4: Novel Experimental Approaches and Novel Theoretical and Computational Approaches

Time: Monday 17:00–19:00 Location: P 105

Invited Talk MO 4.1 Mon 17:00 P 105

A two-color glimpse at nanomatter: ultrafast movies coming soon. — •Alessandro Colombo, Linos Hecht, and Daniela Rupp for the TwoColorCDI-Collaboration — ETH Zurich, Switzerland

Pairs of ultrashort, ultrabright X-ray pulses of distinct wavelengths can now be produced by X-ray Free Electron Lasers (XFELs) [1]. The possibility of precisely controlling their time delay down to the femtosecond regime allows for probing the same system at two different points in time, even down to the natural timescales of electron dynamics. In this talk, we describe how two-color pulses can be combined with diffraction imaging experiments [2], to capture two time-delayed snapshots of a sample and track its light-induced ultrafast changes. In particular, we show results on two-color diffraction patterns acquired at the European XFEL, where two images of the same sample, separated in time by 750 fs, are successfully reconstructed despite the challenging experimental conditions [3]. While improvements on both the instrument and the analysis sides are still necessary to maximize the resolution of the technique, the exciting possibility of two-color diffraction imaging at XFELs, so far considered unviable, opens a new research path for tracking in space and time ultrafast structural and electron dynamics in nanomatter. The long-standing dream of capturing ultrafast movies of nanomatter with an XFEL is finally at hand, along with a new class of experiments yet to be explored.

[1] S. Serkez et al., *Applied Sciences 10, 2728* (2020)
[2] L. Hecht et al., *arXiv:2508.19991* (2025), in review at *Nat Commun*
[3] L. Hecht et al., *arXiv:2508.20153* (2025), in review at *Nat Commun*

MO 4.2 Mon 17:30 P 105

Generation of controlled, dense and shock-frozen protein beams — •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

Single-particle x-ray diffractive imaging (SPI) is a powerful method for probing the structures of gas-phase nanoparticles [1]. Despite the successes in artificial nanoparticles [2] and large viruses [3], its application to proteins remains challenging due to low hit rates, weak scattering, and structural instability. Here, we present a buffer-gas-cell-aerodynamic-lens-stack (BGC-ALS) that is capable of producing shock-frozen and focused protein beams. This approach delivers a large number of hydrated proteins into the tiny x-ray focus, making their native-like structures more likely to be probed. Using strong-field ionization with a velocity-map-imaging spectrometer, we characterized the BGC-ALS and demonstrated its applicability to a broad range of macromolecules including proteins. Such protein beams are promising not only for structural determiniation using SPI but also for pump-probe experiments on protein dynamics.

[1] Barty et al. *Annu. Rev. Phys. Chem.* **9**, 415-435 (2013)
[2] Ayyer et al. *Optica* **8**, 15 (2020)
[3] Seibert et al. *Nature* **470**, 78-81 (2011)

MO 4.3 Mon 17:45 P 105

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 — [2]Department of Physics, Universität Hamburg — [3]Center for Ultrafast Imaging, Universität Hamburg

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)**, 15-23 (2021)
[2] J.C.H. Spence, *et al.*, *Phys. Rev. Lett.* **92**, 198102 (2004)
[3] M. Amin, *et al.*, *J. Am. Chem. Soc.* **147(9)**, 7445 (2025)

MO 4.4 Mon 18:00 P 105

Quantum dynamical properties of Oligocene: from Spectroscopy to Machine Learning — •Viktoria Chatrchyan[1], Fabian Jester[2], Maximilian E. Schommer[1], Philipp Kollenz[1], Oskar Kefer[1], Pavel V. Kolesnichenko[1], Jan Freudenberg[2], Uwe H. F. Bunz[2], and Tiago Buckup[1] — [1]Physikalisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Germany — [2]Organisch-Chemisches Institut, Ruprecht-Karls-Universität Heidelberg, Germany

Femtosecond transient absorption spectroscopy is a powerful technique for probing ultrafast molecular dynamics. However, interpreting the resulting data typically demands extensive human and computational effort to support theoretical models. To address this challenge, we developed a deep neural network capable of real-time analysis of experimental data, enhanced by quantum-mechanical descriptors, to predict the relaxation kinetics of organic chromophores with over 80% accuracy. Evaluation of the neural network on simulated data confirmed the significant improvement of prediction accuracy (6-8%), underscoring the value of hybrid data integration. This model was applied to transient absorption measurements of recently developed oligoacenes due to their intriguing photodimerization properties. The results showed a non-trivial dependence of the multi-step photodimerization efficiency on the number of aromatic rings. The analysis suggests a complicated relationship between formation yield and the stability of the side products for different molecular sizes.

MO 4.5 Mon 18:15 P 105

Novel 340kW continuous-wave enhancement cavity — •Andriana Tsikritea — Department of Physics, TU Dortmund University, 44227, Dortmund, Germany

The design and development of a novel Fabry-Pérot enhancement cavity will be discussed. Using a 43 W continuous-wave input laser at 1064 nm, we report intracavity circulating powers greater than 340 kW and peak laser intensities of 8.7 GW/cm2. Implementing a fast switching scheme, the high-power laser is allowed to circulate the enhancement cavity for specified time durations, spanning 100 μs to 100 ms. The low duty cycle of the switching scheme allows the minimisation of heating effects on the cavity optical components, while simultaneously offering stable and repeatable pulses of the high-power laser.

The enhancement cavity is currently being integrated with a moving magnetic decelerator and superconductive trap apparatus. The high intracavity laser intensity will be used to optically trap polarisable molecular species. For example, for O2 molecules, the reported 340 kW laser power generates a 200 mK deep optical trapping potential. Subsequently, the evaporative cooling of the molecular ensemble will be attempted. With no laser cooling scheme implemented, the optical trapping experiments enabled by the enhancement cavity pave the way for the generation of laser-cooling-free quantum degenerate molecular gases.

MO 4.6 Mon 18:30 P 105

Generation of broad-bandwidth deep ultraviolet pulses using achromatic second harmonic generation — •Nils-Oliver Schütz, Mario Niebuhr, Ulrich Bangert, Felix Selz, Felix Riedel, and Lukas Bruder — Hermann-Herder-Straße 3, 79104 Freiburg, Germany

The generation of deep ultraviolet optical pulses featuring broad spectral bandwidth and short pulse durations is a challenging task, especially when using high repetition rate ($>$ 100kHz) laser systems that provide low pulse energies to drive the nonlinear conversion processes. We present a scheme based on second harmonic generation of the output of a non-collinear optical parametric amplifier. To increase the bandwidth and efficiency of the second harmonic generation we em-

ploy achromatic phase matching [1]. Through ray-tracing simulations, the impact of different geometrical arrangements of the setup on the compression of the UV pulses was investigated. The results, together with the characterization of the UV pulses, are presented.

MO 4.7 Mon 18:45 P 105

Facile production of multiply-charged actinide molecules — •J. Stricker[1,2,3], K. Gaul[1,2], P. Fischer[4], D. Renisch[1,2], D. Budker[1,2,3], F. Schmidt-Kaler[1,2,3], L. von der Wense[1], L. Schweikhard[4], and Ch. E. Düllmann[1,2,3,5] — [1]JGU Mainz — [2]HI Mainz — [3]PRISMA+ Mainz — [4]Universität Greifswald — [5]GSI Darmstadt

We present a new method for producing multiply-charged actinide molecules. Using pulsed laser ablation of micro-targets, we generate ThF_x^{n+} (x = 0-3, n $\leq$ 3) from ThF_4 salt, and UO^{n+} from metallic uranium up to UO^{4+}. The production of ThF^{2+} and UO^{3+} is particularly relevant for searches for nuclear Schiff moments, while UO^{4+} approaches the limit of chemical stability. Relativistic density-functional calculations validate the observed charge states and molecular structures. The technique provides access to a broad range of multiply-charged radioactive molecules for a variety of future precision experiments.