MO 3: Diffraction and Coherences (with A)

Time: Monday 17:00–18:45 Location: N 6

Invited Talk MO 3.1 Mon 17:00 N 6

Single-shot coherent diffractive imaging of individual clusters using a high harmonic source — Nils Monserud[1], Daniela Rupp[2], Bruno Langbehn[2], Mario Sauppe[2], Julian Zimmermann[2], Yevheniy Ovcharenko[2], Thomas Möller[2], Fabio Frassetto[3], Luca Poletto[3], Andrea Trabattoni[4], Francesca Calgari[5], Mauro Misoli[4,5], Katharina Sander[6], Christian Peltz[6], Marc J.J. Vrakking[1], Thomas Fennel[6], and •Arnaud Rouzée[1] — [1]Max-Born-Institut, Berlin, Germany — [2]Institut für Optik und Atomare Physik, Technische Universität Berlin, Berlin, Germany — [3]CNR, Instituto di Fotonica e Nanotecnologie Padova, Padova, Italy — [4]Department of Physics, Politecnico di Milano, Milano, Italy — [5]CNR, Instituto di Fotonica e Nanotecnologie Milano, Milano, Italy — [6]Institut für Physik, Universität Rostock, Rostock, Germany

We present a single-shot coherent diffractive imaging (CDI) experiment based on high harmonic generation of individual He nanodroplets performed with a table-top femtosecond extreme ultraviolet (XUV) light source. Using a laser based HHG source, we are able to demonstrate for the first time the possibility to extract the shape, size, and orientation of free-flying nanoparticles. While most of the recorded diffraction patterns are assigned to the formation of spherical nanodroplets, we observed as well non-point symmetric diffraction patterns which are uniquely assigned to the formation of prolate, pill-shaped He-nanodroplets. Our experiment paves the way towards time-resolved imaging of ultrafast electron motion in individual clusters and nanoparticles with attosecond time resolution.

MO 3.2 Mon 17:30 N 6

Numerical simulations for characterizing and optimizing an aerodynamic lens — •Nils Roth[1], Salah Awel[1,2], Daniel Horke[1,3], and Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science, DESY, Notkestrasse 85, 22607 Hamburg, Germany — [2]Department of Physics, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]The Hamburg Center for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

Atomic resolution single-particle coherent diffractive imaging requires reproducible samples to reconstruct three-dimensional molecular structures from isolated particles [1]. Currently one of the major limiting factors is the inefficient delivery of particles and the correspondingly low number of strong diffraction patterns, collected during typical beam times. We build a numerical simulation infrastructure capable of calculating the flow of gas and the trajectories of particles through an entire aerosol injector, aiming to increase the fundamental understanding and to enable optimization of injection geometries and parameters. The simulation results are compared to literature studies and also validated against experimental data taken in an aerosol beam characterization setup [2]. The simulation yields a detailed understanding of the radial particle distribution and highlights weaknesses of current aerosol injectors. With the aid of these simulations we develop new experimental implementations to overcome current limitations and increase particle densities available for diffractive imaging experiments.

[1] M. M. Seibert, et al, *Nature* **470**, 78 (2011).
[2] Salah et al, *Opt. Exp.* **24**, 6507-6521 (2016)

MO 3.3 Mon 17:45 N 6

Femtosecond Diffractive Imaging of Coherent Nuclear Motion using Relativistic Electrons — Jie Yang[1], •Markus Gühr[2,3], Xiaozhe Shen[3], Renkai Li[3], Theodore Vecchione[3], Ryan Coffee[3], Jeff Corbett[3], Alan Fry[3], Nick Hartmann[3], Carsten Hast[3], Kareem Hegazy[3], Keith Jobe[3], Igor Makasyuk[3], Joseph Robinson[3], Matthew Robinson[1], Sharon Vetter[3], Stephen Weatherby[3], Charles Yoneda[3], Xijie Wang[3], and Martin Centurion[1] — [1]Department of Physics, University of Nebraska-Lincoln,Lincoln, NE, USA — [2]Institut für Physik und Astronomie,Universität Potsdam, Potsdam, Germany — [3]SLAC National Accelerator Laboratory, Menlo Park, CA, USA

Observing ultrafast changes in the molecular geometry after photoexcitation is crucial to understand the conversion of light energy into other energetic degrees of freedom within molecules. We present a time resolved electron diffraction study of a molecular vibrational wavepacket in photoexcited isolated iodine. We determine the time-varying interatomic distance with a precision 0.07 Å and a temporal resolution of 230 fs full width at half maximum. The method is not only sensitive to the position but also the shape of the nuclear wave packet.

MO 3.4 Mon 18:00 N 6

Ultrashort polarization-tailored bichromatic fields — •Stefanie Kerbstadt, Lars Englert, Tim Bayer, and Matthias Wollenhaupt — Carl von Ossietzky Universität Oldenburg, Institut für Physik, Carl-von-Ossietzky-Straße 9-11, 26129 Oldenburg

Ultrashort bichromatic laser fields with commensurable center frequencies, have emerged as a powerful tool to coherently control the dynamics of free electron wave packets [1]. Here we present a novel scheme for the generation of polarization-tailored bichromatic laser fields based on ultrafast pulse shaping techniques. The scheme utilizes a 4f polarization pulse shaper equipped with a composite polarizer in the Fourier plane for independent amplitude and phase modulation of two spectral bands of a whitelight supercontinuum [2]. The setup allows us to sculpture the spectral amplitude, phase and polarization profile of both colors individually, offering an enormous versatility of producible bichromatic waveforms. In addition, the scheme features built-in dispersion management and the option for shaper-based pulse diagnostics. We demonstrate the fidelity of the generated bichromatic fields by optical characterization and present first results of quantum control of bichromatic photoionization of atoms employing photoelectron imaging tomography.

[1] D.B. Milosevic et al., Phys. Rev. A 61 (6) (2000), 063403.
[2] S. Kerbstadt et al., J. Mod. Opt., accepted (2016).

MO 3.5 Mon 18:15 N 6

Electronic decoherence following photoionization: full quantum-dynamical treatment of the influence of nuclear motion — •Caroline Arnold[1,2,3], Oriol Vendrell[1,3,4], and Robin Santra[1,2,3] — [1]Center for Free-Electron Laser Science, DESY, Notkestrasse 85, 22607 Hamburg, Germany — [2]Department of Physics, University of Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany — [3]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany — [4]Department of Physics and Astronomy, Aarhus University, Ny Munkegade 120, 8000 Aarhus, Denmark

Photoionization using attosecond pulses can lead to the formation of coherent superpositions of the electronic states of the parent ion. However, ultrafast electron ejection triggers not only electronic but also nuclear dynamics—leading to electronic decoherence, which is typically neglected on time scales up to tens of femtoseconds. We propose a full quantum-dynamical treatment of nuclear motion in an adiabatic framework, where nuclear wavepackets move on adiabatic potential energy surfaces expanded up to second order at the Franck-Condon point. We show that electronic decoherence is caused by the interplay of a large number of nuclear degrees of freedom and by the relative topology of the potential energy surfaces. Application to H2O, paraxylene, and phenylalanine shows that an initially coherent state evolves to an electronically mixed state within just a few femtoseconds. In these examples, it is not the fast vibrations involving hydrogen atoms, but rather slow vibrational modes that destroy electronic coherence.

MO 3.6 Mon 18:30 N 6

Optimisation of strong laser field-free alignment using tailored light fields — •Evangelos Thomas Karamatskos[1,2], Sebastian Raabe[4], Andrea Trabattoni[1], Terry Mullins[1], Sebastian Trippel[1,2], Arnaud Rouzee[4], and Jochen Küpper[1,2,3] — [1]DESY, Hamburg, Germany — [2]Universität Hamburg, Germany — [3]CUI, Hamburg, Germany — [4]Max-Born Institute, Berlin, Germany

Alignment of molecules with respect to the laboratory fixed frame [1] enables the realization of a large variety of experiments such as the determination of molecular frame photoangular distribution (MFPAD's) [2] or laser induced electron diffraction (LIED) where typically a strong degree of alignment is needed [3]. We present a combined theoretical and experimental effort to optimise the degree of laser field-free alignment of molecules in the gas phase. We start by solving the time-dependent rotational Schrödinger equation coupled to a non-resonant laser field and a static electric field and use an iterative learning-loop algorithm to determine the ideal pulse shape that optimises the degree

of alignment. These calculations serve as a guide to complement the experiments where the alignment laser pulse form is optimally tailored. We discuss the simulation results and the experimental realization of two-pulse impulsive alignment on the example of the linear molecule carbonyl sulfide (OCS) and give an outlook for the use of pulse shaping techniques to achieve strongly aligned asymmetric top molecules.

[1] Stapelfeldt et al., Rev. Mod. Phys. 75, 543 (2003) [2] Hansen et al. Phys. Rev. Lett. 106, 073001 (2011) [3] Pullen et al., Nature Communications 6, 7262 (2015)