MO 10: Poster – Ultrafast Structural Dynamics

Time: Tuesday 17:00–19:00 Location: Philo 1. OG

MO 10.1 Tue 17:00 Philo 1. OG

Direct observation of uracil cation fragmentation via metastable intermediate — •Aditi Pradhan[1,2], Atilay Ayasli[1], Ivo S. Vinklárek[1], Hubertus Bromberger[1], Sebastian Trippel[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 Chemistry, Universität Hamburg, Germany — [3]The Hamburg Center for Ultrafast Imaging (CUI), Universität Hamburg, Germany

Nucleobases are remarkably photostable biomolecules with complex relaxation dynamics at picosecond timescales [1], making them ideal test beds to explore ultrafast fragmentation dynamics with atomic-scale precision. We employ the versatile transportable endstation for controlled molecules (eCOMO) [2] to study isolated uracil molecules as well as hydrated clusters in a size-selected fashion [3]. Our photodissociation experiment in the strong-field regime reveals a metastable fragmentation pathway of uracil cation, enabled by 3D imaging beamplots. The findings are supported by lifetime estimates and accompanied by preliminary theoretical results.

[1]Nachtigallová *et int.* (4 authors), Lischka, *J. Phys. Chem. A*,**21** 115 (2011)

[2]Jin *et int.* (8 authors), Küpper, submitted (2024), arXiv:2406.16491 [physics]

[3]Chang *et int.* (2 authors), Küpper, *Int. Rev. Phys. Chem.*, **34**, 1077838 (2015) arXiv:1505.05632 [physics]

MO 10.2 Tue 17:00 Philo 1. OG

Laser-Induced Electron Recollision in Molecular Targets Studied with a Reaction Microscope — •Martin Garro Gonzalez, Narayan Kundu, Julian Schröter, Janko Umbach, Horst Rottke, Arne Senftleben, and Jochen Mikosch — Institut für Physik, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Laser-driven electron recollision originates from strong-field ionization of atoms, molecules, and solids, where liberated electrons are accelerated by the oscillating laser field and driven back to the parent ion. This process underlies key strong-field phenomena, including non-sequential double ionization, high-harmonic generation, and laser-induced electron diffraction. A question of current interest is in which way electron recollision can be sensitive to the handedness of a chiral molecule. In recent proof of principle experiments, recollision-induced double ionization with elliptically polarized light has been shown to be chiral sensitive, and more recently photoelectron elliptical dichroism, arising from elastic rescattering, has demonstrated high chiral reponse. Here, we report advances in two recollision-driven phenomena. Using a reaction microscope, we investigate recollision-enhanced elliptical dichroism in chiral molecules with femtosecond strong-field studies of fragmentation and double ionization in methyl oxirane and limonene. Second, we will present our advances on controlling intensity- and wavelength-dependent Coulomb explosion of bromoiodomethane, investigating sequential and non-sequential channels.

MO 10.3 Tue 17:00 Philo 1. OG

Phase-dependent modulation of H2 dissociation in a bichromatic laser field — •Nikolas Rapp, Weiyu Zhang, Thomas Pfeifer, and Robert Moshammer — Max-Planck-Institut für Kernphysik, Heidelberg

The ionization and dissociation dynamics of H2 were investigated using a Reaction Microscope (ReMi). A femtosecond laser is shaped by a Spatial Light Modulator (SLM), enabling spectral control of the pulse in terms of amplitude, polarization, and phase. With the SLM, the laser pulse is split into two frequency components, with variable relative phase and temporal delay. The change of different dissociation pathways in terms of energy and yield with varying phase will be presented and compared to TDSE simulations.

MO 10.4 Tue 17:00 Philo 1. OG

Studying UV-induced dynamics in disulfide systems — •Sumukh Venkatesh Makam[1], James Merrick[2], Benoît Richard[3,4,5], Sergey Usenko[1], Robin Santra[3,4,5], Michael Meyer[1], Patrick A. Robertson[6], Matthew S. Robinson[1], and et al[1] — [1]European X-ray Free Electron Laser, Schenefeld, Germany — [2]Department of Chemistry, University of Oxford, Oxford, UK — [3]CFEL, DESY, Hamburg, Germany — [4]Department of Physics, University of Hamburg, Hamburg, Germany. — [5]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany. — [6]School of Chemistry, University of Nottingham, Nottingham, UK

Disulfide bonds (S-S) have a critical role in everyday chemistry, defining the tertiary structure of proteins. However, they undergo ultrafast fission when exposed to UV light leading to protein denaturation [1,2].

1,2-Dithiane is a model system that simulates the structural constraints of S-S bonds in proteins, and theoretical work predicts that it undergoes a cyclic ring-opening/closing process via S-S bond fission following UV (266 nm) excitation [2]. We present recent results obtained at the EuXFEL SQS Instrument in which these dynamics were captured via Coulomb Explosion Imaging.

In addition we also detail future plans to investigate the competing S-S and S-C fission processes following 200 nm absorption.

[1] A.B. Stephansen, et al., J. Am. Chem. Soc. 134, 20279 (2012).

[2] C.D. Rankine, et al., Phys. Chem. Chem. Phys. 18, 27170 (2016).

MO 10.5 Tue 17:00 Philo 1. OG

Formation of transient nanotips from plasmonically superheated silver nanocubes — •Nora Sigrist[1], Thomas Reichenbach[2], Alessandro Colombo[1], Bernd von Issendorf[3], and Daniela Rupp[1] for the SilverCubesAtSwissFEL-Collaboration — [1]ETH Zurich, Zurich, Switzerland — [2]IWM Fraunhofer, Freiburg, Germany — [3]University of Freiburg, Freiburg, Germany

The ultrafast structural dynamics of silver nanocubes are explored after excitation by an optical laser pulse tuned to their surface plasmon resonance. We used the intense X-ray pulses of SwissFEL to obtain single-shot single-particle coherent diffraction images (CDI) of their evolution. Under certain experimental conditions, we find the formation of complex transient geometries, six-legged nanostructures of about twice the size of the original nanocube. Matching this phenomenon with large-scale molecular dynamics simulations enables us to extract physical quantities of warm dense matter on the nanoscale, such as the viscosity of liquid silver at extreme temperatures and pressures, typically hardly accessible in a laboratory environment.