Symposium Coulomb Explosion Imaging (SYCE)

jointly organized by
the Atomic Physics Division (A),
the Molecular Physics Division (MO), and
the Mass Spectrometry Division (MS)

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Coulomb explosion imaging, using intense table-top lasers or x-ray pulses, allows to measure molecular structure and structural dynamics even for dilute gas-phase samples. It combines high temporal resolution, high sensitivity with recently demonstrated high spatial resolution. Especially in combination with conicidence or covariance measurements of the electrons it also allows to obtain higher-order correlations. Thus, it is an ideal tool for the investigation of ultrafast molecular dynamics.

Overview of Invited Talks and Sessions

(Lecture hall Paulussaal)

Invited Talks

SYCE 1.1	Tue	11:00–11:30	Paulussaal	**Dissociation of halogenated organic molecules induced by soft X-rays – pathways and early stages** — •Edwin Kukk
SYCE 1.2	Tue	11:30–12:00	Paulussaal	**X-ray induced Coulomb explosion imaging with channel-selectivity** — •Rebecca Boll
SYCE 1.3	Tue	12:00–12:30	Paulussaal	**Time-resolved Coulomb Explosion Imaging using X-ray Free-Electron Lasers** — •Till Jahnke
SYCE 1.4	Tue	12:30–13:00	Paulussaal	**Dynamics and control of microsolvated biomolecules studied by Coulomb explosion imaging** — •Sebastian Trippel, Jochen Küpper

Sessions

SYCE 1.1–1.4	Tue	11:00–13:00	Paulussaal	**Coulomb-Explosion Imaging**

SYCE 1: Coulomb-Explosion Imaging

Time: Tuesday 11:00–13:00 Location: Paulussaal

Invited Talk SYCE 1.1 Tue 11:00 Paulussaal

Dissociation of halogenated organic molecules induced by soft X-rays – pathways and early stages — •Edwin Kukk — Dept of Physics and Astronomy, Uniersity of Turku, Turku, Finland

While the highly energetic Coulomb explosions of highly charged molecules have received considerable recent interest as a method for probing molecular geometry, a low-charge dissociation of organic molecules is a much gentler process following often quite intricate multi-step pathways. We have studied such processes in halogenated organic molecules, such as thiophene derivatives, using various multi-particle techniques, synchrotron as well as FEL radiation and pump-probe schemes. In this talk, insights obtained from these studies and theoretical modeling are presented. Also, some more applied aspects of such studies, related to radiosensitizers in radiotherapy, are covered.

Invited Talk SYCE 1.2 Tue 11:30 Paulussaal

X-ray induced Coulomb explosion imaging with channel-selectivity — •Rebecca Boll — European XFEL, Schenefeld, Germany

The short and intense X-ray pulses from free-electron lasers are an exquisite tool for Coulomb explosion imaging (CEI) [1-3]. Snapshot images of the complete structure of complex molecules, including all hydrogens, can be captured. The rapid charge-up leads to a violent Coulomb explosion that preserves the information about the molecular structure at the instant of ionization. This allows studying processes such as the influence of transient resonances [4], intramolecular charge rearrangement [1] and molecular fragmentation [3].

Moreover, the multidimensionality of CEI can allow to specifically investigate certain aspects of molecular structural dynamics. We recently demonstrated how X-ray induced CEI can be used to trace a molecular elimination reaction, a minority reaction channel that involves the breaking of two molecular bonds and the formation of a new one [5]. Simultaneously, we mapped light-induced bending vibrations of a bound molecular wave packet, disentangled different dissociation pathways, and directly imaged correlated dynamics leading to ejection of a newly formed molecular fragment.

[1] R. Boll et al., Nat. Phys. 18, 423 (2022)
[2] X. Li et al., Phys. Rev. Res. 4, 013029 (2022)
[3] T. Jahnke et al., Phys. Rev. X 11, 041044 (2021)
[4] X. Li et al., Phys. Rev. A 105, 053102 (2022)
[5] X. Li et al., in preparation (2023)

Invited Talk SYCE 1.3 Tue 12:00 Paulussaal

Time-resolved Coulomb Explosion Imaging using X-ray Free-Electron Lasers — •Till Jahnke — Max-Planck-Institut für Kernphysik, Heidelberg, Germany

Recording real-time movies of dynamical processes in molecules, as, for example, progressing chemical reactions, has been a driving force for many disciplines in fundamental sciences during the last decades. A comparably new experimental technique that addresses single molecules in the gas phase and that involve coincident single-particle detection for imaging these dynamics is Coulomb explosion imaging. This approach uses (for example) ultrashort light pulses to (heavily) fragment the inspected molecules in order to gather such information from the breakup pattern.

X-ray free-electron lasers are able to produce ultrashort light pulses with highest intensity, which are perfectly suitable to perform measurements along these lines. In particular, these light sources allow for time-resolved studies in a pump-probe scheme by adding ultrashort UV pulses that are synchronized with the X-ray flashes (or by employing X-ray pump/X-ray probe schemes). Since almost five years a dedicated COLTRIMS reaction microscope [1,2] is available at the SQS-instrument of the European X-ray free-electron laser, which was used recently to perform time-resolved Coulomb explosion imaging measurements. Some examples will be presented in the talk.

[1] J. Ullrich et al., Rep. Prog. Phys. 66, 1463(2003).
[2] T. Jahnke et al., JESRP 141, 229(2004)

Invited Talk SYCE 1.4 Tue 12:30 Paulussaal

Dynamics and control of microsolvated biomolecules studied by Coulomb explosion imaging — •Sebastian Trippel[1,2] and Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science CFEL, Deutches Elektronen-Synchrotron DESY, Hamburg — [2]Center for Ultrafast Imaging, Universität Hamburg — [3]Department of Physics, Universität Hamburg

Microsolvated biomolecules are promising model systems to study the corresponding light-induced dynamics of molecules in solution [1]. Due to the still manageable complexity of the small clusters, atomic, molecular, and optical physics methods can be used for the analysis and characterization of their dynamics. Coulomb explosion imaging is one of those methods that can be applied to distinguish the various reaction channels present. Furthermore, it allows to determine the orientation of molecules or clusters in the gas phase [2]. In this presentation, our findings on the ionization dynamics of pyrrole-water and water-dimer will be presented. In addition, we will discuss our results on the field-free alignment of complex molecules in the gas phase using pulse shaping [3].

[1] L. He, *et int.* (8 authors), J. Küpper, *J. Phys. Chem. Lett.* **14**, 10499 (2023)
[2] H. Stapelfeldt and T. Seideman, *Rev. Mod. Phys.* **75**, 543 (2003)
[3] T. Mullins, *et int.* (9 authors), J. Küpper *et al.*, *Nat. Commun.* **13**, 1431 (2022)