Multi-particle analysis of ultrafast molecular photoreactions

In the attosecond science and technology group at CFEL (CFEL-ATTO, <u>https://atto.cfel.de</u>), we generate ultrashort laser pulses with attosecond (1 fs = 10^{-18} s) or few-femtosecond (1 fs = 10^{-15} s) duration. We use them to trigger photoreactions in molecules (often biologically relevant ones) and to follow in real-time how the atoms and electrons move and interact. With our research we aim at understanding and potentially manipulating ultrafast processes and, ultimately, the early steps of photochemistry. Such processes are very difficult to simulate accurately even with supercomputers. Experiments are therefore essential for driving this research field and in the long run possibly improve the general ability to design efficient reactions and materials.

The CFEL-ATTO group in Hamburg can host up to two students, who will learn about experimental methods in ultrafast laser and molecular science, as well as the scientific motivations and challenges driving this research field. Due to the COVID-19 pandemic our students will join the group "virtually", with online meetings, training sessions and discussions but most likely without the possibility to work in the laboratory. The student(s) will analyse experiments that have already been performed, but possibly not yet analysed by anyone else. In this context, after initial training they will be involved in the analysis of photon spectra and combined photoion/photoelectron data.

Our main beamline can provide ultrashort pulses in several different spectral ranges: near-infrared, ultraviolet (which is unusual) and extreme-ultraviolet, where the latter gives the finest time resolution and the broadest spectrum. During the past few years, we have studied a wide variety of samples from water (individual molecules or clusters of a few hundred), fullerenes, chiral hydrocarbons and biomolecules such as amino acids and DNA-building blocks.

We are currently extending the capabilities of our lab. During the summer of 2021 the focus will be on generating attosecond pulses with higher photon energy, into the soft x-ray regime which will allow samples in liquid rather than gaseous phase, and where spectral fingerprints of specific atoms within large molecules can give site-specific information. It is thus likely that the students can help develop the ability to analyse the first soft x-ray spectra from a new x-ray spectrometer, as well as participate in the ongoing beamline development via online meetings.

We will provide personal online training in using our software for multi-dimensional data treatment, on top of which you will make program scripts to perform calibration, filtering and produce different types of diagrams. For students interested in more independent programming or details about the spectrometer operation we can adjust the difficulty level. Based on your conclusions and ideas about further questions to investigate, your work will via discussions with us lead to a more refined understanding of one or a few experiments, as well as some typical methods and approaches for studying matter on the time scale of electrons and ultrafast chemical reactions.

Inspirational photos and figures



(Left) The CFEL-ATTO group with two summer students during 2019. (Right) Part of our lab, showing the beamline under construction and the current main beamline.



(Top row) Velocity map images of electrons, and visualizations of time-resolved scans with such data. (Bottom right) time-resolved scan of mass spectra, and (middle right) a diagram of time-dependence for one selected ion.

Contact information

<u>Francesca.Calegari@desy.de</u>, professor and group leader. Tel. 040-8998-6369. <u>Andrea.Trabattoni@desy.de</u>, project leader/team leader. Tel. 040-8998-6048. <u>Vincent.Wanie@desy.de</u>, postdoc/scientist. Tel. 040-8998-3127. <u>Erik.Maansson@desy.de</u>, postdoc/scientist. Tel. 040-8998-6042.