CFEL SCIENCE

SEMINAR

17th February 2021 - 2:00 p.m.

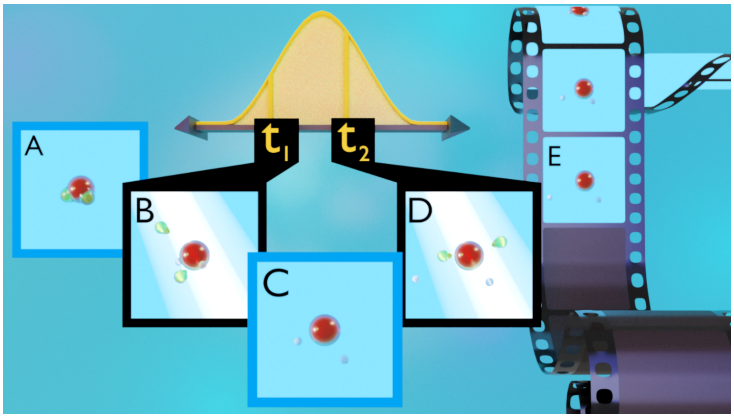
Virtual meeting room in ZOOM (ID: 992 7237 2470 / PW: 755622)

Ludger Inhester

Center for Free-Electron Laser Science, DESY, Germany

Imaging the x-ray induced fragmentation of small molecules

Understanding the radiation induced dynamics of molecules is a crucial step for many research areas. Intense x-ray pulses provide novel tools to image the immediate response of molecules to high-energy radiation. Theoretically following the dynamics after core-shell photoionization and Auger decay is particularly challenging because of the many electronic decay channels and the involved potential energy surfaces on which the molecular geometries evolve. In this talk I want to present my contributions to disentangle the coincident signals in recent XFEL experiments with small molecules, specifically water (H_2O) and nitrogen (N_2). I demonstrate how ab-initio simulations enable us to extract crucial information from coincident data recorded from events involving multiple photoionizations. Even though the data has been recorded employing a single, ultrashort x-ray pulse, time-dependent information on the dynamics triggered by the first photoionization and the ensuing Auger decay can be extracted. For H_2O, I demonstrate that we can image the immediate deformations of the molecule geometry after photoionization and Auger decay. In particular we observe strong unbending and asymmetric stretching. For N_2, I demonstrate that the K-shell photoelectron spectrum exhibits detailed information on the breakage of the chemical bond.



References: T. Jahnke *et al.,* submitted; X. Li *et al.,* Sci. Rep. **11**, 505 (2021); L. Inhester *et al.,* J. Phys. Chem. Lett. **10**, 6536 (2019).

Host: Robin Santra – CFEL-DESY Theory Division