CFEL SCIENCE

SEMINAR

21st December 2022 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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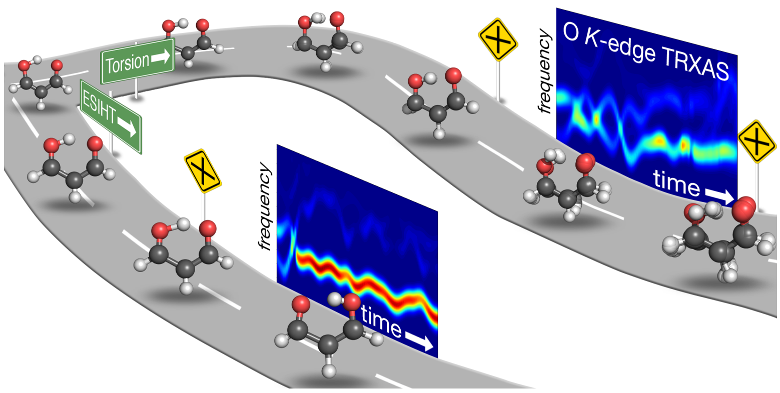
In silico pump-probe experiments of photochemical processes using ultrafast X-ray and electron probes

The importance of photoinduced processes is hard to overstate: they are ubiquitous in nature and represent the prime mechanism powering life on our planet. Indeed, the additional energy introduced by light can drive processes in molecules and materials significantly different from those available under thermal conditions (e.g., charge/energy transfer, chemical transformation or mechanical action). Advances in optics have taught us ways to precisely generate and manipulate light that allow unprecedented control of the optical laser initiation step. The practical use of light then relies critically on our ability to understand the fate of the nonequilibrium state and how it can be controlled.



In this seminar, I review our approach to *in silico* photochemical experiments based on first principles that allows us to simulate what might happen upon photoexcitation. However, simulating the photoinduced dynamics itself does not suffice: whether theory/simulation takes on an exploratory (foregoes experiment) or an interpretative (follows) role, it is critical to also enable a direct link to experiments through the explicit simulation of observables. I will discuss the extension of our theoretical framework to pump-probe schemes involving ultrafast electron and X-ray probes and further examine how the commonly used electric-dipole approximation performs in the X-ray domain. Finally, I will present results from ongoing joint theory–experiment efforts focused on unveiling ultrafast hydrogen motion using X-rays and relativistic electrons.

Host: Robin Santra – CFEL-DESY Theory Division