CFEL SCIENCE

SEMINAR

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

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

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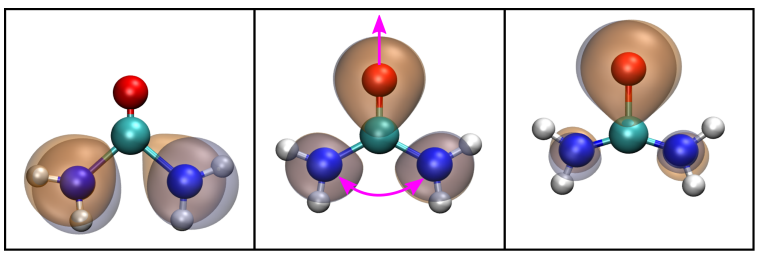
Machine learning reveals the most significant collective coordinate influencing time-resolved x-ray absorption spectra in ionized urea and its dimer

Investigating the early dynamics of chemical systems following ionization is essential for our understanding of radiation damage. Time-resolved x-ray absorption spectroscopy (TRXAS) on a femtosecond timescale, in combination with appropriate simulations, is able to provide crucial insights into the ultrafast processes that occur upon ionization due to its element specific probing nature. However, it can be very challenging to get a clear interpretation of the spectral features, due to the complex nature of the dynamical processes after ionization.

In this talk, I will discuss how machine learning techniques can unravel specific structural dynamics in a molecule that induce time-dependent changes in the x-ray absorption spectra. By applying these techniques, collective coordinates that most influence the spectra are obtained from simulated *ab initio* nonadiabatic trajectories. The ability of TRXAS to reveal rich insights into the dynamics of valence-ionized urea and its dimer is hence shown. For urea, I elucidate the possibility to trace effects of specific molecular vibrations in its TRXAS. For its dimer, where ionization triggers a proton transfer reaction, I show how the spectra can reveal specific details on the progress of proton transfer reaction.



Collective coordinate along with the hole orbital for ionized urea

References:

[1] Shakya *et al.*, submitted.

[2] Loh *et al.*, Science 367, 179–182 (2020).

[3] Khalili *et al.*, Struct. Dyn. 6, 044102 (2019).

Host: Robin Santra – CFEL-DESY Theory Division