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Femtosecond X-ray Experiments: combining local and global observables for chemical dynamics studies

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Abstract:

In solution-phase photochemistry dynamic solute-solvent interactions can drive the reaction pathway, outcome and efficiency of a chemical reaction. Such interactions involving many-body dynamic processes take place on femtosecond (fs) to picosecond (ps) time scales, and involve simultaneous electronic and structural changes both within the molecule and beyond. Ultrafast structural tools sensitive to both the intramolecular electronic (including spin states) and nuclear changes as well as the local solvent structural changes would permit to disentangle the elementary steps in photochemical reactivity. X-ray emission spectroscopy (XES) is sensitive to electronic changes, such as oxidation and spin states, while X-ray Absorption Spectroscopy (XAS) tools deliver information about the local geometric structure around the selected absorbing atom. Combining those with wide-angle X-ray scattering (WAXS) in one single setup in the femtosecond time domain at the X-ray Free Electron Laser (XFEL), we seek to deliver a more complete picture of the ensuing dynamic processes occurring during the course of a light-driven chemical reaction.

I will present the state-of-the-art in selected scientific case examples employing combined femtosecond X-ray scattering and X-ray spectroscopies to study liquid-phase chemical reaction dynamics. These studies guided the design of the FXE (Femtosecond X-ray Experiments) scientific instrument at the European XFEL facility, which is now operational since September 2017 and has been successfully used to carry out first user pump-probe experiments. This scientific instrument aims to deliver a more complete picture of the elementary steps in chemical reactivity, which includes the ultrafast orbital and spin electronic changes together with the actual structure changes.

