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Observing molecular dynamics with ultrafast X-ray spectroscopies and scattering

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Ultrafast structural dynamics is an emerging field aiming to deliver a detailed understanding of the elementary steps in reacting chemical species, which involve changes in their nuclear, electronic and spin states. Such processes are vital ingredients in chemistry and biology, but also in technological applications, including efficient charge transport in light harvesting molecules and ultrafast switchable molecular magnets.
In order to unravel this complex dynamic behavior we have implemented a suite of ultrafast X-ray spectroscopic and scattering tools to zoom into both the electronic and nuclear structures, with the goal to ultimately deliver a molecular movie of ongoing chemical processes. In view of the many potential applications in chemical and biological dynamics it is desirable to increase the signal-to-noise (S/N) level of such experiments as well as to decrease the time resolution into the femtosecond time domain.
We present our benchmark results using a versatile setup that permits simultaneous measurements of ultrafast X-ray absorption and emission spectroscopies combined with X-ray scattering, which has been recently implemented by us at different synchrotrons and XFELs. We applied it to study different photochemical reactions, ranging from nascent radicals in solution, molecular spin transitions and ligand exchange reactions to photocatalytic systems, with the goal to deliver a deeper understanding of the elementary steps in chemical reactivity.

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