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Tracking chemical reactions 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 solar energy converters and ultrafast switchable molecular magnets. In order to unravel the complex dynamic behavior in photoexcited molecules 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 diffuse scattering. This combined scattering and spectroscopic approach has recently been established by us at different synchrotron [1-2] and XFEL [3] lightsources. We applied it to study different photochemical systems in liquid media, ranging from nascent radicals in solution to photocatalytic systems, with the goal to deliver a deeper understanding of the elementary steps in chemical reactivity.

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