Probing dynamics of chemical bonds in organic chromophores by X-ray spectroscopies

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Chemical bonding patterns fundamentally change when molecules dynamically evolve in electronically excited states created by optical excitations. These dynamics give rise to many useful properties and functionalities, which can be resolved in space and time at modern XFEL facilities. In this talk I will overview some possible measurements that can be done with X-ray lasers suggested by computational investigations. In the first example, we use dynamical simulations to compute X-ray Raman signals, which are able to monitor the coherence evolution in molecular photoswitches. Time-resolved X-ray diffraction can further probe key chemical features during the ultrafast dynamics. In the first example, X-ray Circular Dichroism (XCD) can exploit the localized and element-specific nature of X-ray electronic transitions. XCD therefore is more sensitive to local structures and the chirality probed with it can be referred to as local which in contrast to a conventional Optical Circular Dichroism probing the global molecular chirality.

Relevant references

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