

## Ab initio simulations of X-rays probing ultra-fast dynamics

We employ quantum chemical calculations and molecular dynamics simulations in the study of ultra-fast solution dynamics. The theoretical tools are crucial for the interpretation of X-ray and photo-electron spectra of aqueous solutions.

Simulations of photo-induced chemical processes require a computational framework, in which we can calculate spectra in excited states and of molecules undergoing dissociative dynamics. Hence, we have chosen to work with multi-configurational (restricted active space SCF) quantum chemical calculations, which can give a balanced description of many electronic states simultaneously. This is essential both for the description of the dynamical processes and for the spectrum simulations in particular for resonant inelastic X-ray scattering process.

The theoretical tools also allow for the simulation of dynamical effects inherent in the spectroscopies, such as core-hole induces proton-transfer.

Applications to aqueous electrolyte are presented

- the effects of hydrogen bonding around tri-iodide
- the pH dependence in the x-ray emission of simple amino acids
- L-edge x-ray absorption of transition metal complexes

showing the importance of combining experimental and theoretical data for reaching insights into the electronic structure and ultra-fast dynamics.

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