Modelling time-resolved X-ray absorption spectroscopy using ADC

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In recent years, *time-resolved X-ray absorption spectroscopy* (TRXAS) has emerged as a novel experimental technique. It is used to gain insight into electronic structure changes occurring during photochemical processes. However, the interpretation of experimental spectra is challenging and often relies on supporting theoretical simulations.

Here, we present a novel methodology for the electronic structure simulation of TRXAS spectra based on *Algebraic Diagrammatic Construction* (ADC) theory.[1] In this approach, we combine the highly accurate core-valence separation ADC (CVS-ADC) approximation for the description of core-excited states with ADC up to third order for valence-excited states.

The new method is combined with *ab initio* on-the-fly nonadiabatic dynamics calculations for the valence excited states of pyrazine and simulations of the femtosecond time-resolved UV-pump X-ray-probe signal in the doorway-window approximation.[2] The results are compared with recent experimental data for pyrazine.[3]

References

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