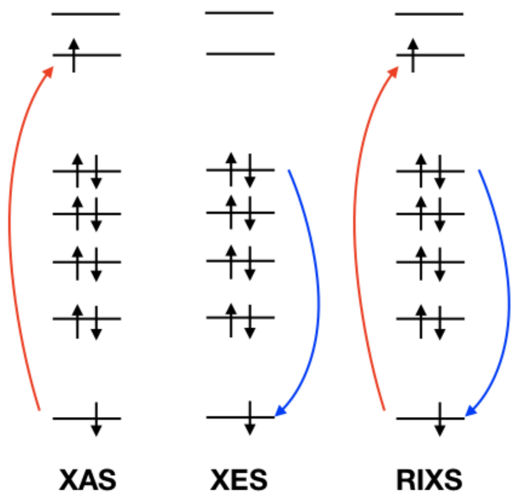
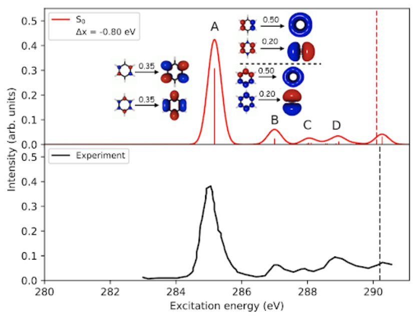
Correlated Methods for Core-Level Spectra



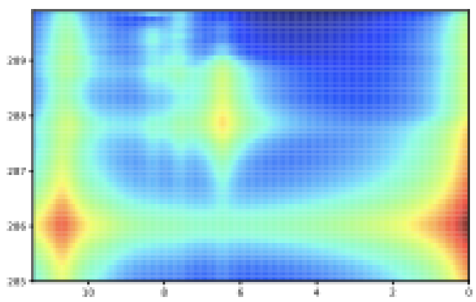
Core-valence separation within the EOM-CC and ADC frameworks enables accurate calculations of core-ionized and core-excited states and relevant spectroscopic properties

Features include:

- XAS (X-ray absorption), XPS (X-ray photoelectron), XES (X-ray emission), and RIXS (resonant inelastic X-ray scattering) spectra;
- Calculations of transition properties between valence and core-level states;
- Natural Transition Orbitals and Dyson orbitals for spectral assignments;
- Solvent effects via QM/MM and EFP.



(a) Simulated XAS for benzene



(b) Simulated RIXS for benzene

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