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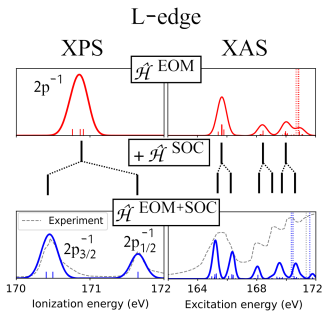
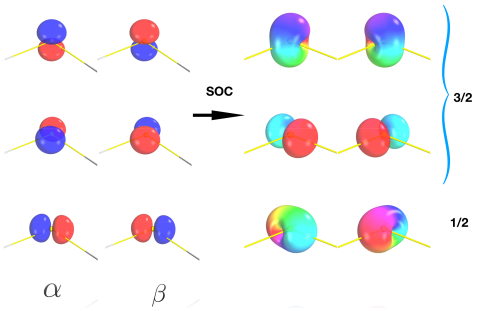
# Simulating L-edge X-ray Absorption and Photoelectron Spectra with Equation-of-Motion Coupled-Cluster Methods

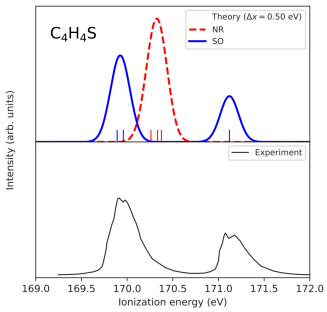


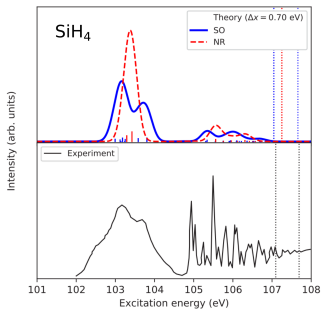

Simulations of L-edge X-ray spectra require inclusion of spin-orbit coupling (SOC), which splits $2p$ core-electron levels. The spectra are computed by a two-step state-interaction procedure:

- Zero-order non-relativistic states are computed using appropriate variants of the EOM-CC family of methods augmented by the fc-CVS scheme to allow access to core-level states (fc: frozen core; CVS: core valence separation). For example, fc-CVS-EOM-IP describes core-ionized states and EOM-EE/SF describes for core-excited states.
- These zero-order states are mixed by SOC perturbation, yielding the SOC-corrected energies and transition properties. SOC matrix elements are evaluated using the Breit-Pauli Hamiltonian and non-relativistic fc-CVS-EOM-CCSD wave functions.

L-edge X-ray absorption spectroscopy (XAS) and X-ray photoelectron spectroscopy (XPS) simulations are supported.




(a) Thiophene ($C_4H_4S$) L-edge XPS




(b) L-edge XAS of $SiH_4$

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