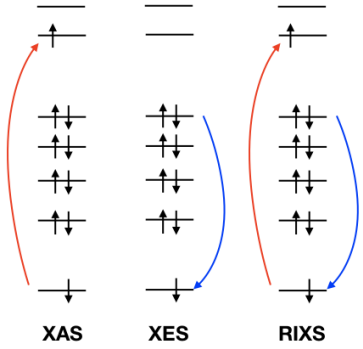
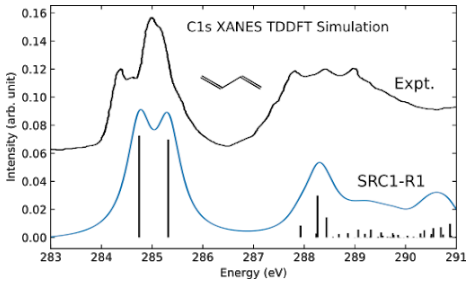
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Simulating X-ray Spectra with Q-Chem

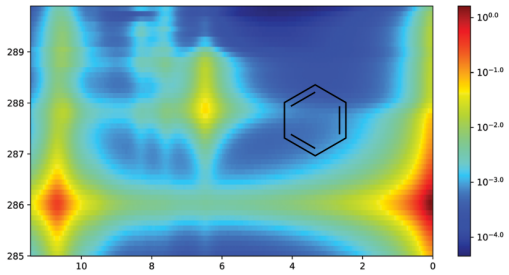


- In Q-Chem, the truncated excitation space and core-valence separation approximations are adopted in the time-dependent density functional theory (TDDFT), equation-of-motion coupled cluster (EOM-CC) and algebraic diagrammatic construction (ADC) frameworks, which enables calculations of core-excited and core-ionized states and relevant spectroscopic properties.
- EOM-CC and ADC are high-level correlated methods which can offer accurate simulated X-ray spectra.
- TDDFT has a good balance between computational accuracy and cost, making it a widely used tool in X-ray spectroscopy simulation.

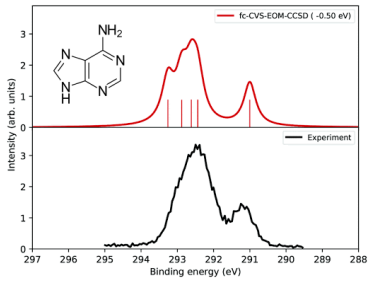
- XAS (X-ray absorption), XPS (X-ray photoelectron), XES (X-ray emission) and RIXS (resonant inelastic X-ray scattering) spectra can be simulated.
- Transition properties between valence and core-level states can be calculated.
- The simulated spectral features can be analyzed with natural transition orbitals and Dyson orbitals, both of which can be visualized with IQmol.
- Solvent effects can be included explicitly via QM/MM and effective fragment potential (EFP).



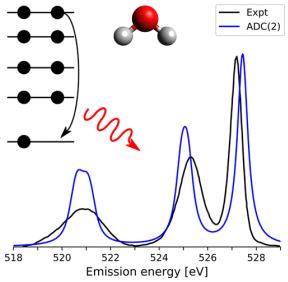
Simulated XAS of butadiene using TDDFT



Simulated C K-edge RIXS of benzene using EOM-CC



Simulated C K-edge XPS of adenine using EOM-CC



Simulated O K-edge XES of H2O using ADC

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