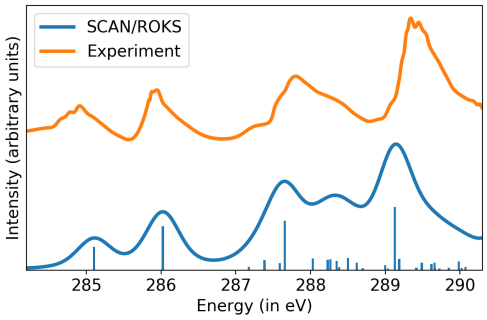
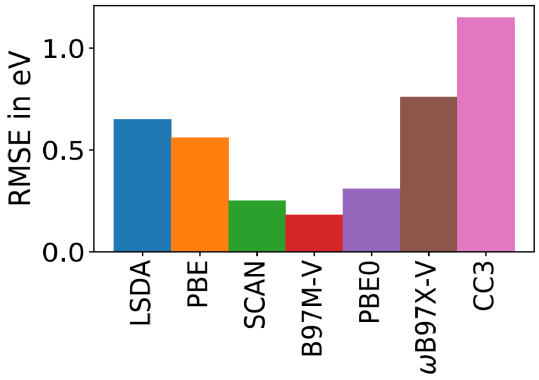
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

X-Ray Absorption Spectroscopy with ΔSCF/ROKS



(a) XAS spectrum of thymine

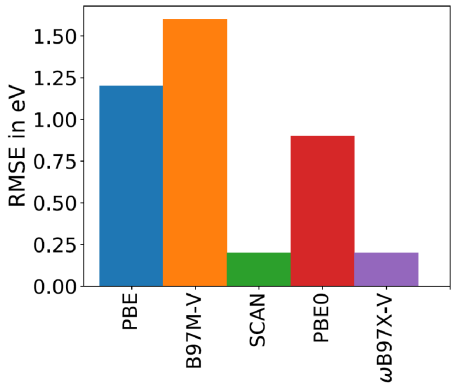


(b) ΔSCF benchmark for double excitations

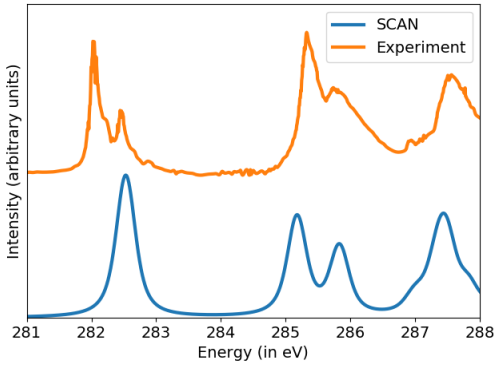
ΔSCF/ROKS ansätze enables KS-DFT calculations of excited states. Square Gradient Minimization (SGM) algorithm affords cheap (at the ground-state scaling) and reliable (without collapsing to ground-state orbitals) optimization of excited-state orbitals.

Highlights:

- Effective for states that TDDFT either misses (double excitations) or catastrophically fails to describe (charge-transfer, core excitations);
- Computes XAS (X-ray absorption spectra) for closed-shell and radical species, without empirical shifts;
- Can be used to compute excitation energies, optimized geometries, and frequencies;
- Can be applied to large systems due to low computational cost.



(a) RMSE of ROKS for K-edge core-excitation energies



(b) XAS of allyl radical

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