P5007: An Edge-Specific Scheme For Equation-of-motion Coupled-Cluster calculations of X-Ray Absorption Spectra

Xuechen Zheng, Chaoqun Zhang, Lan Cheng, Johns Hopkin University

Augmenting the standard correlation-consistent basis sets for the target atom is an efficient method to treat core-excited Rydberg states.

Triple excitations are important to give an accurate relative shift between 1s -> π^* and first Rydberg transition.

CVS-EOM-CC/cc-pVTZ+4spd calculations managed to provide a good assignment of the experimental spectrum for ESCA molecule.