AN EDGE-SPECIFIC SCHEME FOR EQUATION-OF-MOTION COUPLED-CLUSTER CALCULATIONS OF X-RAY ABSORPTION SPECTRA

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We present an edge-specific scheme for calculating near edge x-ray absorption fine structure (NEXAFS) spectra using core-valence separated equation-of-motion coupled-cluster (CVS-EOM-CC) theory. [1,2] Standard correlation-consistent basis set for the atom where targeted core excitation takes place is systematically augmented with diffuse s-, p-, and d-type functions to accurately describe Rydberg-type core excitations with diffuse character. It is also shown that triple excitations in CVS-EOM-CC methods not only are important for obtaining accurate absolute values of core excitation energies, but also make significant contributions to relative shifts between local and Rydberg core excitations. Quadruples excitations are shown to be relevant when aiming at high-accuracy calculations of absolute values.

Reference

[1] L. S. Cederbaum, W. Domcke, J. Schirmer, and W. von Niessen, Phys. Scripta 21, 481 (1980).
[2] S. Coriani, and H. Koch, J. Chem. Phys. 143, 181103 (2015).