Towards accurate calculations of core-level spectroscopy using relativistic coupled-cluster techniques

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The presentation focuses on the performance and applicability of techniques based on coupled-cluster theory [1] including scalar-relativistic delta-coupled-cluster (ΔCC) methods [2, 3] and equation-of-motion coupled-cluster (EOMCC) methods [4-6] in calculations of core-level spectroscopy. Formulation and implementation of core-valence separation scheme [7] is analyzed in detail for both ΔCC and EOM-CC methods aiming to obtain high accuracy in computed core ionization and excitation energies. Molecular applications presented here are focused on single and double core ionization energies.

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