Equation-of-motion and response-theory coupled-cluster approaches to linear and non-linear spectroscopic effects across different frequency regions.

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Coupled-cluster (CC) wave-function based methods play an important role in theoretical chemistry as they serve as accurate frameworks for simulating molecular properties and benchmarking computationally cheaper theoretical approaches. We summarize here our recent development of CC methods for the simulation of various linear and non-linear spectroscopic effects in the UV-vis and X-ray frequency regions. These include EOM-CCSD protocols to simulate ground and excited state electronic circular dichroism [1], x-ray natural circular dichroism at K- and L-edges [1], and x-ray two-photon absorption [2], as well as a damped response RI-CC2 framework for magnetic circular dichroism [3] and RI-CC2 studies of nuclear spin-induced circular dichroism [4]. Our results serve to illustrate the range of spectroscopies available for investigation via coupled-cluster theory.

References

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