

Advances in Relativistic Time-Dependent Configuration Interaction Methods

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Real-time electronic structure methods describe the direct response of a quantum mechanical system to a time-dependent perturbation without the usual constraints of time-dependent perturbation theory (i.e. response theory). Such approaches enable the investigation of strong-field dynamics and ultrafast spectroscopy directly in the time domain. Time-dependent configuration interaction algorithms in particular can be readily modified to include heuristic ionization models, spin-orbit coupling, and multiconfigurational reference wave functions. Advances in the implementation and application of these methods are discussed, with a focus on relativistic corrections in small molecules.