

Cavity quantum electrodynamics via time-dependent configuration interaction theory

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Resonances between an electronic excitation in a molecule and a photonic mode of a cavity produce hybrid electron-photon states, known as polaritonic states, which have a number of useful photochemical properties. We implement the effects of a resonant cavity into the time-dependent configuration interaction (TDCI) method to model strong light-matter interactions. The TDCI method is a real-time quantum electron dynamics method based on an expansion of the time-dependent wavefunction in the time-independent CI eigenstates. Transitions between states are induced via an external electric field, and the effects of a resonant cavity are introduced via a model Hamiltonian. This method is used to study the cavity-induced dipole-switching dynamics in small polar molecules.