Title: The Simplest Possible Approach for Simulating S_0-S_1 Conical Intersections with DFT/TDDFT — Adding *One* Doubly Excited Configuration

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Abstract:
A simple combination of DFT/TDDFT and configuration interaction is presented to fix up the incorrect topology of the S_0-S_1 conical intersection (CI) and allow a description of bond making and bond breaking in photo-induced dynamics. The proposed TDDFT-1D method includes one lone optimized doubly excited configuration in addition to the DFT/TDDFT singly-excited states within the context of a large configuration interaction Hamiltonian. Results for ethylene and stilbene are provided to demonstrate that this ansatz can yield physically meaningful potential energy surfaces near S_0-S_1 avoided crossings, without changing the vertical excitation energies far from the relevant crossings. We also investigate the famous linear water example (Levine *et al.*, Mol. Phys., 104, 1039 (2006)) to show that the algorithm calculates the correct topology of the S_0-S_1 CI and yields the correct geometric phase.