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Self-interaction-free TDDFT for nonperturbative treatment of multiphoton processes of heteronuclear diatomic molecular systems in intense laser fields JOHN HESLAR, SHIH-I. CHU, University of Kansas — We present a *self-interaction-free* time-dependent density-functional theory (TDDFT) with proper asymptotic *long-range* potential for nonperturbative treatment of multiphoton processes of many-electron heteronuclear molecular systems in intense laser fields. A *time-dependent generalized pseudospectral* method is developed with the use of a new mass-weighted prolate spheroidal coordinate system for accurate solution of the electronic structure and TDDFT equations for two-center heteronuclear diatomic systems. The procedure allows *nonuniform* and optimal spatial grid discretization of the Hamiltonian in the adapted prolate spheroidal coordinates and a split operator scheme in *energy* representation is used for the time propagation of individual molecular spin orbital's in space and time. The theory is applied to a detailed *all-electron* study of high-order harmonic generation (HHG) and multiphoton ionization processes of CO in intense laser fields. Both even and odd-order harmonics are predicted for the CO molecule.

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