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High-Order Harmonic Generation of Homonuclear and Heteronuclear Diatomic Molecules: Exploration of Multiple Orbital Contributions[1] JOHN HESLAR, National Taiwan University, Taiwan, DMITRY A. TELNOV, St. Petersburg State University, Russia, SHIH-I CHU, University of Kansas — We extend the *self-interaction-free* time-dependent density functional theory (TDDFT) approach with proper asymptotic long-range potential for nonperturbative treatment of high-order harmonic generation (HHG) of diatomic molecules. A time-dependent two-center generalized pseudospectral method in prolate spheroidal coordinate system is used for accurate and efficient treatment of the TDDFT equations in space and time. The theory is applied to a detailed *all-electron* nonperturbative investigation of HHG processes of homonuclear (N_2 and F_2) and heteronuclear (CO, BF, and HF) molecules in intense ultrashort laser pulses with the emphasis on the role of multiple molecular orbitals (MOs). The results reveal intriguing and substantially different nonlinear optical response behaviors for homonuclear and heteronuclear molecules. In particular, we found that the HHG spectrum for homonuclear molecules features a destructive interference of MO contributions while heteronuclear molecules show mostly constructive interference of orbital contributions.

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