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Multielectron Effects in High Harmonic Generation: A Time-Dependent Density Functional Theory Approach PAUL ABANADOR, FRANCOIS MAUGER, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, KENNETH LOPATA, Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana 70803, METTE GAARDE, KENNETH SCHAFER, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803 — Multielectron effects are expected to play a prominent role in processes involving the interaction of molecules with strong laser fields, such as high harmonic generation (HHG). We employ a two-active-orbital model using time-dependent density functional theory (TDDFT) framework for HHG from a diatomic molecule in one-dimension. We find that incorporating dynamical multielectron effects within TDDFT for this prototypical molecular model can lead to a higher cutoff of the harmonic plateau compared to what is expected from a single-active-orbital model. This feature in the HHG spectrum is associated to recombination of the ionized electron wave packet to the orbital with higher ionization potential. We aim to compare the TDDFT results with an extension of our semiclassical model [Phys. Rev. A 93, 043815 (2016)] to multiple active orbitals in order to investigate the role of multielectron effects in the HHG process.

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