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Single-Active-Electron Approximation for Describing Molecules in Ultrashort Laser Pulses ALEJANDRO SAENZ, MANOHAR AWASTHI, YULIAN VANNE, Humboldt University Berlin, 10117 Berlin (Germany), ALBERTO CASTRO, Free University Berlin, 14 195 Berlin (Germany), PIERO DECLEVA, University of Trieste, 34127 Trieste (Italy) — A numerical approach that allows for the solution of the time-dependent Schrödinger equation (TDSE) describing molecules exposed to intense short laser pulses was developed. The molecular response to the strong field is described within the single-active electron approximation (SAE). The method is applied to molecular hydrogen and the validity of the SAE is investigated by comparing the ionization and electronic excitation yields to full two-electron solutions of the TDSE. The present results are also used to investigate the validity of approximate SAE methods like the molecular Ammosov-Delone-Krainov and the strong-field approximation. Finally, results for larger molecules like O_2, N_2, and C_2H_2 (acetylene) are presented.

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