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Comparison of high-order harmonic generation of Ar atoms and H_2 molecules in intense 780 nm laser fields[1] DMITRY A. TELNOV, St. Petersburg State University, Russia, SHIH-I CHU, University of Kansas — We analyze the high-order harmonic generation (HHG) of Ar atoms and H_2 molecules in 780 nm laser fields with the pulse duration about 30 fs and various peak intensities by means of the self-interaction-free time-dependent density functional theory (TDDFT). Since the ionization potentials of Ar and H_2 are close to each other, the cutoff position of the HHG spectra for the specific intensity is expected approximately at the same harmonic order, according to the three-step model. In general, our TDDFT calculations agree with this prediction; however, in the high-energy part of the HHG spectra, the harmonic signal from H_2 is considerably lower than that from Ar. On the other hand, the HHG spectrum of Ar has a prominent minimum at the photon energy 50 eV, especially for lower laser intensities. This minimum has the same nature as the well-known Cooper minimum in Ar observed in photoionization cross sections.

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