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High-order harmonic generation of aligned CO molecules: a TDDFT approach[1] SHIH-I CHU, University of Kansas, DMITRY A. TELNOV, St. Petersburg State University, Russia, JOHN HESLAR, National Taiwan University, Taiwan — We have performed time-dependent density functional (TDDFT) calculations of high-order harmonic generation (HHG) by aligned CO molecules subject to intense 800 nm laser pulses. We make use of LBα exchange-correlation potential which proved its accuracy in time-independent electronic structure calculations. The time-dependent Kohn-Sham equations are efficiently solved by the time-dependent generalized pseudospectral method (TDGPS) in prolate spheroidal coordinates. We have found that the high-energy part of the HHG spectrum exhibits a strong dependence on the alignment angle between the molecular axis and the polarization direction of the laser field with the sharp minimum at the perpendicular alignment. An analysis of the HHG spectra at the perpendicular alignment revealed also two minima, one of them corresponding to the photon energy in the range 37 eV to 45 eV, and another one in the range 63 eV to 69 eV. Positions of both minima only slightly depend on the peak intensity of the laser field.

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