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Effect of nuclear vibration on high-order harmonic generation of aligned H_2^+ molecules[1] DMITRY A. TELNOV, St. Petersburg State University, Russia, JOHN HESLAR, National Taiwan University, SHIH-I CHU, University of Kansas — High-order harmonic generation (HHG) spectra have been calculated for H_2^+ molecules aligned in the direction parallel to the polarization of the laser field. We make use of the Jacobi coordinates and neglect the rotation of the nuclei. The remaining time-dependent Schrödinger equation is 3D in spatial coordinates, one of them being the internuclear separation and the other two describing the electronic motion. The problem is solved using the accurate and efficient time-dependent generalized pseudospectral method in prolate spheroidal coordinates for the electronic coordinates and Fourier grid method for the internuclear separation. Laser pulses with the carrier wavelength of 800 nm, duration of 10 optical cycles, and several peak intensities have been used in the calculations. Our HHG spectra obtained fully beyond the Born-Oppenheimer approximation generally exhibit a significant deviation from those calculated for the fixed internuclear separations. The low-energy regions of the spectra, however, resemble those for the nuclei fixed at larger separations while the high-energy regions are closer to those for the nuclei fixed at smaller internuclear distances. The dynamics of the nuclear vibrational wave packet is also obtained and analyzed.

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