

Abstract Submitted  
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**Orientation-Dependent High-Order Harmonic Generation of N<sub>2</sub> and F<sub>2</sub> in Intense 800 nm Laser Pulses<sup>1</sup>** DMITRY A. TELNOV, Department of Physics, St. Petersburg State University, St. Petersburg, Russia, SHIH-I CHU, Department of Chemistry, University of Kansas, Lawrence, Kansas — We present time-dependent density functional calculations of high-order harmonic generation (HHG) of diatomic molecules N<sub>2</sub> and F<sub>2</sub> with arbitrary orientation of the molecular axis by intense linearly-polarized laser pulses with the wavelength 800 nm [1]. HHG is more intense for the orientations where multiphoton ionization reaches its maximum. This happens at the parallel orientation for N<sub>2</sub> and at the orientation 40° for F<sub>2</sub>. The high-order harmonics are very sensitive to the interference of the contributions from multiple electronic shells. Due to one-photon resonance, the highest-occupied molecular orbital (HOMO) and the next occupied orbital (HOMO–1) in N<sub>2</sub> are strongly coupled by the laser field at nonparallel orientations, and the HHG radiation results from their combined response to the field. In any case, the account of the multielectron effects can change the resulting harmonic radiation energy by orders of magnitude, as compared with the HHG spectrum produced by HOMO only.

[1] D. A. Telnov and S. I. Chu, Phys. Rev. A **80**, 043412 (2009).

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Shih-I Chu  
Department of Chemistry, University of Kansas, Lawrence, Kansas

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