

Abstract Submitted
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Contributions of inner valence molecular orbitals and multiphoton resonances to high harmonic generation: A TDDFT study¹ XI CHU, University of Montana, GERRIT GROENENBOOM, Radboud University Nijmegen — Using a TDDFT method, we calculated the high harmonic generation (HHG) spectra of N₂ in 800 nm and 1300 nm intense lasers. The calculations reproduce the experimentally observed minimum near 40 eV and the shift of the minimum due to interference of different molecular orbitals. They also support the proposed shape resonance near 30 eV. The TDDFT method allows us to analyze the involvement of different electronic configurations in the HHG process. We identified a significant role of Rydberg states and autoionizing states in enhancing HHG. This finding is consistent with studies of photoelectron spectra in a similar energy range. Moreover, we discover a significant contribution of the $2\sigma_g$ orbital above 40 eV, demonstrating the complexity of electronic structure information contained in molecular HHG. At high energy not only the HOMO and HOMO-1 are important, as suggested by earlier studies, but the HOMO-3 contributes substantially as well.

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