

Abstract Submitted
for the DAMOP11 Meeting of
The American Physical Society

Role of multiphoton excitation and two-electron effects in high harmonic generation of H₂: a TDDFT calculation¹ XI CHU, PATRICK MEMOLI, The University of Montana — Using two different TDDFT methods, we study the role of electronically excited states and two-electron dynamics in high harmonic generation (HHG) of H₂. The two methods produce slightly different electronic structures as reflected in the calculated ionization potentials. They nevertheless give similar HHG spectra. The difference between the two methods increases with the laser intensity, while their predictions remain qualitatively consistent. Our results suggest that two-electron dynamics can extend the HHG cutoff. Specifics of such an extension depends on the internuclear distance and the laser intensity. We propose an ion excitation plus tunneling ionization mechanism to explain these extensions. The involvement of excited states is further revealed when we analyze each harmonic as a function of the internuclear distance. We see resonant peaks that are due to multiphoton excitation. These peaks exist above the ionization threshold as well.

¹This work is supported by the National Science Foundation Award No. PHY-0855676.

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Date submitted: 04 Feb 2011

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