Abstract Submitted
for the DAMOP11 Meeting of
The American Physical Society

High Harmonic Generation from 2D Diatomic Molecules[1] MITSUKO MURAKAMI, TOM KIRCHNER, MARKO HORBATSCH, Department of Physics and Astronomy, York University, Toronto, Ontario, Canada M3J 1P3 — We propose a simple model to calculate high harmonic spectra from diatomic molecules based on an independent-particle description of molecular orbitals. High harmonics are calculated from the numerical solution of the time-dependent Schrödinger equation in a two-dimensional geometry. According to this model, harmonic spectra from individual orbitals generally follow the semi-classical cutoff law, but their relative strengths vary depending on molecular orientations and driving laser intensities. In particular, when the contributions from multiple orbitals are comparably strong, their net spectra will extend to the inner-orbital cutoffs but may appear to have a local minimum where the harmonic intensity of the highest occupied molecular orbital begins to fall off. This mechanism might be the underlying cause for the intensity-dependent minima in molecular harmonics observed in a recent experiment by Wörner et.al. [1].

[1] H. J. Wörner *et.al.*, Phys. Rev. Lett. **104**, 233904 (2010).

[1]This work has been supported by NSERC Canada and SHARCNET.

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Date submitted: 03 Mar 2011 Electronic form version 1.4