Abstract Submitted
for the DAMOP08 Meeting of
The American Physical Society

**Multi-electron Effects in High-Order Harmonic Generation: Homonuclear vs. Heteronuclear Diatomic Molecules** JOHN HESLAR, SHIH-I CHU, Dept. of Chemistry, Univ. of Kansas, Lawrence, KS 66045 USA — We present a *self-interaction-free* time-dependent density-functional theory (TDDFT) with proper asymptotic *long-range* potential for nonperturbative treatment of very-high-order nonlinear response of multi-electron molecular systems to intense laser fields. A time-dependent generalized pseudospectral method is developed in prolate spheroidal coordinate system for accurate solution of both the electronic structure and TDDFT equations for homonuclear and heteronuclear diatomic molecules. The theory is applied to a detailed *all-electron* study of high-order harmonic generation (HHG) processes of CO, $N_2$, $F_2$, BF, and HF in intense laser fields. We found distinctive difference between the responses of homonuclear vs. heteronuclear diatomic molecules. First, while the homonuclear diatomics show only the odd harmonics, both even and odd harmonics are observed for heteronuclear diatomics. Second, destructive interference in HHG is observed in some MOs for homonuclear diatomics but not for heteronuclear diatomics. More detailed results will be presented in the conference.

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Date submitted: 26 Jan 2008 Electronic form version 1.4