Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

A Simulation of Strong-Field Attosecond Electron Dynamics: Effects of Pulse Shape STANLEY SMITH, DMITRI ROMANOV, Temple University, XIAOSONG LI, University of Washington, H. BERNHARD SCHLEGEL, Wayne State University, ROBERT LEVIS, Temple University — As the complexity of systems increases from atoms to molecules, the exploration of non-adiabatic electron dynamics in strong fields requires a leap in understanding and in the principles of description. Recently, a time-dependent Hartree-Fock approach (TDHF) was developed to study the dynamics of individual electrons in multielectron systems. We have used this TDHF approach to numerically simulate the non-adiabatic electron dynamics of a few small molecules and polyacenes using basis sets ranging from AUG-cc-pVTZ for smaller molecules to 6-31G(d,p) for larger molecules. The electric field was applied in the direction of the long molecular axis and the attosecond response of the electrons during and after the laser pulse has been obtained. To determine the effects of ionization, electron dynamics for both neutrals and ions was also simulated. As a function of pulse shape, there are significant differences in the excitation spectrum and volume for each molecule.

Stanley Smith
Temple University

Date submitted: 05 Dec 2007 Electronic form version 1.4