Abstract Submitted
for the TSF05 Meeting of
The American Physical Society

Response of Biological Molecules to Ultrafast Laser Pulses[1] PETRA SAUER, ROLAND ALLEN, Texas A&M University — Our earlier work on organic molecules containing only carbon and hydrogen has been extended to biological molecules which also contain nitrogen and oxygen. We will present preliminary results, with animations, for the response of dipicolinic acid and retinal to femtosecond-scale laser pulses. We will also discuss how a realistic model was developed which (1) provides a reasonably accurate representation of chemical bonding in complex molecules and (2) is computationally efficient enough to permit simulations of the coupled electronic and nuclear dynamics with a time step of order 10 attoseconds. One starts with a diatomic molecule, fitting the Hamiltonian to the principal electronic energy gap, and an effective repulsive potential to the bond length and vibrational frequency. However, the model must work more globally, in a variety of different chemical environments, and to achieve this broader goal requires further refinements and testing. There are various subtleties. For example, with a minimal basis set, the highest energy state is unphysically senstive to changes in bond length, because it is not pushed down by higher-lying states. We will discuss preliminary work on quantum control of molecules via changes in the duration, intensity, polarization, and other laser pulse parameters.

[1]Supported by Robert A. Welch Foundation (Grant A-0929).

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Date submitted: 14 Sep 2005 Electronic form version 1.4