

Abstract Submitted
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Response of Biomolecules to Ultrafast Laser Pulses¹ ROLAND ALLEN, ROBERT MURAWSKI, PETRA SAUER , Texas A&M University, YUSHEUG DOU, Nicholls State University, TRAIAN DUMITRICA, Rice University, JOHN R.H. XIE , Texas A&M University — Using two complementary techniques – semiclassical electron-radiation-ion dynamics (SERID) and time-dependent density functional theory (TDDFT) – we are studying the response of various biologically relevant molecules to femtosecond-scale laser pulses. Our simulations provide microscopic information on mechanisms for photoisomerization [1] and other molecular transformations [2] and on spectroscopic identification of pathogens with schemes like FAST CARS [3]. The coupled dynamics of electrons and nuclei is determined by solving the time-dependent Schrödinger equation and using Ehrenfest’s theorem, with a 30 attosecond time step. Results will be shown for molecules including stilbene, benzene, and dipicloninc acid. [1] Y. Dou and R. E. Allen, *Chemical Physics Letters* 378, 323 (2003).2] B. Torralva and R. E. Allen, *Journal of Modern Optics* 49, 593 - 625 (2002).3] M. O. Scully et al., *Proc. Nat. Acad. Sci.* 99, 10994 (2002).

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Roland Allen
Texas A&M University

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