Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Photoisomerization selectivity in conjugated π-bond systems through local microenvironment AARON VIRSHUP, Dept. of Physics, Univ. of Illinois at Urbana-Champaign, TODD MARTINEZ, Dept. of Chemistry, Univ. of Illinois at Urbana-Champaign — Photoisomerization represents one of the simplest means to convert light energy into mechanical motion on the molecular scale. Theoretical models of photobiology often require description of not only a small photochemically active chromophore, but also the effects of the much larger solvent or protein environment containing the chromophore. We have recently developed a program for carrying out excited state QM/MM studies of photodynamics using *ab initio* quantum chemistry techniques for the QM region, and modeling the time evolution of the system with the Full Multiple Spawning method for molecular dynamics. With this method, we show how local charge environments can be used to manipulate and enhance the photoisomer selectivity of small conjugated molecules.

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Date submitted: 20 Nov 2006 Electronic form version 1.4