

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

NA-ESMD modeling of photoinduced dynamics in conjugated molecules TAMMIE NELSON, Los Alamos National Laboratory, SEBASTIAN FERNANDEZ-ALBERTI, Universidad Nacional de Quilmes, VLADIMIR CHERNYAK, Wayne State University, ADRIAN ROITBERG, University of Florida, SERGEI TRETIAK, Los Alamos National Laboratory — The evolution of electronic excitations in optically active molecules can generally be defined by non-adiabatic (NA) dynamics. A number of fundamental and complex processes are associated with NA dynamics. To treat ultrafast excited state dynamics we have developed a non-adiabatic excited state molecular dynamics (NA-ESMD) framework incorporating quantum transitions. Our calculations combine the Collective Electronic Oscillator (CEO) package with the Tully's fewest switches algorithm for surface hopping, and the actual potential energy surfaces of the excited states are used. This method is applied to model the photoinduced dynamics of distyrylbenzene. Our analysis shows intricate details of vibronic relaxation and identifies specific slow and fast nuclear motions that are strongly coupled to the electronic degrees of freedom. Non-adiabatic relaxation of the highly excited mAg state is predicted to occur on a femtosecond timescale at room temperature and on a picosecond timescale at low temperature.

Tammie Nelson
Los Alamos National Laboratory

Date submitted: 20 Oct 2010

Electronic form version 1.4