Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Photoexcited energy transfer in a weakly coupled dimer TAMMIE NELSON, Los Alamos National Lab, LAURA ALFONSO HERNANDEZ, Universidad Nacional de Quilmes, SERGEI TRETIAK, Los Alamos National Lab, SEBASTIAN FERNANDEZ ALBERTI, Universidad Nacional de Quilmes — Nonadiabatic excited-state molecular dynamics (NA-ESMD) simulations have been performed to study the time dependent exciton localization during energy transfer between two chromophore units of the weakly coupled dimer dithia-anthracenophane (DTA). The initial photoexcitation creates an exciton which is primarily localized on a single monomer unit. Subsequently, the exciton experiences an ultrafast energy transfer becoming localized on either one unit or the other whereas delocalization between both monomers never occurs. In half of the trajectories, the electronic transition density becomes completely localized on the same monomer as the initial excitation, while in the other half, it becomes completely localized on the opposite monomer. Here we present an analysis of the energy transfer dynamics and the effect of thermally induced geometry distortions on the exciton localization. Finally, simulated fluorescence anisotropy decay curves for both DTA and the monomer dimethyl anthracene (DMA) reveal that changes in the transition density localization caused by energy transfer in DTA is not the only source of depolarization and relaxation within a single monomer unit can also cause reorientation of the transition dipole.

Tammie Nelson
Los Alamos National Lab

Date submitted: 13 Nov 2014

Electronic form version 1.4