Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Exciton Transport Simulations in Phenyl Cored Thiophene Dendrimers[1] KWISEON KIM, MUHAMMET ERKAN KOSE, PETER GRAF, NIKOS KOPIDAKIS, GARRY RUMBLES, National Renewable Energy Laboratory, SEAN E. SHAHEEN, University of Denver — Phenyl cored 3-arm and 4-arm thiophene dendrimers are promising materials for use in photovoltaic devices. It is important to understand the energy transfer mechanisms in these molecules to guide the synthesis of novel dendrimers with improved efficiency. A method is developed to estimate the exciton diffusion lengths for the dendrimers and similar chromophores in amorphous films. The approach exploits Fermi's Golden Rule to estimate the energy transfer rates for an ensemble of bimolecular complexes in random orientations. Using Poisson's equation to evaluate Coulomb integrals led to efficient calculation of excitonic couplings between the transition densities. Monte-Carlo simulations revealed the dynamics of energy transport in the dendrimers. Experimental exciton diffusion lengths of the dendrimers range $10 \sim 20$ nm, increasing with the size of the dendrimer. Simulated diffusion lengths correlate well with experiments. The chemical structure of the chromophore, the shape of the transition densities and the exciton lifetime are found to be the most important factors that determine the exciton diffusion length in amorphous films.

[1]Supported by NREL's LDRD program

Kwiseon Kim
National Renewable Energy Lab

Date submitted: 21 Nov 2008 Electronic form version 1.4