Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A Multiscale Approach to Realistic Simulation of Organic Photovoltaic Devices[1] DANIEL OLDS, PHILLIP DUXBURY, Michigan State University, JON KIEL, MICHAEL MACKAY, University of Delaware — We have generated three dimensional bulk heterostructures consistent with neutron reflectivity data from polymer-fullerene systems and have used these nanostructures in fully three dimensional simulations of solar cells fabricated from these materials. The simulations are based on a multiscale model of organic photovoltaic devices, incorporating exciton generation and dis-association, photoinduced charge transport, dark current injection from contacts, and losses due to charge recombination and trapping. Through the use of precalculated charge-pair escape probabilities based upon likely local internal morphologies, interface effects, and associated electric fields, the most computationally intensive parts of many other dynamic Monte Carlo device simulators can be efficiently approximated. Comparison with continuum device models and experimental data will be used to illustrate the aspects that require a fully three dimensional atomistic model.

[1]We acknowledge a Strategic Partnership Grant at Michigan State University

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Date submitted: 18 Nov 2009 Electronic form version 1.4