Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Petascale Molecular Dynamics Simulations of Thermal Annealing of P3HT:PCBM Active Layers in Bulk Heterojunctions[1] JAN-MICHAEL CARRILLO, RAJEEV KUMAR, MONOJOY GOSWAMI, Oak Ridge National Laboratory, S. MICHAEL KILBEY II, Department of Chemistry, University of Tennessee, BOBBY SUMPTER, W. MICHAEL BROWN, Oak Ridge National Laboratory — Using petascale coarse-grained molecular dynamics simulations, we have investigated the thermal annealing of poly(3-hexylthiophene) (P3HT) and Phenyl-C61-butyric acid methyl ester (PCBM) blends in the presence of a silicon substrate. The simulations were run on the Titan supercomputer using 21% of the capacity of the machine. This is in contrast to recent studies, which were unable to obtain results representative of the entire thermal annealing process because of limited simulation time and size. The simulations are in agreement with neutron reflectivity (NR) and near edge X-ray fine structure (NEXAFS) experiments and reveal a vertical composition profile of the bulk heterojunction normal to the substrate with enrichment of PCBM near the substrate. We demonstrate that the addition of short P3HT chains, as a third component of the blend, can be used to alter the morphology of the active layer.

[1]U.S. DOE Contract No. DE-AC05-00OR22725

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Date submitted: 15 Nov 2013 Electronic form version 1.4