

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Systematic Multiscale Modeling of Polymers ROLAND FALLER, UC Davis, DAVID HUANG, Univ of Adelaide, BESTE BAYRAMOGLU, ADAM MOULE, UC Davis — The systematic coarse-graining of heterogeneous soft matter systems is an area of current research. We show how the Iterative Boltzmann Inversion systematically develops models for polymers in different environments. We present the scheme and a few applications. We study polystyrene in various environments and compare the different models from the melt, the solution and polymer brushes to validate accuracy and efficiency. We then apply the technique to a complex system needed as active layer in polymer-based solar cells. Nano-scale morphological information is difficult to obtain experimentally. On the other hand, atomistic computer simulations are only feasible to studying systems not much larger than an exciton diffusion length. Thus, we develop a coarse-grained (CG) simulation model, in which collections of atoms from an atomistic model are mapped onto a smaller number of “superatoms.” We study mixtures of poly(3-hexylthiophene) and C₆₀. By comparing the results of atomistic and CG simulations, we demonstrate that the model, parametrized at one temperature and two mixture compositions, accurately reproduces the system structure at other points of the phase diagram. We use the CG model to characterize the microstructure as a function of polymer:fullerene mole fraction and polymer chain length for systems approaching the scale of photovoltaic devices.

Roland Faller
UC Davis

Date submitted: 12 Nov 2010

Electronic form version 1.4