Center for Quantum Science and Engineering (CQSE)

Weekly Seminar
May 20, 2011 (Friday)

TIME May 20, 14:30 ~ 15:30
TITLE Probe Nanoscale Morphologies of Bulk Heterojunction Polymer Solar Cell from Multiscale Molecular Simulations
SPEAKER Dr. Chun-Wei Pao 包淳偉博士
Research Center for Applied Sciences, Academia Sinica
PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

Bulk heterojunction (BHJ) polymer solar cells are promising renewable energy sources because of their low production cost, high mechanical flexibility, and light-weight. The BHJ layer featuring a nanoscale interpenetrating network of electron donor/acceptor phases is critical for the overall device performance. Hence, characterization of the structure of BHJ layer is crucial for connecting various processing conditions with resultant device performance; however, this is never a trivial task from experimental perspective. In this study, we employed multiscale molecular simulations to study morphologies of the P3HT:PCBM blend during thermal annealing. From multiscale molecular simulations, we can study systems with size compatible with experiments, and extract morphological properties that are difficult to extract from experiments; furthermore, by reverse-mapping the atomistic details can be retrieved to study atomic packing and transport properties. By analyzing blend morphologies, we demonstrate that thermal annealing can substantially improve the crystallinity of P3HT, and the optimal blend ratio 1:1 for the P3HT:PCBM blend can be attributed to its highest interface-to-volume ratio, and most balanced charge transport among all blending ratios investigated. Hence, this article provides a multiscale molecular simulation framework which can be extended to any BHJ systems to help researchers characterize and design BHJ cells with superior efficiency.