

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Correlation of Fullerene Structure to its Miscibility in P3HT and OPV Function MARK DADMUN, HUIPENG CHEN, University of Tennessee, JEFF PEET, Konarka — The miscibility of four fullerenes, bis-PCBM, ICBA, Thio-PCBM and PC₇₀BM in poly(3-hexylthiophene) (P3HT) is determined by neutron reflectivity by monitoring the intermixing of P3HT and fullerene bilayers with thermal annealing. The miscibility limit of these fullerenes in P3HT ranges from 11% to 26%, where the bis-adduct fullerenes exhibit a lower miscibility in P3HT than singly functionalized fullerenes. The correlation of miscibility to device performance indicates that sufficient polymer/fullerene miscibility is crucial to rationally optimize organic photovoltaic active layers. Low miscibility of conjugated polymer and fullerene in the amorphous phase decreases the probability of exciton dissociation and enhances the recombination of free charge-carriers. Moreover, the results indicate that the average surface-to-surface distance between fullerenes must be less than approximately of 5-7 Å to minimize charge traps and allow sufficient charge transport in the mixed phase to improve photovoltaic performance.

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Date submitted: 08 Nov 2012

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