Supporting information

Solubility of PCBM and Optimal Blending Ratio of Bulk Heterojunction Polymer Solar Cells

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Back-mapping Procedure

In order to retrieve atomistic details from configurations generated from CGMD, the following procedure was employed: (1) prepare equilibrium atomistic structures of a PBTTT monomer and a PCBM molecule, (2) replace the CG model with the atomistic structures, (3) rotate a PBTTT monomer and PCBM molecule as a Monte Carlo trial move, (4) determine if the trial move is accepted by using the Metropolis Monte Carlo algorithm,[1] (5) repeat steps 3 and 4 until the whole system relaxes, (6) run MD simulation again to relax the whole system from back-mapping.

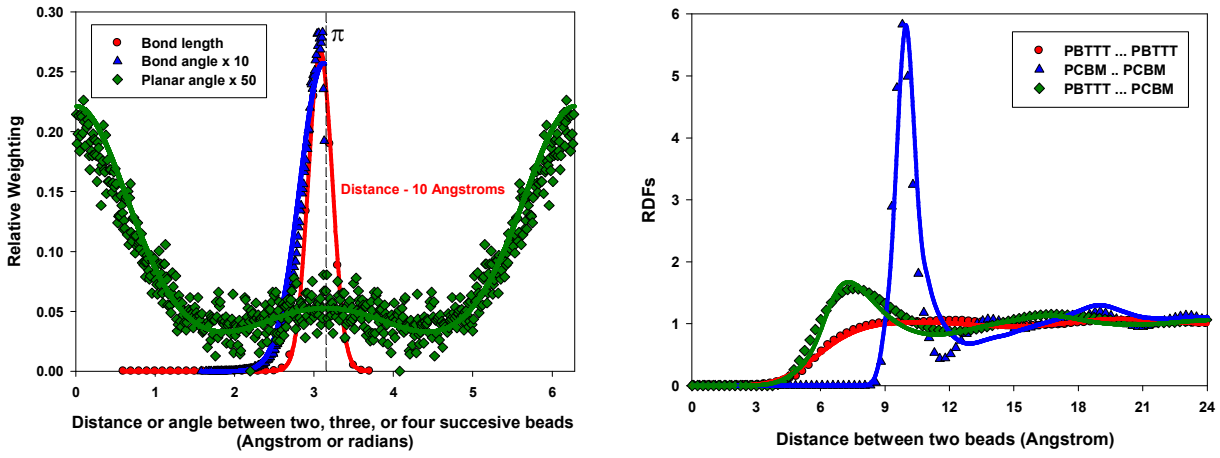
All-atom Molecular Dynamics Simulation Procedures for Fitting CG Potentials

The AMD simulations were performed using DL_POLY_4 MD simulation packages[2] and incorporated DREIDING force fields.[3] The Nosé-Hoover *NVT* ensemble (423 K) and periodic boundary condition were employed with a time step of 1 fs and a cutoff distance of 15 Å for all non-bonding interactions. To ensure that the data collected for the atomistic model accurately described the equilibrium distributions of the CG particle bond length r, bond angle θ, and planar angle ϕ. the initial chain conformations for the original atomistic model were created with a Monte Carlo scheme[1] and subsequently equilibrated with an AMD simulation for 10 ns.

Movie files

M1: the 360° view of the three-dimensional structure of PBTTT:PCBM blend with blending ratio 1:3. PBTTT chains and PCBM particles are colored in yellow and blue, respectively. In the second half of this movie, PCBM molecules are set to be transparent so that the structure of self-assembled PBTTT nanostructure can be visualized.

M2: the 360° view of the three-dimensional structure of P3HT:PCBM blend with blending ratio 1:1. P3HT chains and PCBM particles are colored in red and blue, respectively. In the second half of this movie, PCBM molecules are set to be transparent so that the structure of self-assembled P3HT nanostructure can be visualized.



(a) (b)

Figure S1. (a) Distribution functions of the bond length r, bond angle θ, and planar angle ϕ of an isolated 10-mer of PBTTT at 423 K; (b) radial distribution functions (RDFs), $G(r)$, at 423 K and 1 atm, of the particle bath consisting of PBTTT monomers, PCBM, and a mixture of the two. AMD and CGMD simulation data are displayed as symbols and lines, respectively.

Supplemental References

(1) Landau, D. P.; Binder, K. *A Guide to Monte Carlo Simulations in Statistical Physics*; Cambridge University Press: New York, 2001.
(2) Todorov, I. T.; Smith, W. *The DL_POLY_4 User Manual*; STFC Daresbury Laboratory: Daresbury, 2011.
(3) Mayo, S. L.; Olafson, B. D.; Goddard, W. A. *J. Phys. Chem.* **1990**, *94*, 8897-8909.