

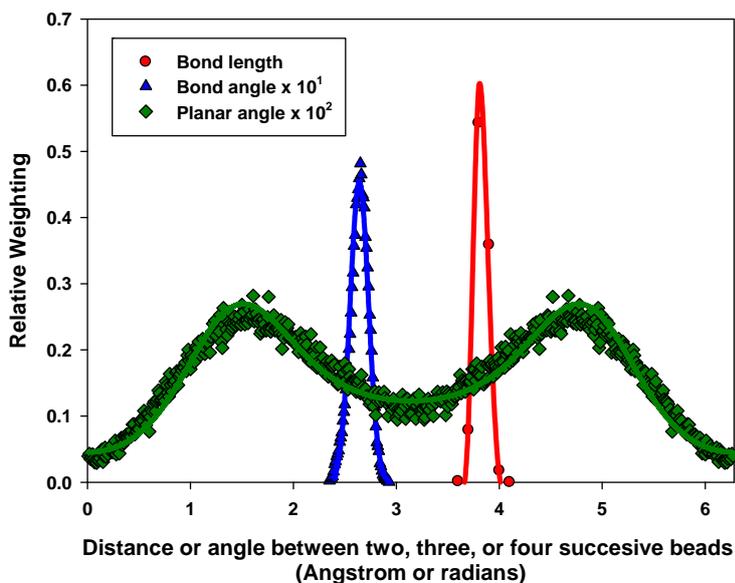
Supplementary Material (ESI) for Energy & Environmental Science

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Supplementary material for “Multiscale Molecular Simulations of the Nanoscale Morphologies of P3HT:PCBM Blends for Bulk Heterojunction Organic Photovoltaic Cells”

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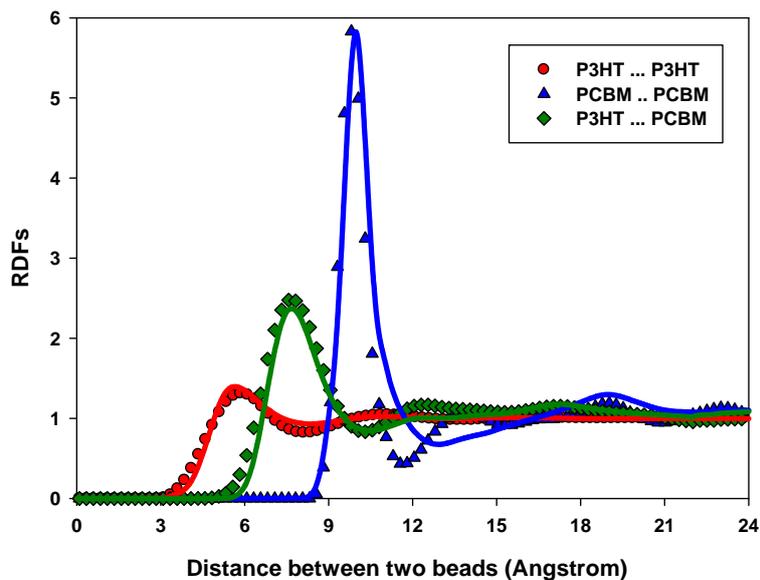


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Fig. S1 Distribution functions of the bond length r , bond angle θ , and planar angle ϕ of an isolated 10-mer of P3HT at 423 K; AMD and CGMD simulation data are displayed as symbols and lines, respectively.

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Fig. S2 Radial distribution functions ($RDFs$), $G(r)$, at 423 K and 1 atm, of the particle bath consisting of P3HT monomers, PCBM, and a mixture of the two; AMD and CGMD simulation data are displayed as symbols and lines, respectively.