

## Supplementary material for “Correlation of nanoscale organizations of polymer and nanocrystals in polymer/inorganic nanocrystal bulk heterojunction hybrid solar cells: insights from multiscale molecular simulations”

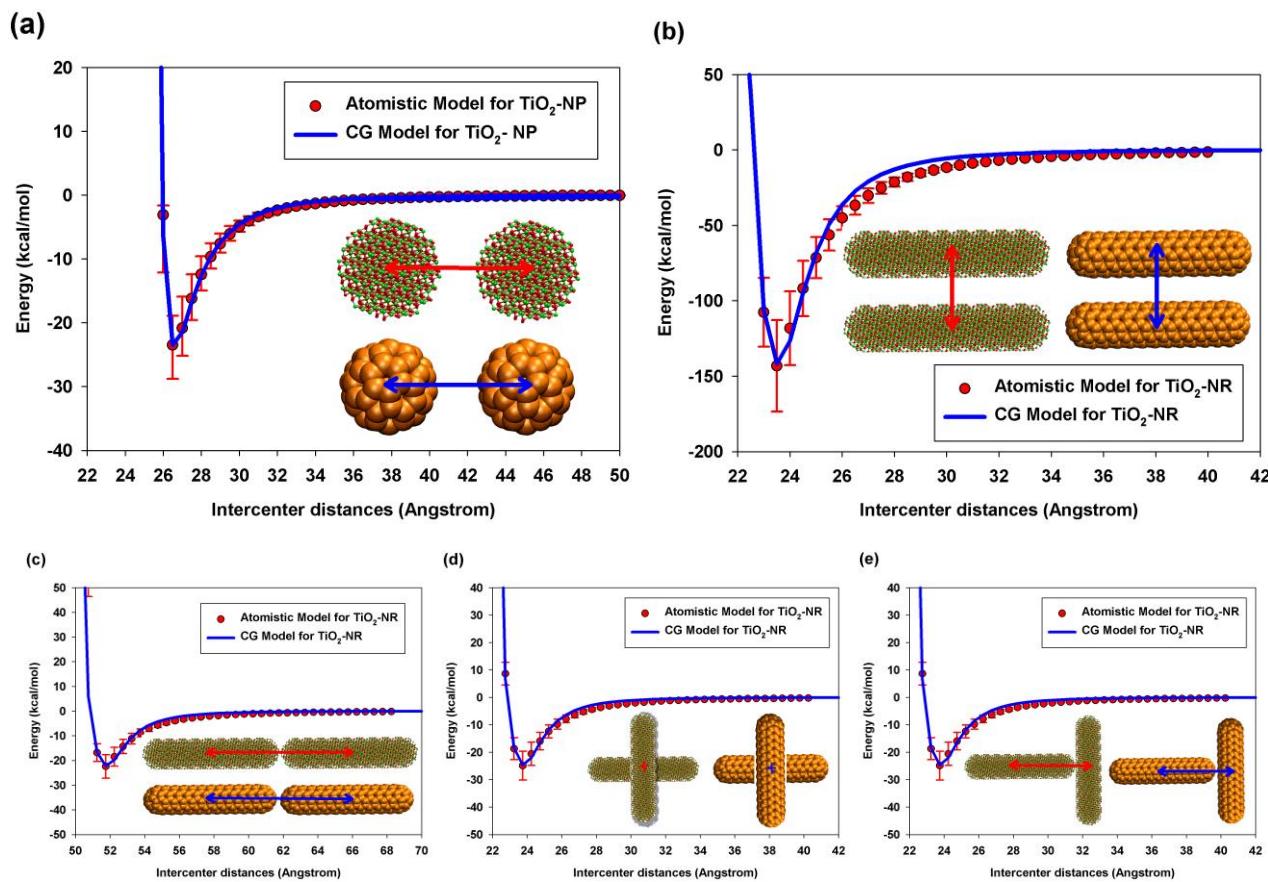
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### Method for Autocorrelation function (ACR) Analysis:

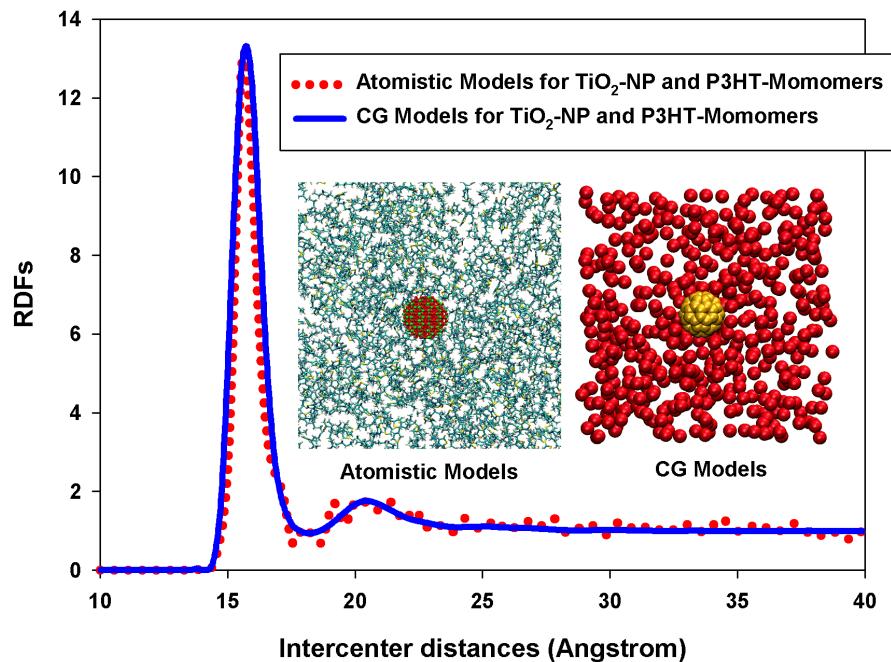
The autocorrelation length can be defined as<sup>1</sup>

$$ACR(x') = \frac{1}{L_x} \int_0^{L_x} I(x)I(x-x')dx, \quad (S1)$$

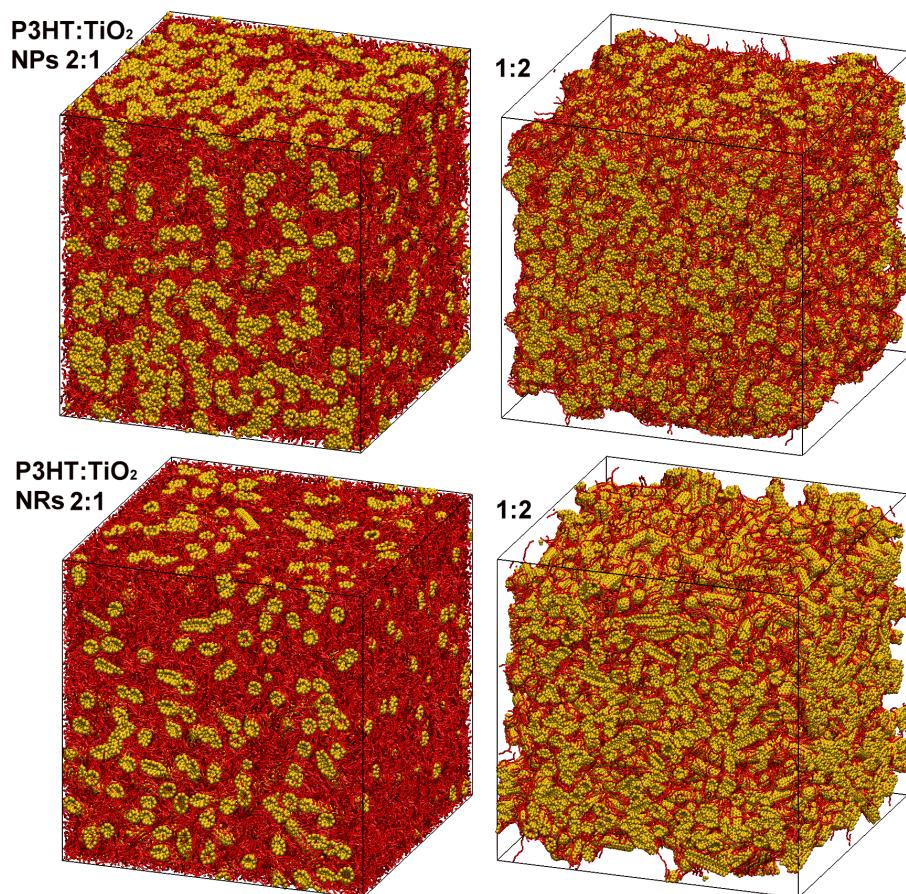
where  $L_x$  is the simulation cell size, and  $I(x)$  is a phase function determining whether a point  $x$  in the simulation belonging to polymer phases.  $I(x) = 1$  or -1 if a point  $x$  belongs to polymer or nanocrystal phases, respectively.



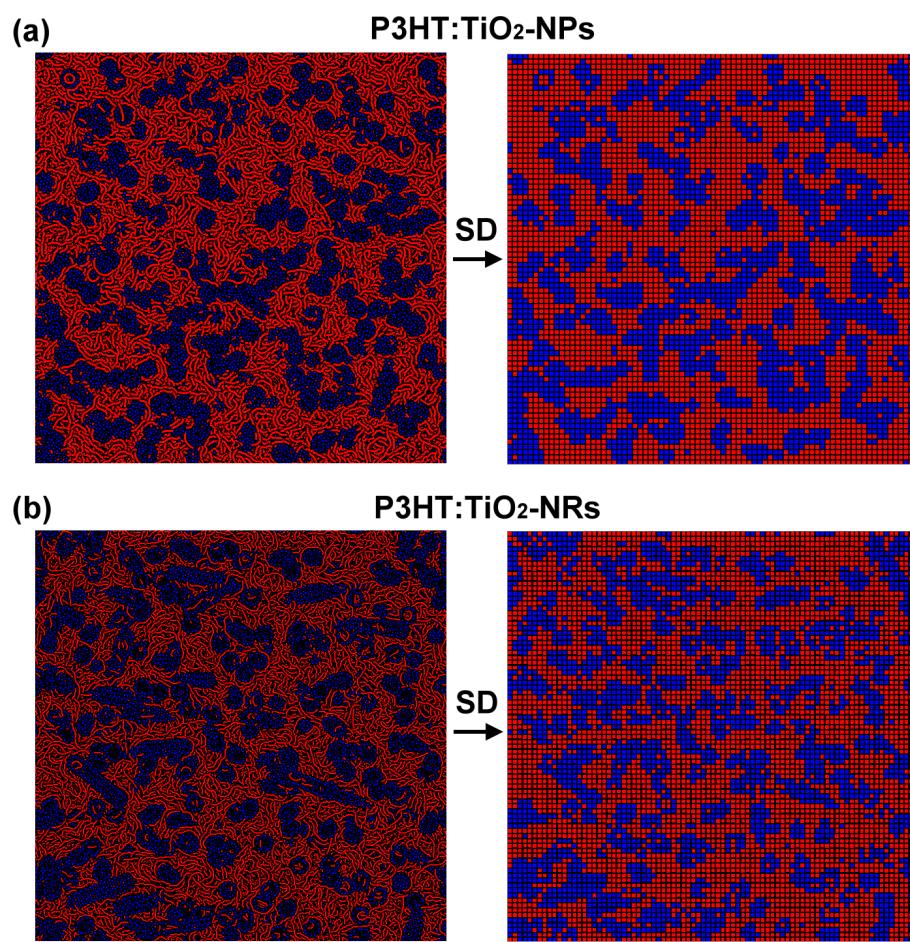
**Fig. S1** Potential energy surface between two  $\text{TiO}_2$  NPs (a) and  $\text{TiO}_2$  NRs with side-to-side (b), end-to-end (c), cross (d), and T-shape (e) stackings. Symbols and error bars represent the averaged potential energy and its fluctuation due to  $\text{TiO}_2$  crystal orientations at given interparticle separation. The blue lines are the inter-particle potential energy surfaces from our CG potential fitted.



**Fig. S2** The radial distribution functions (RDFs) of P3HT monomers surrounding a  $\text{TiO}_2$  nanoparticle from atomistic MD (symbols) and CGMD simulation.



**Fig. S3** The three-dimensional morphologies of P3HT:TiO<sub>2</sub> NPs (upper panels) and P3HT:TiO<sub>2</sub> NRs (lower panels) with different blending ratios. TiO<sub>2</sub> CG particles are colored in orange and P3HT CG particles are colored in red.



**Fig. S4** The P3HT:TiO<sub>2</sub> NP (a) and P3HT:TiO<sub>2</sub> NR (b) blends before (left panels) and after (right panels) spatial-discretization (SD)<sup>2, 3</sup> processes for evaluating morphological properties. P3HT molecules and cubes are colored in red, whereas TiO<sub>2</sub> CG particle and cubes are colored in blue.

**Table S1.** Analytic forms and parameters used for CG model potential of P3HT-TiO<sub>2</sub>

intra-/intermolecular potentials		notation (units)	parameters
Bond length:	$U_{\text{bond}} = \frac{1}{2} k_b (r_{ij} - r_0)^2$	$k_b$ : force constant (kcal mol <sup>-1</sup> Å <sup>-2</sup> ) $r_0$ : equilibrium bond length (Å)	$k_{b,\text{P3HT}} = 216.19$ $r_{0,\text{P3HT}} = 3.82$
bond angle:	$U_{\text{angle}} = \frac{1}{2} k_\theta (\theta_{jik} - \theta_0)^2$	$k_\theta$ : force constant (kcal mol <sup>-1</sup> rad <sup>-2</sup> ) $\theta_0$ : equilibrium bond angle (rad)	$k_{\theta,\text{P3HT}} = 130.25$ $\theta_{0,\text{P3HT}} = 2.65$
dihedral angle:	$U_{\text{dihed}} = \frac{1}{2} V_1 (1 + \cos \phi) + \frac{1}{2} V_2 (1 - \cos 2\phi) + \frac{1}{2} V_3 (1 + \cos 3\phi)$	$V_1, V_2, V_3$ : constants (kcal mol <sup>-1</sup> )	$V_{1,\text{P3HT}} = 0.56$ $V_{2,\text{P3HT}} = -1.08$ $V_{3,\text{P3HT}} = 0.28$ $\varepsilon_{\text{P3HT-P3HT}} = 0.26$
van der Waals:	$U_{\text{LJ}} = 4\varepsilon \left[ \left( \sigma / r_g \right)^{12} - \left( \sigma / r_g \right)^6 \right]$	$\varepsilon$ (kcal mol <sup>-1</sup> ) and $\sigma$ (Å) are Lennard-Jones parameters	$\sigma_{\text{P3HT-P3HT}} = 4.95$ $\varepsilon_{\text{P3HT-NP}} = 0.85$ $\sigma_{\text{NP-NP}} = 2.77$ $\varepsilon_{\text{P3HT-NP}} = 4.74$ $\sigma_{\text{NP-NP}} = 4.52$ $\varepsilon_{\text{P3HT-NR}} = 0.62$ $\varepsilon_{\text{NR-NR}} = 1.49$ $\sigma_{\text{P3HT-NR}} = 4.44$ $\sigma_{\text{NR-NR}} = 3.93$

#### Supplemental References

1. J. S. Moon, J. K. Lee, S. Cho, J. Byun and A. J. Heeger, *Nano Lett.*, 2009, **9**, 230.
2. C. K. Lee, C. W. Pao and C. W. Chu, *Energy Environ. Sci.*, 2011, **4**, 4124.
3. C. K. Lee and C. W. Pao, *J. Phys. Chem. C*, 2012, **116**, 12455.