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:
\[
ACR(x') = \frac{1}{L_x} \int_0^{L_x} I(x)I(x-x')dx,
\]
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 TiO\(_2\) NPs (a) and TiO\(_2\) NRs with side-to-side (b), end-to-end (c), cross (c), and T-shape (e) stackings. Symbols and error bars represent the averaged potential energy and its fluctuation due to TiO\(_2\) crystal orientations at given inter-particle 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 TiO$_2$ nanoparticle from atomistic MD (symbols) and CGMD simulation.

Fig. S3 The three-dimensional morphologies of P3HT:TiO$_2$ NPs (upper panels) and P3HT:TiO$_2$ NRs (lower panels) with different blending ratios. TiO$_2$ CG particles are colored in orange and P3HT CG particles are colored in red.
Fig. S4 The P3HT:TiO$_2$ NP (a) and P3HT:TiO$_2$ NR (b) blends before (left panels) and after (right panels) spatial-discretization (SD)\textsuperscript{2,3} processes for evaluating morphological properties. P3HT molecules and cubes are colored in red, whereas TiO$_2$ CG particle and cubes are colored in blue.

Table S1. Analytic forms and parameters used for CG model potential of P3HT-TiO$_2$

<table>
<thead>
<tr>
<th>intra-/intermolecular potentials</th>
<th>notation (units)</th>
<th>parameters</th>
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<tbody>
<tr>
<td>Bond length:</td>
<td>$U_{\text{bond}} = \frac{1}{2} k_b \left( r - r_0 \right)^2$</td>
<td>$k_b$: force constant (kcal mol$^{-1}$ Å$^2$) and $r_0$: equilibrium bond length (Å)</td>
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<td>Bond angle:</td>
<td>$U_{\text{angle}} = \frac{1}{2} k_\theta \left( \theta - \theta_0 \right)^2$</td>
<td>$k_\theta$: force constant (kcal mol$^{-1}$ rad$^2$) and $\theta_0$: equilibrium bond angle (rad)</td>
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<td>Dihedral angle:</td>
<td>$U_{\text{dihed}} = \frac{1}{2} V_1 (1 + \cos \phi) + \frac{1}{2} V_2 (1 - \cos 2\phi) + \frac{1}{2} V_3 (1 + \cos 3\phi)$</td>
<td>$V_1$, $V_2$, $V_3$: constants (kcal mol$^{-1}$)</td>
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<tr>
<td>van der Waals:</td>
<td>$U_{\text{vdW}} = 4\varepsilon \left[ \left( \frac{\sigma}{r_0} \right)^{12} - \left( \frac{\sigma}{r_0} \right)^{6} \right]$</td>
<td>$\varepsilon$: (kcal mol$^{-1}$) and $\sigma$: (Å) are Lennard-Jones parameters</td>
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Supplemental References

