Electronic Supplementary Material (ESI) for Soft Matter

Supporting Information for

Correlating fullerenes diffusion with the polythiophene morphology: molecular dynamics simulations

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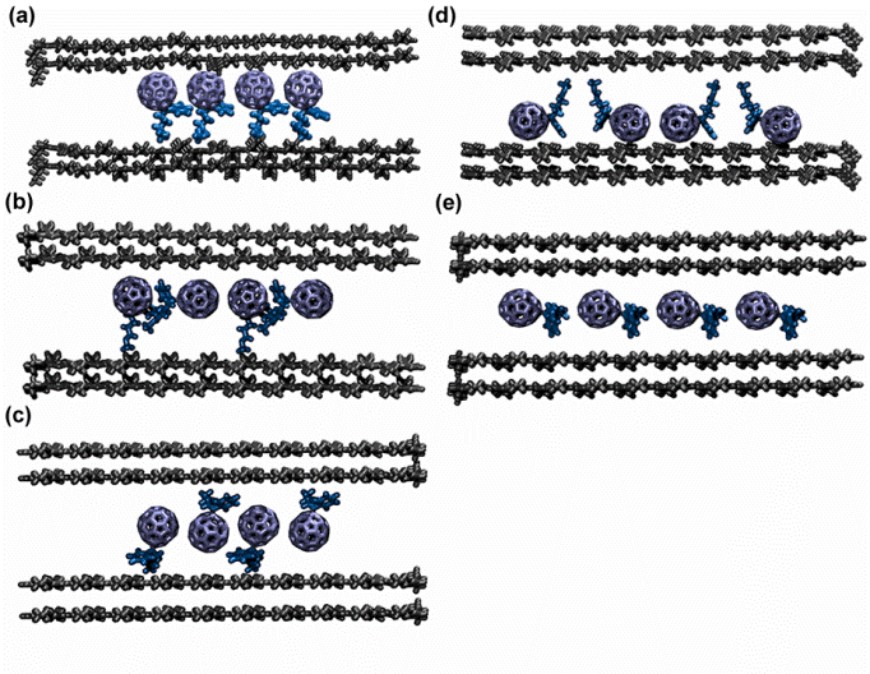

Figure S1. Five models with different orientations of the PCBMs functional group, *i.e* [6,6]-Phenyl butyric acid methyl ester, with respect to the P3HT chains were used. The terminology used for each initial configuration refers to the orientation of PCBM tail with respect to the P3HT chain, where 'd' denotes down, 'r' denotes right, 'u' denotes up, and 'l' denotes left. Initial snapshots of each initial configuration are (a) dddd (b) dldl (c) dudu (d) rlrl and (e) rrrr. For example, "dddd" denotes the configuration of 4 PCBM molecules with their functionalized group pointed down towards the P3HT chain and "rrrr" denotes the PCBM functionalized group lying parallel to the P3HT chains with the functional groups pointing right.

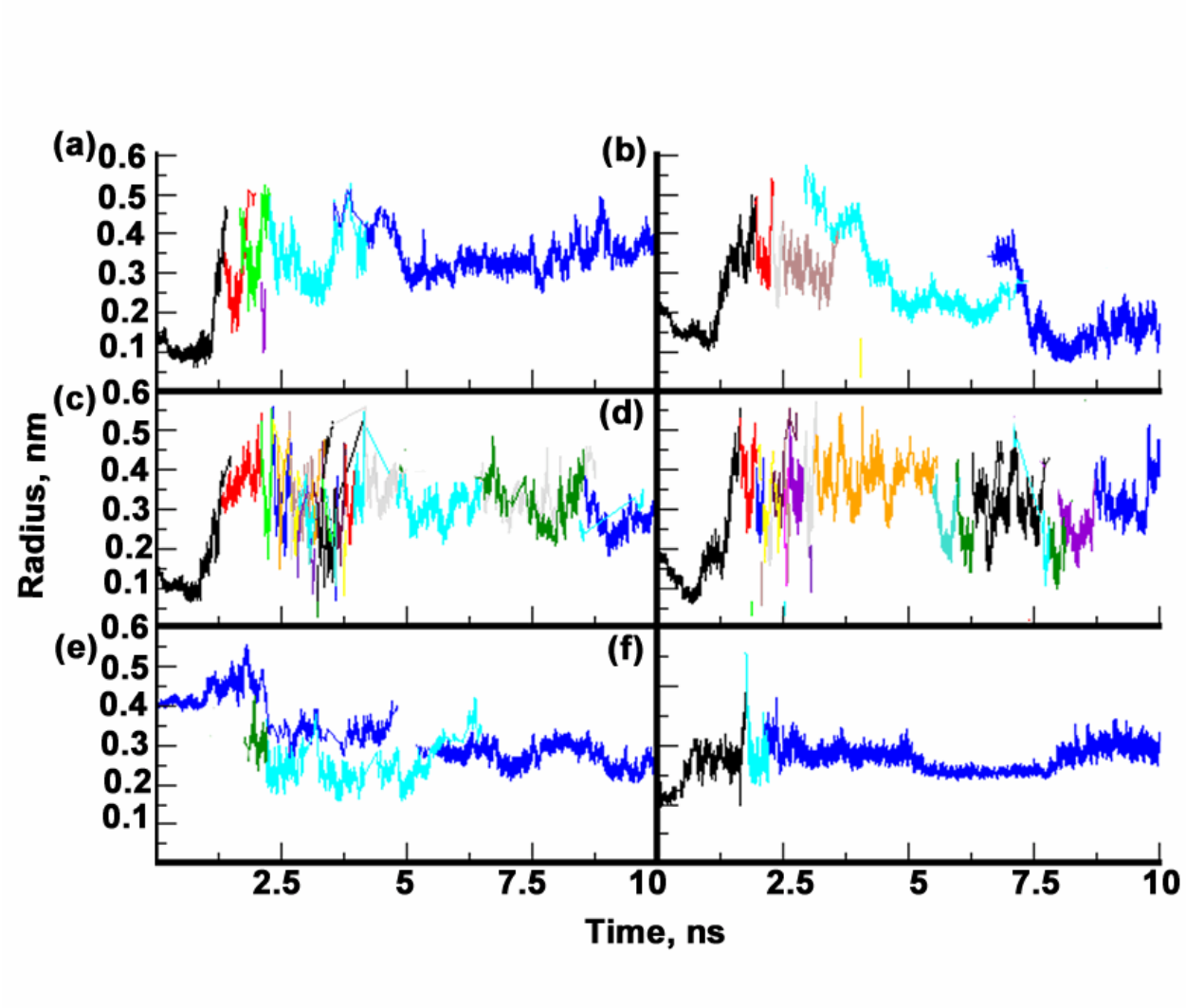

Figure S2. Cluster of populations for all configurations of PCBM in the Bulk simulations,(a)'dddd'(downward),(b)'dldl'(downward and left orientation),(c)'dudu'(downward and upward orientation),(d)'rlrl'(right and left orientation),(d) 'rrrr'(right orientation). We compared simulations with and without restraint on the P3HT side chains. Unrestraint side chains lead to accelerated dynamics of PCBM molecules (Figure 3h), which resulted in broader occupancy peaks of the PCBM molecules on the P3HT surface,(Figure 3c). However, the dynamics of the side chains is not essential as PCBMs tend to interact with and diffuse along the P3HT backbone on (010) surface.

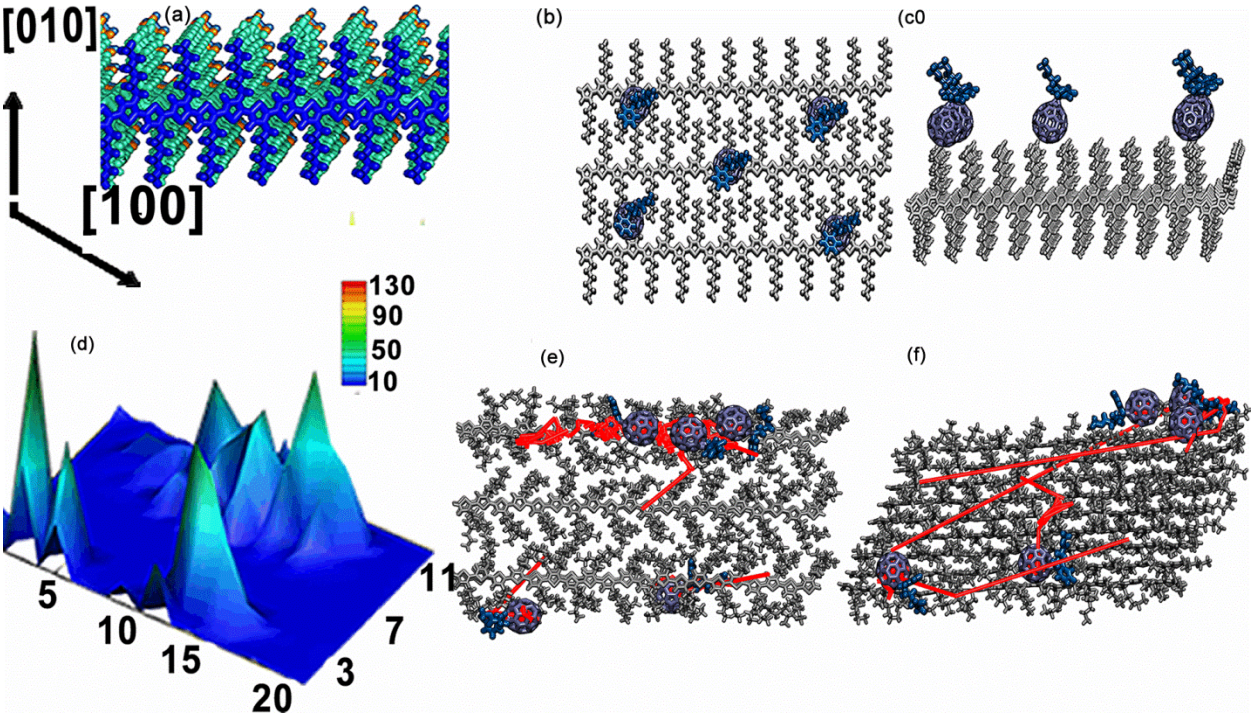

Figure S3. (a) Schematic of P3HT surface (b)-(c) Initial location of PCBM on the P3HT face-on and edge-on orientation (d) Occupancy time of the PCBM nanoparticles along the P3HT face with no restraints on P3HT side chains (e)-(f) Diffusion of PCBM on the P3HT face-on and edge-on orientation without restraints on the P3HT side chains.

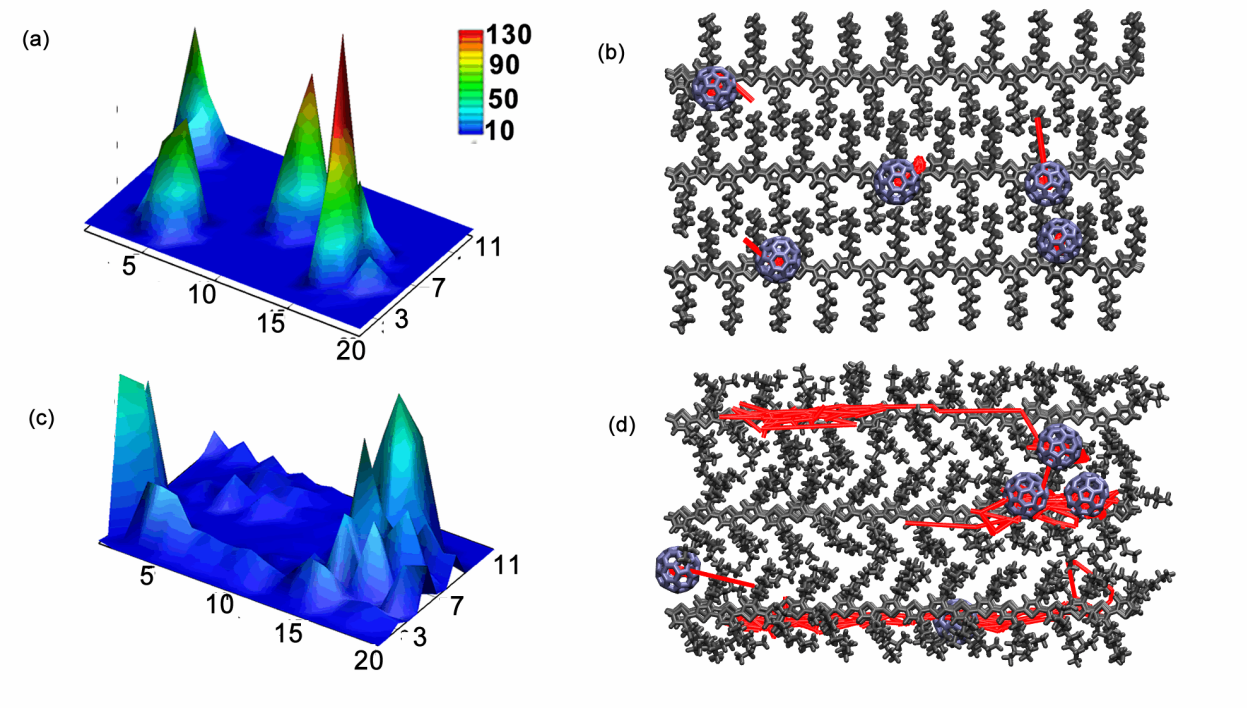

Figure S4. (a)-(c) Occupancy time of C_{60} on different sites of P3HT face-on orientation with restraints on P3HT surface and without restraints on P3HT side chains (b)-(d) Corresponding diffusion path of the C_{60} on P3HT face-on orientation with restraints on P3HT surface and without restraints on P3HT side chains.

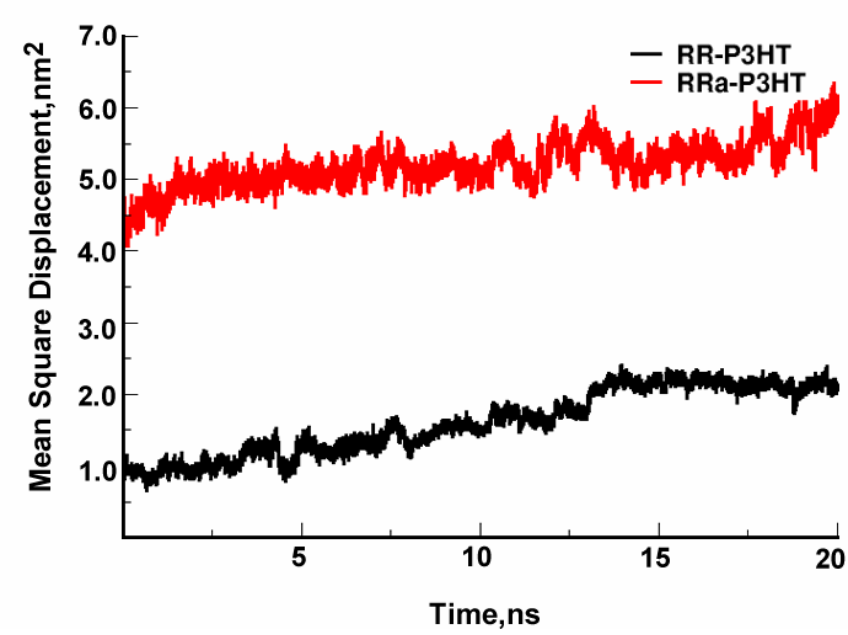

Figure S5. Mean square displacement of PCBM molecules on the P3HT (100) formed of regioregular P3HT chains and regiorandom P3HT chains.

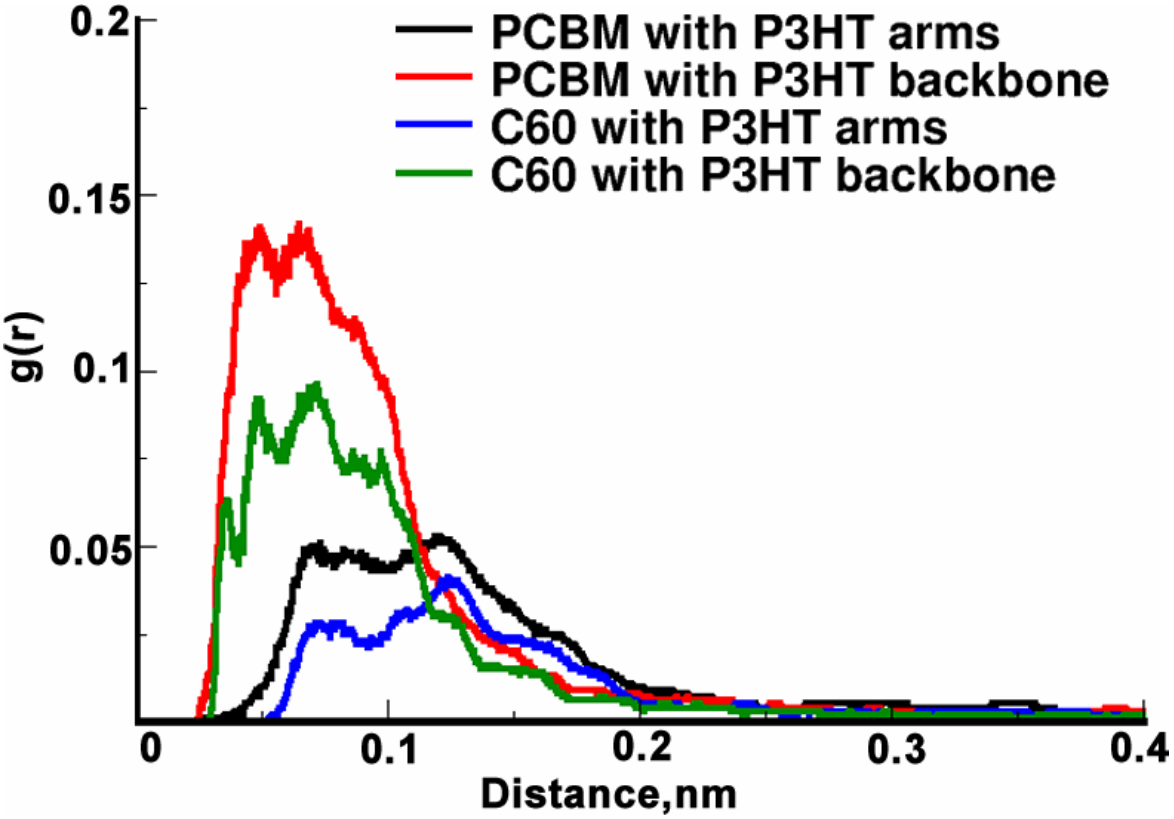

Figure S5. Radial distribution and structural order of PCBM and C_{60} nanoparticles with the P3HT arms and P3HT backbone in the models representing crystalline P3HT.

Table S1. Binding energy of PCBM and C60 with P3HT side chains and backbone [kcal/mole]

At 423K	PCBM on P3HT side chain	PCBM on P3HT backbone	PCBM tail of PCBM on side chain	PCBM tail of PCBM on backbone	C60 on P3HT side chain	C60 on P3HT backbone
With P3HT side chain	-7.66±0.84	-12.06±0.65	-1.21±0.81	-1.85±0.45	-3.7±0.23	-8.1±0.37
With P3HT backbone	-14.08±1.23	-15.66±1.7	-4.34±0.98	-4.46±1.52	-10.04±0.79	-11.72±0.66
With P3HT chain	-21.74±2.07	-27.72±2.35	-5.55±1.79	-6.31±1.97	-13.74±1.02	-19.82±1.03
At 300K						
With P3HT side chain	-8.22±0.47	-15.15±0.62	-1.25±0.39	-4.42±0.44	-4.04±0.16	-8.4±0.33
With P3HT backbone	-15.56±1.04	-16.69±0.67	-5.68±0.84	-5±0.5	-10.17±0.63	-11.89±0.53
With P3HT chain	-23.78±1.51	-31.84±1.29	-6.93±1.23	-9.42±0.94	-14.21±0.79	-20.29±0.86