Supporting information for "Improved force field for molecular modeling of poly(3-hexylthiophene)"

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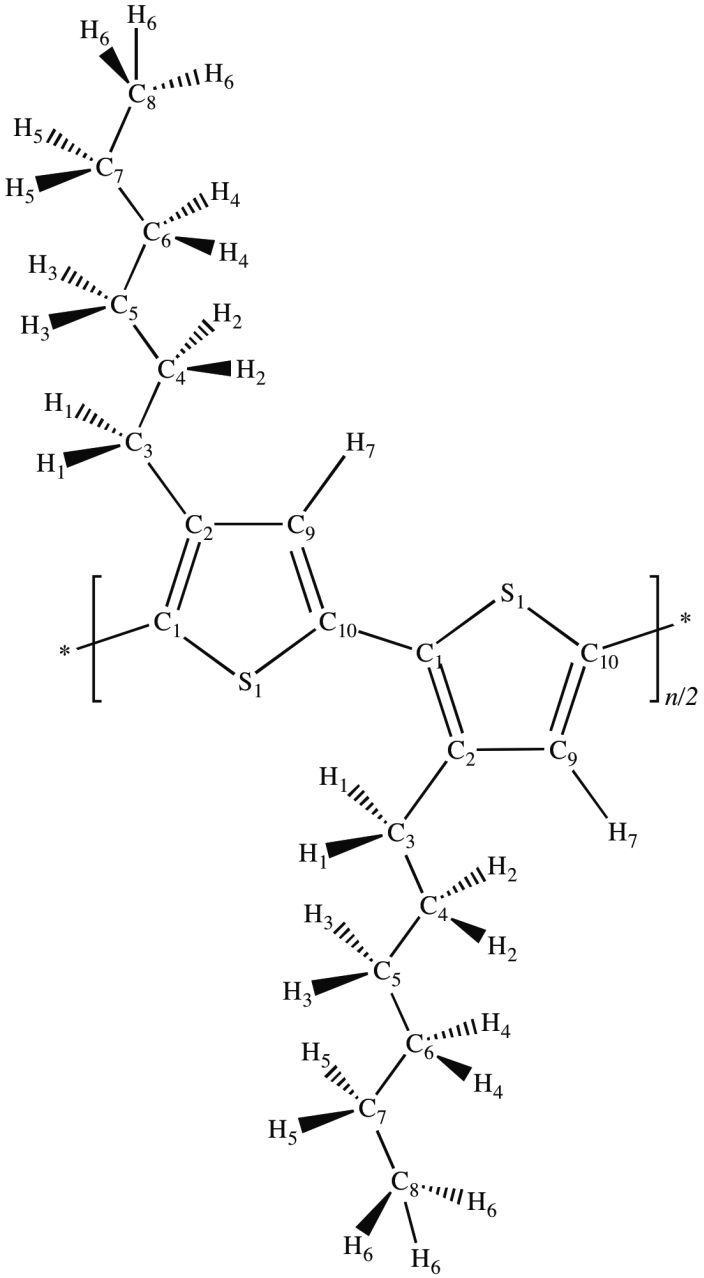

Fig. S1: Chemical structure of central two-monomer unit in a P3HT chain. Atom types are labeled with different numerical suffixes.

Table S1: Non-bonded parameters used in MD simulation of P3HT. P3HT atom types are defined in Fig. S1.

Atom type	σ(Å)[a,b]	ε(kcal mol^{-1})[a,b]	$q(e)$[c]
C1	3.550	0.070	-0.0441
S1	3.550	0.250	-0.2171
C2	3.550	0.070	0.0318
C3	3.500	0.066	0.1278
H1	2.500	0.030	0.0039
C4	3.500	0.066	-0.0926
H2	2.500	0.030	0.0290
C5	3.500	0.066	0.0189
H3	2.500	0.030	0.0036
C6	3.500	0.066	0.0289
H4	2.500	0.030	0.0069
C7	3.500	0.066	-0.1396
H5	2.500	0.030	0.0536
C8	3.500	0.066	-0.0670
H6	2.500	0.030	0.0200
C9	3.550	0.070	-0.3128
H7	2.420	0.030	0.2356
C10	3.550	0.070	0.1762

[a]From Ref. [1]
[b]From Ref. [2]
[c]This work

Table S2: Bond-stretching parameters. Bond-stretching potential is defined by harmonic expression; $E\_bond = k_r(r - r_{eq})^2$.

Bond type	r_{eq}(Å)	k_r(kcal mol^{-1} Å^{-2})
C9-H7[a]	1.0822	370.63
C1/C10-S1[a]	1.73373	291.25
C1-C2[a]; C9-C10[a]	1.37368	514.27
C2-C3[b]	1.50884	299.82
C2-C9[a]	1.43277	453.1
C3-H1[b]	1.09827	327.545
C3-C4[c]; C4-C5[c]; C5-C6[c]; C6-C7[c]; C7-C8[c]	1.54158	268
C4-H2[c]; C5-H3[c]; C6-H4[c]; C7-H5[c]; C8-H6[c]	1.09527	340
C1-C10	1.45	392.29

[a]From Ref. [1]
[b]This work
[c]From Ref. [2]

Table S3: Angle-bending parameters. Angle-bending potential is defined by harmonic expression; $E\_angle = k_\theta(\theta - \theta_{eq})^2$.

Angle type	θ_{eq}(degree)	k_θ(kcal mol^{-1} deg^{-2})
C1-S1-C10[a]	92.774	86.36
S1-C1-C2[a]; S1-C10-C9[a]	110.292	86.36
C1-C2-C9[a]; C2-C9-C10[a]	113.322	39.582
C2-C9-H7[a]	123.7	35.263
C1-C10-C9[a]; C2-C1-C10[a]	130.14	54.694
H7-C9-C10[a]	122.979	35.263
S1-C1-C10[a]; S1-C10-C1[a]	119.569	41.74
C3-C2-C9[b]	123.378	166.545
C1-C2-C3[b]	124.554	166.32
C2-C3-C4[b]	115.44	120.14
C2-C3-H1[b]	109.189	74.06
C3-C4-C5[c]; C4-C5-C6[c]; C5-C6-C7[c]; C6-C7-C8[c]	112.7	58.35
H1-C3-C4[c]; C3-C4-H2[c]; H2-C4-C5[c]; C4-C5-H3[c];	110.7	37.5
H3-C5-C6[c]; C5-C6-H4[c]; H4-C6-C7[c]; C6-C7-H5[c];	110.7	37.5
H5-C7-C8[c]; C7-C8-H6[c]	110.7	37.5
H1-C3-H1[c]; H2-C4-H2[c]; H3-C5-H3[c]; H4-C6-H4[c];	107.8	33
H5-C7-H5[c]; H6-C8-H6[c]	107.8	33

[a]From Ref. [1]
[b]This work
[c]From Ref. [2]

Table S4: Torsional parameters[a]. Torsional potential is defined by multi-harmonic expression; $E\_torsion = \sum_{n=0}^{4} V_n \cos^n \phi$.

Dihedral type	V_0(kcal mol^{-1})	V_1(kcal mol^{-1})	V_2(kcal mol^{-1})	V_3(kcal mol^{-1})	V_4(kcal mol^{-1})
S1-C10-C1-S1[b]	2.9533	0.1571	-4.2326	0.3979	1.8855
C9-C2-C3-C4[b]	0.3175	1.127	14.143	-22.297	6.7188
C2-C1-S1-C10;	126.32	-109.81	-19.738	-25.303	28.53
C1-S1-C10-C9;	126.32	-109.81	-19.738	-25.303	28.53
C1-C2-C9-C10;	126.32	-109.81	-19.738	-25.303	28.53
C2-C9-C10-S1	126.32	-109.81	-19.738	-25.303	28.53
C2-C3-C4-C5	2.4469	-6.3946	10.747	30.695	11.139
C3-C4-C5-C6	1.9475	-3.7121	1.388	8.6305	1.6008
C4-C5-C6-C7	1.8922	-3.4904	1.4665	7.1418	0.2859
C5-C6-C7-C8	1.9788	-3.8476	1.1614	7.419	0.4146
S1-C10-C1-C2	2.9533	-0.1571	-4.2326	-0.3979	1.8855
C3-C2-C9-C10	117.65	238.26	205.96	112.81	27.467
C2-C9-C10-C1	75.595	116	42.679	-1.528	-3.8137
C10-C1-S1-C10	158.7	418.34	521.33	376.73	115.12

[a]This work
[b]From Ref. [3]

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