

## Supporting information for “Improved force field for molecular modeling of poly(3-hexylthiophene)”

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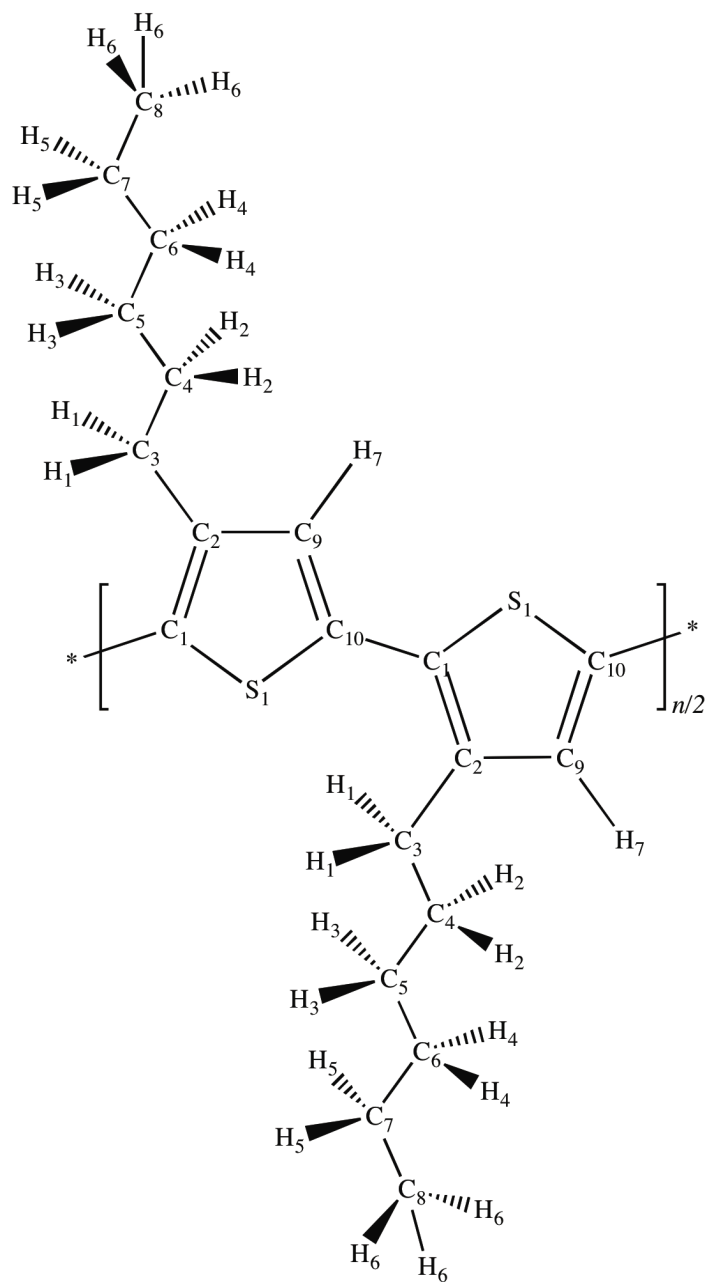


Fig. S1: Chemical structure of central two-monomer unit in a P3HT chain. Atom types are labeled with different numerical suffixes.

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

Atom type	$\sigma(\text{\AA})^{\text{a,b}}$	$\epsilon(\text{kcal mol}^{-1})^{\text{a,b}}$	$q(e)^{\text{c}}$
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

<sup>a</sup>From Ref. [1]

<sup>b</sup>From Ref. [2]

<sup>c</sup>This work

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

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

<sup>a</sup>From Ref. [1]

<sup>b</sup>This work

<sup>c</sup>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	$\theta_{eq}$ (degree)	$k_{\theta}$ (kcal mol <sup>-1</sup> deg <sup>-2</sup> )
C1-S1-C10 <sup>a</sup>	92.774	86.36
S1-C1-C2 <sup>a</sup> ; S1-C10-C9 <sup>a</sup>	110.292	86.36
C1-C2-C9 <sup>a</sup> ; C2-C9-C10 <sup>a</sup>	113.322	39.582
C2-C9-H7 <sup>a</sup>	123.7	35.263
C1-C10-C9 <sup>a</sup> ; C2-C1-C10 <sup>a</sup>	130.14	54.694
H7-C9-C10 <sup>a</sup>	122.979	35.263
S1-C1-C10 <sup>a</sup> ; S1-C10-C1 <sup>a</sup>	119.569	41.74
C3-C2-C9 <sup>b</sup>	123.378	166.545
C1-C2-C3 <sup>b</sup>	124.554	166.32
C2-C3-C4 <sup>b</sup>	115.44	120.14
C2-C3-H1 <sup>b</sup>	109.189	74.06
C3-C4-C5 <sup>c</sup> ; C4-C5-C6 <sup>c</sup> ; C5-C6-C7 <sup>c</sup> ; C6-C7-C8 <sup>c</sup>	112.7	58.35
H1-C3-C4 <sup>c</sup> ; C3-C4-H2 <sup>c</sup> ; H2-C4-C5 <sup>c</sup> ; C4-C5-H3 <sup>c</sup> ;	110.7	37.5
H3-C5-C6 <sup>c</sup> ; C5-C6-H4 <sup>c</sup> ; H4-C6-C7 <sup>c</sup> ; C6-C7-H5 <sup>c</sup> ;	110.7	37.5
H5-C7-C8 <sup>c</sup> ; C7-C8-H6 <sup>c</sup>	110.7	37.5
H1-C3-H1 <sup>c</sup> ; H2-C4-H2 <sup>c</sup> ; H3-C5-H3 <sup>c</sup> ; H4-C6-H4 <sup>c</sup> ;	107.8	33
H5-C7-H5 <sup>c</sup> ; H6-C8-H6 <sup>c</sup>	107.8	33

<sup>a</sup>From Ref. [1]

<sup>b</sup>This work

<sup>c</sup>From Ref. [2]

Table S4: Torsional parameters<sup>a</sup>. 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 <sup>-1</sup> )	$V_1$ (kcal mol <sup>-1</sup> )	$V_2$ (kcal mol <sup>-1</sup> )	$V_3$ (kcal mol <sup>-1</sup> )	$V_4$ (kcal mol <sup>-1</sup> )
S1-C10-C1-S1 <sup>b</sup>	2.9533	0.1571	-4.2326	0.3979	1.8855
C9-C2-C3-C4 <sup>b</sup>	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

<sup>a</sup>This work

<sup>b</sup>From Ref. [3]

References:

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