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Supplementary Information for "A comparative MD study of the local structure of polymer semiconductors P3HT and PBTTT"

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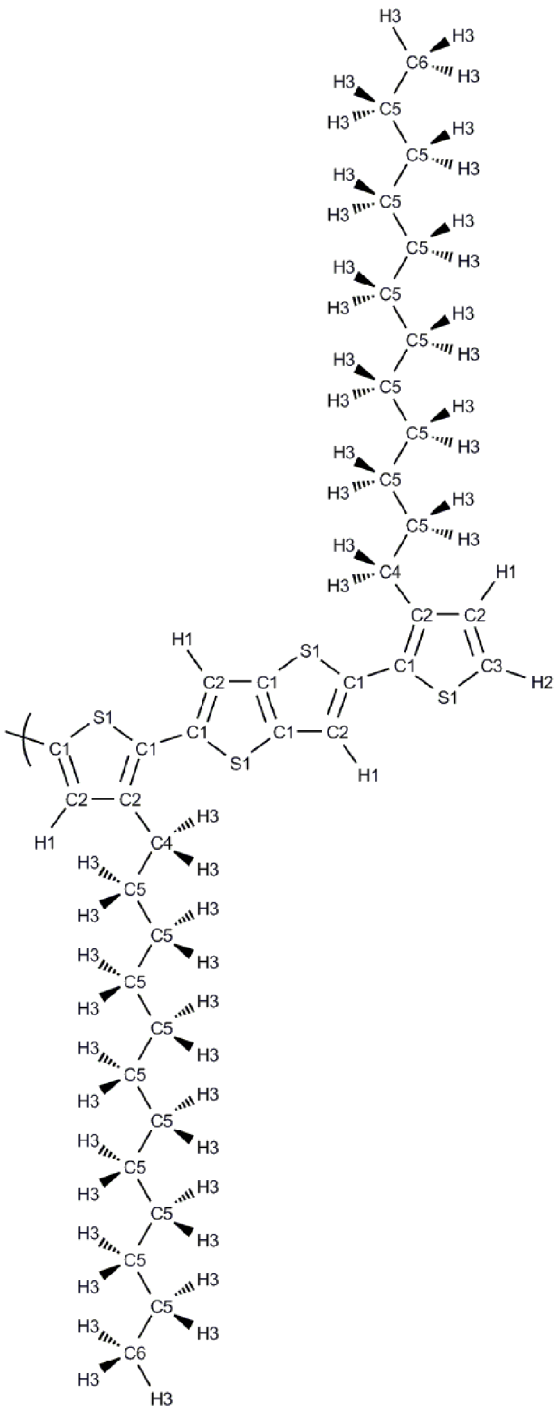

Fig. S1 Chemical structure of the end monomer in a poly(2,5-bis(3-alkylthiophen-2-yl)thieno[3,2-b]thiophene) (PBTTT) chain. Atoms of different type on our atomistic model are labelled with different numerical suffixes.

Table S1 Non-bonded parameters (LJ diameter σ_{ii}, LJ interaction strength ε_{ii}, and charge q_i) used in atomistic simulation models of PBTTT. PBTTT atom types are defined in Fig. S1.

Atom type i	σ_{ii}/Å	ε_{ii}/kcal mol^{-1}	q_i/e
S1[a]	3.550	0.250	-0.1496
C1[a]	3.550	0.070	0.0748
C2[a]	3.550	0.070	-0.1817
C3[a]	3.550	0.070	-0.1412
C4[b]	3.500	0.066	0.0617
C5[c]	3.500	0.066	-0.1200
C6[c]	3.500	0.066	-0.1800
H1[a]	2.420	0.030	0.1817
H2[a]	2.420	0.030	0.2160
H3[c]	2.500	0.030	0.0600

[a] Adapted from Ref. [1] (see our previous work for details [3]), with LJ parameters from OPLS-AA model [2].
[b] From OPLS-AA model [2], with charge adjusted for monomer neutrality.
[c] From OPLS-AA model [2].

Table S2 Parameters used in harmonic bond length potential $V_{\text{bond}}(l) = k_l(l - l_0)^2/2$ in atomistic simulation models of PBTTT. PBTTT atom types are defined in Fig. S1.

Bond type	l_0/Å	k_l/kcal mol^{-1} Å^{-2}
S1-C1[a]	1.732	582.50
C1-C2[a]	1.364	1028.54
C2-C2[a]	1.428	906.20
C2-H1[a]	1.080	741.26
C1-C1[a]	1.430	784.58
C3-H2[a]	1.080	741.26
C2-C4[b]	1.510	634.00
C4/C5-C5/C6[b]	1.529	536.00
C4/C5/C6-H3[b]	1.090	680.00

[a] Adapted from Ref. [1] (see our previous work for details [3]).
[b] From Ref. [2].

Table S3 Parameters used in harmonic bond angle potential $V_{\text{angle}}(\theta) = k_\theta(\theta - \theta_0)^2/2$ in atomistic simulation models of PBTTT. PBTTT atom types are defined in Fig. S1.

Angle type	θ_0/deg.	k_θ/kcal mol^{-1} rad^{-2}
C1-S1-C1[a]	92.774	172.720
S1-C1-C2[a]	110.292	172.720
C1-C2-C2[a]	113.322	79.164
C2-C2-H1[a]	123.700	70.526
C2-C1-C1[a]	130.140	109.388
C2-C3-H2[a]	125.100	70.526
C1-C2-H1[a]	122.979	70.526
S1-C1-C1[a]	119.569	83.480
S1-C3-H2[a]	124.609	57.574
C2-C2-C4[b]	123.700	140.000
C1-C2-C4[b]	122.979	140.000
C2-C4-C5[c]	114.000	126.000
C2-C4-H3[c]	109.500	70.000
C4/C5-C5-C5/C6[c]	112.700	116.700
C4/C5/C6-C4/C5/C6-H3[c]	110.700	75.000
H3-C4/C5/C6-H3[c]	107.800	66.000

[a] Adapted from Ref. [1] (see our previous work for details [3]).
[b] θ_0 adapted from Ref. [1]; k_θ from Ref. [2].
[c] From Ref. [2].

References

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