Electronic Supplementary Material (ESI) for Nanoscale

Supplementary Information for "Coarse-grained simulations of the solution-phase self-assembly of poly(3-hexylthiophene) nanostructures"

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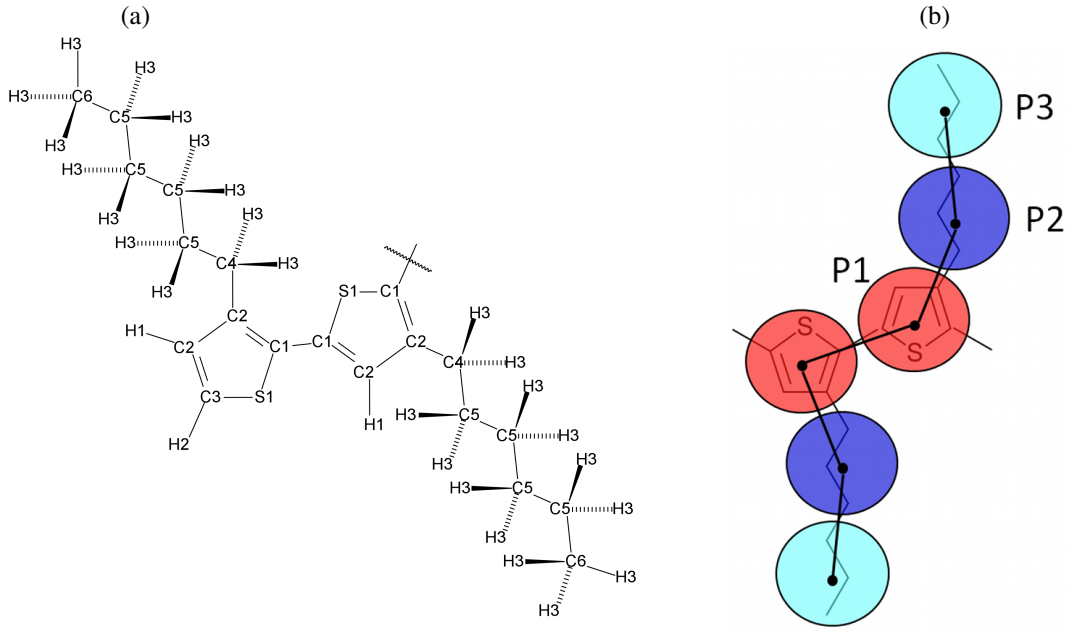

Fig. S1 (a) Chemical structure of last two monomers in a poly(3-hexylthiophene) chain. Atoms of different type on our atomistic model are labelled with different numerical suffixes. (b) Chemical structures of P3HT with sites in coarse-grained models depicted and labelled.

Table S1 Parameters used in non-bonded potential* $V_{\mathrm{nb}}(r_{ij}) = 4\varepsilon_{ij}\left[(\sigma_{ij}/r_{ij})^{12} - (\sigma_{ij}/r_{ij})^{6}\right] + q_i q_j/(4\pi\varepsilon_0 r_{ij})$ in atomistic simulation model of P3HT. P3HT atom types are defined in Figure S1(a).

Atom type i	σ_{ii} (Å)	ε_{ii} (kcal/mol)	q_i (e)
S1*	3.550	0.250	-0.1496
C1*	3.550	0.070	0.0748
C2*	3.550	0.070	-0.1817
C3*	3.550	0.070	-0.1412
C4†	3.500	0.066	0.0617
C5‡	3.500	0.066	-0.1200
C6‡	3.500	0.066	-0.1800
H1*	2.420	0.030	0.1817
H2*	2.420	0.030	0.2160
H3‡	2.500	0.030	0.0600

* σ_{ii} = LJ diameter (homonuclear); ε_{ii} = LJ interaction strength (homonuclear); q_i = charge; $\sigma_{ij} = \sqrt{\sigma_{ii}\sigma_{jj}}$, $\varepsilon_{ij} = \sqrt{\varepsilon_{ii}\varepsilon_{jj}}$.

* Adapted from Ref. 1 (see text for details), with LJ parameters from OPLS-AA model.[2]

† From OPLS-AA model,[2] with charge adjusted for monomer neutrality.

‡ From OPLS-AA model.[2]

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Table S2 Parameters used in harmonic bond length potential $V_{\text{bond}}(l) = k_l(l - l_0)^2/2$ in atomistic simulation model of P3HT. P3HT atom types are defined in Figure S1(a).

Bond type	l_0 (Å)	k_l (kcal/mol/Å^2)
S1–{C1,C3}*	1.732	582.50
{C1,C3}–C2*	1.364	1028.54
C2–C2*	1.428	906.20
C2–H1*	1.080	741.26
C1–C1*	1.430	784.58
C3–H2*	1.080	741.26
C2–C4†	1.510	634.00
{C4,C5}–{C5,C6}†	1.529	536.00
{C4,C5,C6}–H3†	1.090	680.00

* Adapted from Ref. 1 (see text for details).
† 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 model of P3HT. P3HT atom types are defined in Figure S1(a).

Angle type	θ_0 (Å)	k_θ (kcal/mol/rad^2)
C1–S1–{C1,C3}*	92.774	172.720
S1–{C1,C3}–C2*	110.292	172.720
{C1,C3}–C2–C2*	113.322	79.164
C2–C2–H1*	123.700	70.526
C2–C1–C1*	130.140	109.388
C2–C3–H2*	125.100	70.526
{C1,C3}–C2–H1*	122.979	70.526
S1–C1–C1*	119.569	83.480
S1–C3–H2*	124.609	57.574
C2–C2–C4†	123.700	140.000
C1–C2–C4†	122.979	140.000
C2–C4–C5‡	114.000	126.000
C2–C4–H3‡	109.500	70.000
{C4,C5}–C5–{C5,C6}‡	112.700	116.700
{C4,C5,C6}–{C4,C5,C6}–H3‡	110.700	75.000
H3–{C4,C5,C6}–H3‡	107.800	66.000

* Adapted from Ref. 1 (see text for details).
† Bond angle θ_0 adapted from Ref. 1; k_θ from Ref. 2.
‡ From Ref. 2.

Table S4 Parameters used in proper dihedral potential $U_{\mathrm{dihed}}(\phi) = \sum_{i=0}^{n} k_i \cos^i(\phi)$ in atomistic simulation models of P3HT (all k_i in kcal/mol).† P3HT atom types are defined in Figure S1(a).

Dihedral angle type	k_0	k_1	k_2	k_3	k_4	k_5	k_6	k_7	k_8
S1–C1–C1–S1*	1.6857	-0.1551	-0.7668	0.8848	-4.5490	-1.8898	7.9805	1.0988	-4.4117
C2–C1–C1–C2*	1.6857	-0.1551	-0.7668	0.8848	-4.5490	-1.8898	7.9805	1.0988	-4.4117
C2–C1–C1–S1*	1.6857	0.1551	-0.7668	-0.8848	-4.5490	1.8898	7.9805	-1.0988	-4.4117
C1–C2–C4–C5	0	0	0	0	0	-	-	-	-
C2–C2–C4–C5	0	0	0	0	0	-	-	-	-
C2–C4–C5–C5	0.7000	0.3500	0.0500	0.4000	0	-	-	-	-
{C4,C5}–C5–C5–{C5,C6}	0.7000	0.3500	0.0500	0.4000	0	-	-	-	-
C1–C2–C4–H3	0	0	0	0	0	-	-	-	-
C2–C2–C4–H3	0	0	0	0	0	-	-	-	-
C2–C4–C5–H3	0.2310	-0.6930	0	0.9241	0	-	-	-	-
{C4,C5,C6}–C5–{C4,C5,C6}–H3	0.1500	-0.4500	0	0.6000	0	-	-	-	-
H3–{C4,C5,C6}–{C4,C5,C6}–H3	0.1500	-0.4500	0	0.6000	0	-	-	-	-

* Besides these dihedrals, parameters for all others in the table were taken from the OPLS-AA model[2,3] and are identical to those in Ref. 4.
† Following the OPLS-AA model[5], ring planarity was maintained by applying proper and improper dihedral potentials from the AMBER94 force field[6] of the form $U_{\mathrm{dihed}}(\phi) = k[1 + d\cos(n\phi)]$. For the proper dihedrals (S1–{C1,C3}–C2–C2, {C1,C3}–C2–C2–C1, C2–{C1,C3}–S1–{C1,C3}, {C1,C3}–S1–{C1,C3}–C2, C4–C2–C2–H1, C4–C2–C2–{C1,C3}, C4–C2–C1–S1, C4–C2–C1–C1, H2–C3–C2–H1, H2–C3–C2–C2, H2–C3–S1–C1, C1–C2–C2–H1, C2–C2–C1–C1, S1–{C1,C3}–C2–H1, and {C1,C3}–S1–C1–C1), $k = 3.625$ kcal/mol, $d = -1$, and $n = 2$. For the improper dihedrals (C2–C1–C2–C4, C2–{C1,C3}–H1–C2, C3–C2–S1–H2, and C1–S1–C2–C1), $k = 1.1$ kcal/mol, $d = -1$, and $n = 2$. These parameters differ from those used in Ref. 4, in which only improper dihedral potentials were applied to ring atoms.

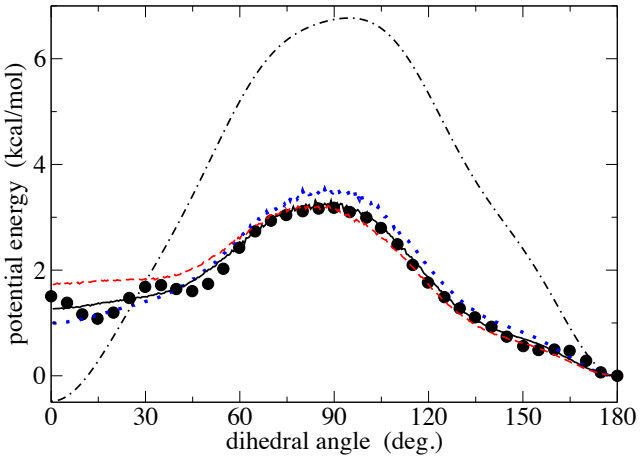

Fig. S2 Potential energy profile for rotation around the central inter-monomer bond in a 3-methylthiophene oligomer vs the inter-monomer sulfur-carbon-carbon-sulfur dihedral angle from DFT calculations of a 14-mer[7] (circles) and estimated as $-k_{\mathrm{B}}T\ln P_{\mathrm{dihed}}(\phi)$ from constant-temperature gas-phase MD simulations of a hexamer at 200 K (dotted line), 300 K (solid line), and 400 K (dashed line) in which the total applied "intrinsic" potential was the dot-dashed line.

Table S5 Parameters used in bond length potential $U_{\text{bond}}(l) = \sum_{i=2}^{n} c_i (l - l_0)^i$ in coarse-grained simulation model of P3HT. Site types are defined in Figure S1(b).

	P1–P1	P1–P2	P2–P3
l_0 (Å)	3.8817	4.0773	3.8297
c_2 (kcal/mol/Å^2)	58.228	56.4094	44.618
c_3 (kcal/mol/Å^3)	-	175.556	278.203
c_4 (kcal/mol/Å^4)	-	148.733	436.270

Table S6 Parameters used in bond angle potential $U_{\text{angle}}(\theta) = \sum_{i=2}^{n} c_i (\theta - \theta_0)^i$ in coarse-grained simulation model of P3HT. Site types are defined in Figure S1(b).

	P1–P1–P1	P1–P2–P3	P1–P1–P2*	P2–P1–P1*
θ_0 (deg.)	166.746	158.086	129.094	76.260
c_2 (kcal/mol/rad^2)	26.5042	12.3621	2.7338	22.9487
c_3 (kcal/mol/rad^3)	109.837	16.546	17.5095	-6.75983
c_4 (kcal/mol/rad^4)	148.883	6.94524	73.6114	0.497818

* Because regioregular P3HT chains have directionality, the P1–P1–P2 and P2–P1–P1 angles (labelled from the tail to the head end of the chain) differ and were parametrised separately.

Table S7 Parameters used in proper dihedral angle potential $U_{\text{dihed}}(\phi) = \sum_{i=0}^{4} c_i \cos^i(\phi)$ in coarse-grained simulation model of P3HT.† Site types are defined in Figure S1(b).

	P1–P1–P1–P1	P2–P1–P1–P2	P1–P1–P2–P3*	P3–P2–P1–P1*
c_0 (kcal/mol)	0.64032	1.49237	0.15825	0.00897
c_1 (kcal/mol)	0.38505	0.24725	-0.51422	0.11540
c_2 (kcal/mol)	0.16429	-2.14918	0.24975	0.37918
c_3 (kcal/mol)	-0.71093	0.12574	0.33530	0.04050
c_4 (kcal/mol)	-0.47873	1.02980	-0.07288	-0.07528

* Because regioregular P3HT chains have directionality, the P1–P1–P2–P3 and P3–P2–P1–P1 dihedrals (labelled from the tail to the head end of the chain) differ and were parametrised separately.

† P1–P2–P1–P1 improper dihedral potential: $U_{\text{improp}}(\xi) = c_\xi (\xi - \xi_0)^2$, where $c_\xi = 45.3281$ kcal/mol/rad^2 and $\xi_0 = 0$.

Table S8 Parameters used in non-bonded interaction potentials $U_{\mathrm{nb}}(r)$ in coarse-grained simulation models of P3HT. Site types are defined in Figure S1(b).

r (Å)	$U^{\mathrm{P1..P1}}$	$U^{\mathrm{P1..P2}}$	$U^{\mathrm{P1..P3}}$	$U^{\mathrm{P2..P2}}$	$U^{\mathrm{P2..P3}}$	$U^{\mathrm{P3..P3}}$
			(kcal/mol)			
3.01	74.90000000	26.50000000	59.50000000	44.00000000	40.20000000	74.90000000
3.11	53.70000000	18.90000000	42.50000000	32.10000000	28.90000000	53.70000000
3.21	38.70000000	13.50000000	30.60000000	23.60000000	21.00000000	38.70000000
3.31	27.80000000	9.64000000	21.80000000	17.40000000	15.20000000	27.80000000
3.41	20.00000000	7.03000000	15.60000000	12.90000000	11.00000000	20.00000000
3.51	14.50000000	4.62000000	11.40000000	9.66000000	8.19000000	14.60000000
3.61	10.50000000	2.42000000	8.03000000	7.24000000	5.84000000	10.50000000
3.71	7.63000000	0.95200000	5.09000000	5.56000000	3.49000000	7.41000000
3.81	5.06000000	0.62100000	3.20000000	3.42000000	2.44000000	5.15000000
3.91	2.80000000	0.43700000	1.86000000	1.41000000	1.76000000	3.02000000
4.01	1.38000000	0.14900000	0.94200000	0.86700000	1.07000000	0.71700000
4.11	1.18000000	0.05400000	0.40200000	0.74200000	0.58100000	0.24300000
4.21	1.10000000	0.00961000	0.19400000	0.60000000	0.39800000	0.19800000
4.31	0.81300000	-0.09810000	0.13000000	0.39200000	0.27200000	0.10900000
4.41	0.57400000	-0.20800000	-0.02340000	0.27600000	0.10400000	-0.02820000
4.51	0.31600000	-0.31300000	-0.16500000	0.16300000	-0.06120000	-0.17600000
4.61	-0.07550000	-0.35800000	-0.27100000	0.01030000	-0.19400000	-0.31200000
4.71	-0.23300000	-0.35900000	-0.35400000	-0.13000000	-0.28700000	-0.41800000
4.81	-0.36400000	-0.36900000	-0.40000000	-0.22300000	-0.31600000	-0.45300000
4.91	-0.48900000	-0.39900000	-0.41900000	-0.25600000	-0.30900000	-0.46600000
5.01	-0.50300000	-0.42600000	-0.45700000	-0.27900000	-0.33700000	-0.48300000
5.11	-0.51400000	-0.42900000	-0.48300000	-0.28200000	-0.34300000	-0.50000000
5.21	-0.58000000	-0.39700000	-0.47100000	-0.26300000	-0.33200000	-0.51000000
5.31	-0.59400000	-0.38400000	-0.42600000	-0.26700000	-0.32800000	-0.48400000
5.41	-0.58600000	-0.35700000	-0.40600000	-0.24800000	-0.30500000	-0.46000000
5.51	-0.56300000	-0.31400000	-0.41500000	-0.19200000	-0.27400000	-0.44400000
5.61	-0.52100000	-0.28700000	-0.38700000	-0.17500000	-0.24300000	-0.40000000
5.71	-0.48100000	-0.26100000	-0.35200000	-0.17000000	-0.21100000	-0.35400000
5.81	-0.44200000	-0.23400000	-0.31400000	-0.17000000	-0.17400000	-0.30600000
5.91	-0.40000000	-0.21000000	-0.26500000	-0.11200000	-0.19300000	-0.30900000
6.01	-0.35200000	-0.17300000	-0.23700000	-0.08090000	-0.15000000	-0.25100000
6.11	-0.29800000	-0.12000000	-0.22800000	-0.06440000	-0.06280000	-0.15500000
6.21	-0.29500000	-0.10300000	-0.19700000	-0.01290000	-0.06790000	-0.15500000
6.31	-0.22400000	-0.07130000	-0.15100000	0.00244000	-0.03400000	-0.14500000
6.41	-0.13500000	-0.03760000	-0.10500000	0.00348000	0.00427000	-0.12000000
6.51	-0.11800000	-0.03640000	-0.07890000	0.04100000	0.02510000	-0.04990000
6.61	-0.09110000	-0.01220000	-0.04820000	0.04410000	0.04010000	-0.00039100
6.71	-0.05650000	0.01260000	-0.01670000	0.04320000	0.05550000	0.02950000
6.81	0.00139000	0.02770000	0.01330000	0.05670000	0.09300000	0.04690000
6.91	0.01530000	0.04140000	0.01740000	0.06290000	0.09120000	0.05950000
7.01	0.02190000	0.05280000	0.02110000	0.07410000	0.08730000	0.07260000

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r (Å)	$U^{P1..P1}$	$U^{P1..P2}$	$U^{P1..P3}$	$U^{P2..P2}$	$U^{P2..P3}$	$U^{P3..P3}$
			(kcal/mol)			
7.11	0.03790000	0.05240000	0.06200000	0.13100000	0.11300000	0.09210000
7.21	0.07010000	0.09310000	0.08680000	0.14300000	0.11600000	0.09110000
7.31	0.10200000	0.11400000	0.09610000	0.12300000	0.12200000	0.09430000
7.41	0.11900000	0.10500000	0.08520000	0.07870000	0.14400000	0.13300000
7.51	0.11900000	0.09500000	0.10200000	0.10400000	0.12700000	0.12000000
7.61	0.11400000	0.08510000	0.10900000	0.13200000	0.10900000	0.11200000
7.71	0.10500000	0.07710000	0.08630000	0.14600000	0.10200000	0.11600000
7.81	0.11100000	0.08800000	0.11100000	0.11600000	0.11500000	0.09780000
7.91	0.12300000	0.10300000	0.10900000	0.09800000	0.12900000	0.09150000
8.01	0.13700000	0.11300000	0.08150000	0.09980000	0.13700000	0.09910000
8.11	0.11600000	0.09790000	0.07880000	0.06390000	0.10000000	0.11900000
8.21	0.10500000	0.09010000	0.06160000	0.05040000	0.07860000	0.10500000
8.31	0.10400000	0.09150000	0.03870000	0.04770000	0.07400000	0.05420000
8.41	0.06450000	0.05550000	0.01730000	0.04760000	0.04090000	0.02060000
8.51	0.05570000	0.03860000	0.01170000	0.02830000	0.03510000	0.02430000
8.61	0.05880000	0.02960000	0.02340000	-0.01060000	0.04310000	0.05640000
8.71	0.04590000	0.02200000	0.00196000	-0.00051200	0.01650000	0.00075400
8.81	0.03560000	0.01750000	-0.00634000	-0.01350000	0.00272000	-0.01260000
8.91	0.02490000	0.01450000	-0.01300000	-0.03000000	-0.00585000	-0.01850000
9.01	-0.01200000	0.00649000	-0.02620000	-0.03340000	-0.00980000	-0.03040000
9.11	-0.01450000	-0.00849000	-0.04340000	-0.02670000	-0.02670000	-0.04530000
9.21	-0.01230000	-0.02540000	-0.05820000	-0.02130000	-0.04390000	-0.05680000
9.31	-0.01080000	-0.03880000	-0.02970000	-0.03480000	-0.04110000	-0.03100000
9.41	-0.02670000	-0.02900000	-0.04680000	-0.03130000	-0.03020000	-0.02770000
9.51	-0.04810000	-0.01660000	-0.06030000	-0.02700000	-0.02300000	-0.03590000
9.61	-0.05580000	-0.02980000	-0.03770000	-0.02610000	-0.03520000	-0.05680000
9.71	-0.05840000	-0.02350000	-0.04950000	-0.01620000	-0.02310000	-0.04260000
9.81	-0.06170000	-0.02190000	-0.05790000	-0.00645000	-0.01010000	-0.02810000
9.91	-0.07000000	-0.03170000	-0.05920000	-0.00156000	-0.00160000	-0.04020000
10.02	-0.09100000	-0.02530000	-0.06560000	0.01020000	-0.01050000	-0.00185000
10.12	-0.09960000	-0.01850000	-0.06850000	0.01730000	-0.01170000	0.00761000
10.22	-0.07940000	-0.01150000	-0.06160000	0.01620000	-0.00429000	-0.04680000
10.32	-0.08920000	-0.01710000	-0.07220000	0.01050000	0.00207000	-0.01970000
10.42	-0.08470000	-0.01690000	-0.06680000	0.01280000	0.00163000	-0.01500000
10.52	-0.06640000	-0.01060000	-0.04020000	0.02370000	-0.01410000	-0.03090000
10.62	-0.07270000	-0.00699000	-0.04210000	0.03070000	-0.01440000	0.00230000
10.72	-0.07450000	-0.00827000	-0.03920000	0.02960000	-0.00087300	0.00818000
10.82	-0.07110000	-0.01320000	-0.03490000	0.02280000	0.01950000	0.00054000
10.92	-0.05350000	-0.00794000	-0.04240000	0.01390000	0.01800000	0.00390000
11.02	-0.06000000	-0.00452000	-0.04780000	0.01940000	0.00560000	-0.01090000
11.12	-0.08160000	-0.00301000	-0.04370000	0.03370000	-0.00683000	-0.03440000
11.22	-0.05910000	-0.00492000	-0.02920000	0.01990000	0.00807000	-0.00219000
11.32	-0.05370000	-0.01050000	-0.01520000	0.00953000	0.01010000	0.01080000
11.42	-0.05170000	-0.01540000	-0.00362000	0.00295000	0.00911000	0.01020000
11.52	-0.01630000	0.00042800	-0.02100000	0.00036200	0.01650000	-0.00537000

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r (Å)	$U^{P1..P1}$	$U^{P1..P2}$	$U^{P1..P3}$	$U^{P2..P2}$	$U^{P2..P3}$	$U^{P3..P3}$
			(kcal/mol)			
11.62	-0.03150000	0.00408000	-0.01030000	-0.00301000	0.00397000	-0.00240000
11.72	-0.05030000	0.00615000	0.00271000	-0.00431000	-0.01220000	0.00136000
11.82	-0.02960000	0.01600000	-0.01740000	0.01800000	0.00802000	-0.00714000
11.92	-0.02750000	0.00337000	-0.00326000	0.00982000	-0.00907000	-0.00855000
12.02	-0.02530000	-0.01390000	0.00557000	0.00012900	-0.01930000	-0.00396000
12.12	-0.02080000	-0.01770000	-0.01000000	-0.00448000	-0.01140000	0.00875000
12.22	-0.01990000	-0.00434000	-0.00600000	-0.01150000	-0.00816000	0.00706000
12.32	-0.01560000	0.00098500	-0.00544000	-0.01330000	-0.00745000	-0.00044600
12.42	0.00600000	-0.00989000	-0.01080000	0.00916000	-0.01050000	-0.01150000
12.52	-0.00931000	-0.00927000	-0.00910000	-0.01590000	-0.00380000	0.00299000
12.62	-0.01080000	-0.01100000	-0.00581000	-0.02600000	-0.00390000	0.01150000
12.72	0.00302000	-0.01840000	-0.00208000	-0.01930000	-0.01160000	0.01060000
12.82	0.01160000	-0.00201000	0.00191000	-0.00666000	-0.02160000	0.00733000
12.92	0.00365000	-0.00274000	0.00149000	-0.00664000	-0.02640000	0.00994000
13.02	-0.02930000	-0.02110000	-0.00998000	-0.01800000	-0.01850000	0.01770000
13.12	0.00223000	-0.02420000	0.00325000	-0.02500000	-0.00307000	0.02430000
13.22	0.01190000	-0.01570000	-0.00182000	-0.02640000	0.00052900	0.02490000
13.32	0.00718000	-0.00351000	-0.01650000	-0.02390000	-0.00518000	0.01650000
13.42	-0.00794000	-0.01290000	-0.00933000	-0.02770000	-0.01450000	0.00632000
13.52	-0.00539000	-0.01580000	-0.00215000	-0.02630000	-0.01320000	0.00419000
13.62	0.00302000	-0.01570000	0.00450000	-0.02140000	-0.00405000	0.00677000
13.72	0.00853000	-0.01410000	-0.00774000	-0.01530000	-0.01610000	0.00457000
13.82	0.00765000	-0.01280000	-0.00598000	-0.00859000	-0.01300000	0.00163000
13.92	0.00452000	-0.01140000	-0.00064700	-0.00396000	-0.00333000	-0.00218000
14.02	0.03550000	-0.00716000	-0.01780000	-0.04110000	0.01160000	-0.01110000
14.12	0.02410000	-0.01070000	-0.01020000	-0.02820000	0.00514000	-0.00778000
14.22	0.00921000	-0.01610000	-0.00253000	-0.01210000	-0.00905000	0.00322000
14.32	0.00712000	-0.01280000	-0.01120000	-0.01510000	-0.01180000	0.01770000
14.42	0.00312000	-0.01810000	-0.01110000	-0.01190000	-0.00399000	-0.00324000
14.52	0.00116000	-0.02100000	-0.00754000	-0.01150000	-0.00093700	-0.02220000
14.62	0.01130000	-0.01120000	-0.00053100	-0.01480000	-0.00934000	-0.01490000
14.72	0.00091300	-0.01510000	-0.00314000	-0.01900000	-0.01300000	-0.00177000
14.82	-0.00459000	-0.01700000	-0.01040000	-0.02200000	-0.01070000	0.00213000
14.92	-0.00159000	-0.01620000	-0.02020000	-0.01840000	0.00348000	-0.01740000
15.02	-0.00243000	-0.01620000	-0.00822000	-0.01010000	-0.01020000	-0.01660000
15.12	-0.00197000	-0.01190000	-0.00236000	-0.00192000	-0.01650000	-0.01550000
15.22	0.00117000	0.00275000	-0.00727000	0.00280000	-0.01470000	-0.01440000
15.32	-0.00928000	0.00041600	-0.01790000	-0.00511000	-0.01110000	0.00511000
15.42	-0.01330000	-0.00324000	-0.01820000	-0.01110000	-0.00809000	0.00738000
15.52	-0.01150000	-0.00711000	-0.00603000	-0.01350000	-0.00628000	-0.00925000
15.62	-0.00732000	-0.00953000	-0.00348000	-0.01290000	-0.00741000	-0.00610000
15.72	-0.00678000	-0.00483000	-0.00971000	-0.00689000	-0.00634000	0.00338000
15.82	-0.01200000	0.00568000	-0.01900000	0.00425000	-0.00453000	0.01420000
15.92	-0.02290000	-0.00146000	-0.01470000	-0.01650000	-0.00273000	-0.00936000
16.02	-0.02110000	-0.00418000	-0.00690000	-0.01240000	-0.00546000	-0.01190000

(Continued on next page.)

r (Å)	$U^{P1..P1}$	$U^{P1..P2}$	$U^{P1..P3}$	$U^{P2..P2}$	$U^{P2..P3}$	$U^{P3..P3}$
			(kcal/mol)			
16.12	-0.01200000	-0.00560000	0.00050900	0.00168000	-0.01270000	-0.00896000
16.22	-0.01350000	-0.01340000	-0.01740000	-0.01390000	0.00266000	-0.00605000
16.32	-0.02010000	-0.00854000	-0.01280000	-0.00496000	-0.00664000	-0.00748000
16.42	-0.02570000	0.00106000	-0.00523000	0.00529000	-0.01840000	-0.01180000
16.52	-0.02590000	-0.01810000	-0.00608000	-0.01020000	-0.01370000	-0.00443000
16.62	-0.02470000	-0.00765000	-0.00836000	-0.01080000	-0.00588000	-0.00929000
16.72	-0.01960000	0.00144000	-0.01170000	-0.00685000	0.00215000	-0.01370000
16.82	0.00278000	-0.01610000	-0.01890000	-0.00017700	0.00971000	0.00313000
16.92	-0.00110000	-0.01130000	-0.01220000	0.00010800	0.00389000	-0.00413000
17.02	-0.00492000	-0.00755000	-0.00195000	0.00112000	-0.00589000	-0.00750000
17.12	0.00251000	-0.00790000	0.00381000	0.01410000	-0.00757000	0.00673000
17.22	-0.00515000	-0.00469000	-0.00157000	-0.00046900	-0.00491000	0.00133000
17.32	-0.00741000	-0.00245000	-0.00948000	-0.01510000	-0.00259000	-0.00291000
17.42	0.00418000	-0.00511000	-0.01810000	-0.01810000	-0.00240000	-0.00221000
17.52	-0.00536000	-0.01630000	-0.00692000	-0.00683000	-0.01110000	-0.02110000
17.62	-0.00883000	-0.01920000	-0.00526000	0.00432000	-0.01120000	-0.02450000
17.72	-0.00713000	-0.00596000	-0.01920000	0.01310000	0.00713000	-0.00843000
17.82	-0.00403000	-0.01470000	-0.01610000	0.00147000	-0.00337000	-0.00840000
17.92	0.00008130	-0.01180000	-0.00632000	-0.00218000	-0.00268000	-0.00574000
18.02	0.00561000	0.00203000	0.00291000	0.00259000	0.00654000	-0.00196000
18.12	-0.01420000	-0.01290000	-0.00235000	-0.00764000	-0.00557000	-0.00503000
18.22	-0.01240000	-0.01310000	-0.00745000	-0.00796000	-0.00607000	-0.00470000
18.32	0.00014600	-0.00754000	-0.01150000	-0.00165000	-0.00160000	-0.00252000
18.42	0.00119000	-0.01310000	-0.00682000	0.00965000	-0.00477000	-0.00677000
18.52	-0.00021300	-0.01310000	-0.00513000	0.01020000	0.00146000	-0.00630000
18.62	-0.00231000	-0.00913000	-0.00440000	-0.00010200	0.01060000	-0.00410000
18.72	-0.00561000	0.00071300	0.00158000	-0.01720000	-0.00714000	-0.00619000
18.82	-0.01330000	-0.00293000	0.00111000	-0.01290000	-0.00723000	-0.00139000
18.92	-0.02110000	-0.01110000	-0.00224000	-0.00093100	-0.00480000	0.00504000
19.02	0.00255000	-0.00880000	-0.00657000	0.00495000	-0.00276000	0.00109000
19.12	-0.01160000	0.00176000	-0.00906000	-0.00653000	-0.00356000	0.00596000
19.22	-0.02240000	0.00803000	-0.00897000	-0.01830000	-0.00867000	0.00868000
19.32	-0.00833000	-0.00381000	-0.00652000	0.00367000	-0.01790000	-0.00288000
19.42	-0.00517000	-0.00396000	-0.00683000	-0.01080000	-0.01440000	-0.00134000
19.52	-0.00591000	-0.00437000	-0.00713000	-0.01600000	-0.00985000	0.00086200
19.62	-0.00965000	-0.00805000	-0.00574000	0.00256000	-0.00957000	0.00304000
19.72	-0.00671000	0.00063100	-0.01210000	0.00190000	-0.00235000	-0.00433000
19.82	-0.00373000	0.00235000	-0.01520000	0.00220000	-0.00063800	-0.00771000
19.9	-0.00424000	-0.01420000	-0.01090000	0.00386000	-0.01150000	-0.00095500
20	-0.01890000	-0.00853000	-0.00044500	0.00038100	-0.00963000	-0.00323000

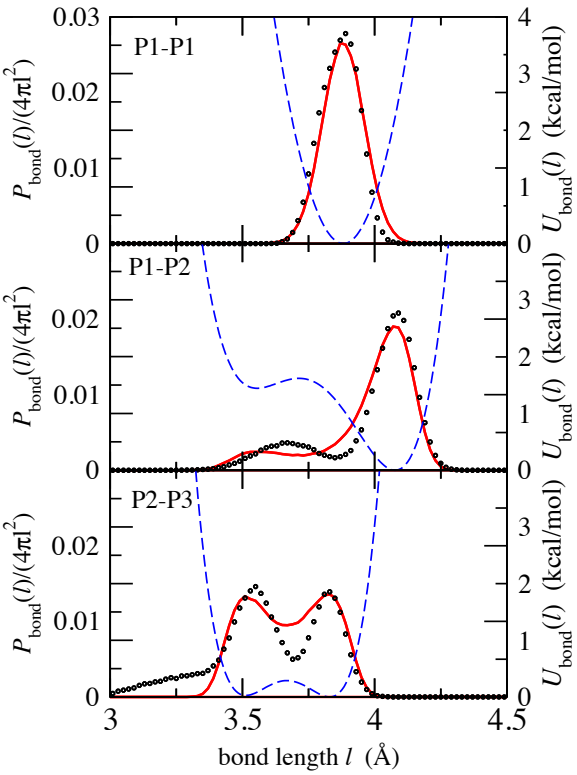

Fig. S3 Bond length probability distributions, $U_{bond}(l)$, computed from a constant NPT simulation at 353 K and 1 atm of four P3HT 10-mers and 1134 anisole molecules (circles) and from a constant NVT simulation at 353 K of an equivalent CG system (solid lines) using optimised CG interaction potentials, $U_{bond}(l)$ (dashed lines). Site type definitions are given in Figure S1(b).

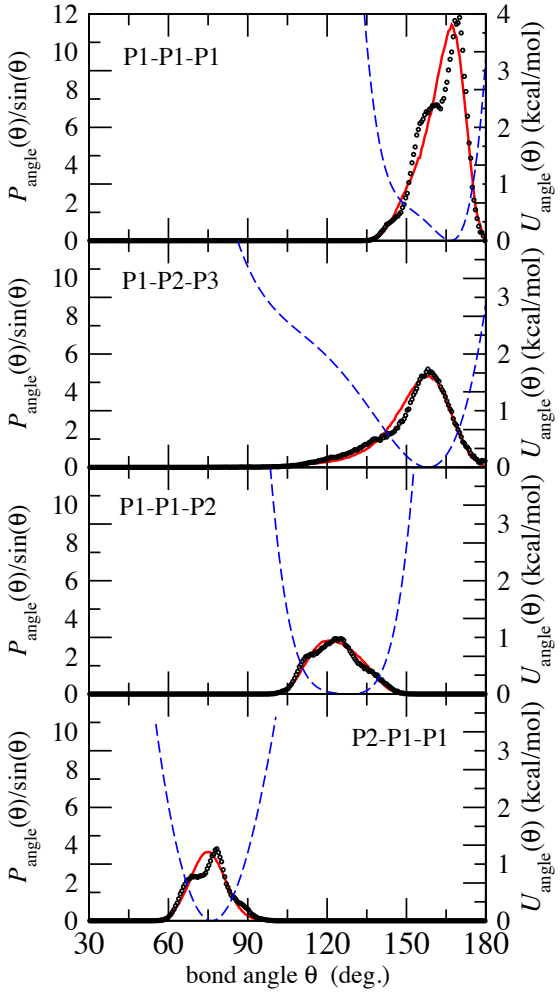

Fig. S4 Bond angle probability distributions, $P_{angle}(\theta)$, computed from a constant NPT simulation at 353 K and 1 atm of four P3HT 10-mers and 1134 anisole molecules (circles) and from a constant NVT simulation at 353 K of an equivalent CG system (solid lines) using optimised CG interaction potentials, $U_{angle}(\theta)$ (dashed lines). Site type definitions are given in Figure S1(b).

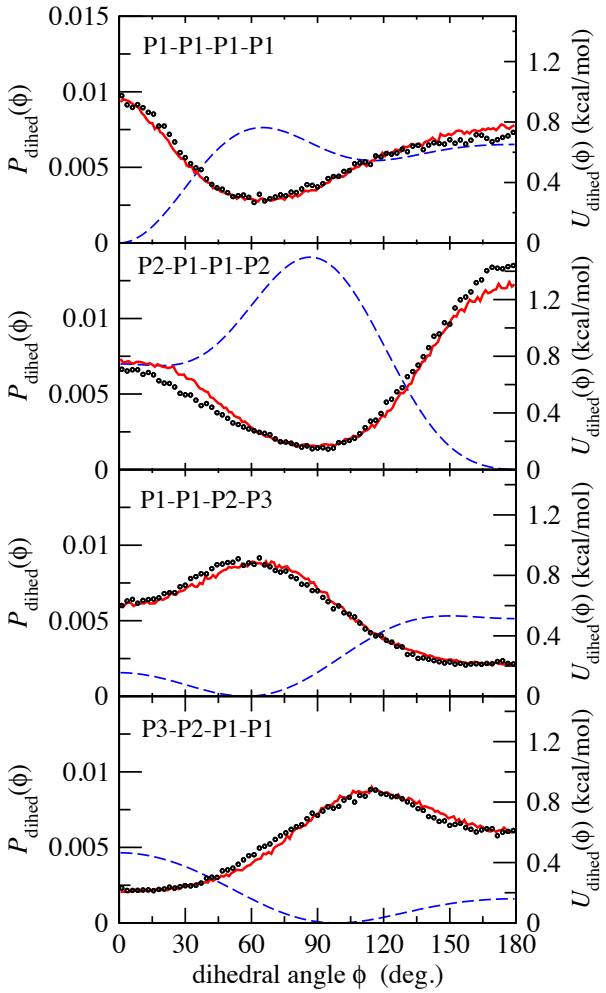

Fig. S5 Proper dihedral angle probability distributions, $P_{\text{dihed}}(\phi)$, computed from a constant NPT simulation at 353 K and 1 atm of four P3HT 10-mers and 1134 anisole molecules (circles) and from a constant NVT simulation of an equivalent CG system at 353 K (solid lines) using optimised CG interaction potentials, $P_{\text{dihed}}(\phi)$ (dashed lines). Site type definitions are given in Figure S1(b).

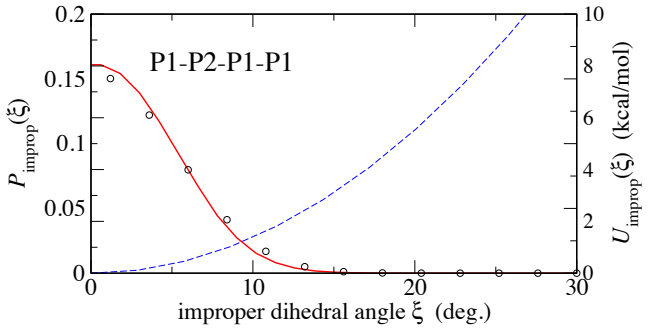

Fig. S6 Improper dihedral angle probability distribution, $P_{\text{improp}}(\xi)$, computed from a constant NPT simulation at 353 K and 1 atm of four P3HT 10-mers and 1134 anisole molecules (circles) and from a constant NVT simulation of an equivalent CG system at 353 K (solid lines) using optimised CG interaction potentials, $U_{\text{improp}}(\xi)$ (dashed lines). Site type definitions are given in Figure S1(b).

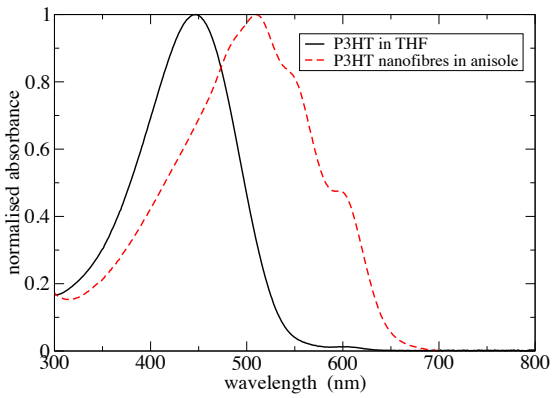

Fig. S7 Experimentally measured normalized UV-vis absorption spectra of non-aggregated P3HT in THF (solid line) and of P3HT nanowires in anisole (dashed line).

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