Supporting Information:

Effect of substituting non-polar chains with polar chains on the structural dynamics of small organic molecule and polymer semiconductors

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Table S1. Crystal data and structure refinement for PTTP-TEG.

Identification code	PTTP-TEG
Empirical formula	C68 H84 O16 S4
Formula weight	1285.59
Temperature	100(2) K
Wavelength	1.54184 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 22.9690(10) A alpha = 90 deg.
	b = 8.1561(3) A beta = 100.575(4) deg.
	c = 8.6458(3) A gamma = 90 deg.
Volume	1592.17(11) A^3
Z, Calculated density	1, 1.341 Mg/m^3
Absorption coefficient	1.942 mm^-1
F(000)	684
Crystal size	0.03 mm × 0.04 mm × 0.05 mm
Theta range for data collection	3.916 to 68.221 deg.
Limiting indices	-27<=h<=27, 0<=k<=9, 0<=l<=10

Reflections collected / unique	2916 / 2916 [R(int) = 0.041]
Completeness to theta = 67.684	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1 and 0.682
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2916 / 0 / 209
Goodness-of-fit on F^2	1.084
Final R indices [I>2sigma(I)]	R1 = 0.0488, wR2 = 0.1288
R indices (all data)	R1 = 0.0584, wR2 = 0.1338
Extinction coefficient	n/a
Largest diff. peak and hole	0.513 and -0.339 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for PTTP-TEG. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
S(1)	9638(1)	-735(1)	2081(1)	29(1)
O(1)	7558(1)	-307(2)	6705(2)	31(1)
O(2)	7101(1)	501(2)	9483(2)	33(1)
O(3)	6250(1)	3131(2)	9669(2)	38(1)
O(4)	5347(1)	5250(5)	7994(3)	92(1)
C(1)	9744(1)	207(3)	350(2)	28(1)
C(2)	9307(1)	1298(3)	-156(3)	33(1)
C(3)	8877(1)	1395(3)	817(3)	31(1)
C(4)	8987(1)	348(3)	2089(3)	28(1)
C(5)	8629(1)	124(3)	3319(2)	27(1)
C(6)	8048(1)	708(3)	3084(3)	29(1)
C(7)	7704(1)	562(3)	4236(3)	29(1)
C(8)	7938(1)	-198(3)	5659(2)	27(1)
C(9)	8514(1)	-797(3)	5923(3)	31(1)
C(10)	8855(1)	-629(3)	4755(3)	30(1)
C(11)	7781(1)	-1001(3)	8222(3)	32(1)
C(12)	7274(1)	-1096(3)	9101(3)	36(1)
C(13)	6604(1)	411(3)	10250(3)	38(1)
C(14)	6471(1)	2029(3)	10913(3)	37(1)
C(15)	6039(1)	4587(4)	10282(3)	48(1)
C(16)	5863(2)	5786(4)	8994(5)	67(1)
C(17A)	5188(4)	6880(14)	7121(11)	66(3)
C(17B)	5081(3)	5871(16)	6483(12)	58(3)

Table S3. Bond lengths [A] and angles [deg] for PTTP-TEG.

S(1)-C(4)	1.738(2)
S(1)-C(1)	1.738(2)
O(1)-C(8)	1.370(3)
O(1)-C(11)	1.434(3)
O(2)-C(12)	1.419(3)
O(2)-C(13)	1.423(3)
O(3)-C(14)	1.421(3)
O(3)-C(15)	1.421(3)
O(4)-C(16)	1.403(5)
O(4)-C(17B)	1.430(8)
O(4)-C(17A)	1.538(8)
C(1)-C(2)	1.353(3)
C(1)-C(1)#1	1.458(4)
C(2)-C(3)	1.412(3)
C(3)-C(4)	1.378(3)
C(4)-C(5)	1.469(3)
C(5)-C(6)	1.396(3)
C(5)-C(10)	1.397(3)
C(6)-C(7)	1.385(3)
C(7)-C(8)	1.394(3)
C(8)-C(9)	1.391(3)
C(9)-C(10)	1.394(3)
C(11)-C(12)	1.504(3)
C(13)-C(14)	1.493(4)
C(15)-C(16)	1.482(5)
C(4)-S(1)-C(1)	92.05(11)
C(8)-O(1)-C(11)	117.68(17)
C(12)-O(2)-C(13)	110.14(18)

C(14)-O(3)-C(15)	110.17(19)
C(16)-O(4)-C(17B)	128.6(5)
C(16)-O(4)-C(17A)	97.5(5)
C(2)-C(1)-C(1)#1	128.7(3)
C(2)-C(1)-S(1)	110.87(17)
C(1)#1-C(1)-S(1)	120.4(2)
C(1)-C(2)-C(3)	113.7(2)
C(4)-C(3)-C(2)	113.3(2)
C(3)-C(4)-C(5)	127.6(2)
C(3)-C(4)-S(1)	110.04(17)
C(5)-C(4)-S(1)	122.35(17)
C(6)-C(5)-C(10)	117.9(2)
C(6)-C(5)-C(4)	119.9(2)
C(10)-C(5)-C(4)	122.2(2)
C(7)-C(6)-C(5)	121.5(2)
C(6)-C(7)-C(8)	119.7(2)
O(1)-C(8)-C(9)	124.9(2)
O(1)-C(8)-C(7)	115.0(2)
C(9)-C(8)-C(7)	120.1(2)
C(8)-C(9)-C(10)	119.4(2)
C(9)-C(10)-C(5)	121.4(2)
O(1)-C(11)-C(12)	107.58(19)
O(2)-C(12)-C(11)	110.3(2)
O(2)-C(13)-C(14)	111.8(2)
O(3)-C(14)-C(13)	109.78(19)
O(3)-C(15)-C(16)	109.6(2)
O(4)-C(16)-C(15)	109.9(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for PTTP-TEG.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	39(1)	28(1)	22(1)	4(1)	9(1)	4(1)
O(1)	40(1)	35(1)	19(1)	2(1)	10(1)	3(1)
O(2)	42(1)	31(1)	28(1)	1(1)	13(1)	5(1)
O(3)	46(1)	40(1)	27(1)	-4(1)	6(1)	9(1)
O(4)	52(1)	147(3)	80(2)	65(2)	19(1)	31(2)
C(1)	41(1)	26(1)	18(1)	-1(1)	7(1)	0(1)
C(2)	45(1)	32(1)	23(1)	4(1)	11(1)	5(1)
C(3)	43(1)	28(1)	23(1)	3(1)	9(1)	7(1)
C(4)	38(1)	23(1)	23(1)	-2(1)	7(1)	-2(1)
C(5)	39(1)	22(1)	22(1)	-3(1)	8(1)	-3(1)
C(6)	39(1)	27(1)	20(1)	-1(1)	5(1)	-2(1)
C(7)	35(1)	28(1)	24(1)	-2(1)	6(1)	-1(1)
C(8)	38(1)	24(1)	21(1)	-3(1)	10(1)	-3(1)
C(9)	44(1)	27(1)	21(1)	2(1)	8(1)	2(1)
C(10)	38(1)	27(1)	24(1)	0(1)	8(1)	1(1)
C(11)	45(1)	34(1)	20(1)	3(1)	12(1)	6(1)
C(12)	51(2)	30(1)	29(1)	4(1)	15(1)	7(1)
C(13)	45(1)	42(2)	30(1)	2(1)	17(1)	5(1)
C(14)	46(1)	43(2)	24(1)	0(1)	9(1)	7(1)
C(15)	51(2)	45(2)	48(2)	-10(1)	10(1)	13(1)
C(16)	69(2)	54(2)	85(3)	12(2)	39(2)	18(2)
C(17A)	81(5)	65(7)	51(4)	21(4)	8(4)	17(4)
C(17B)	50(4)	67(7)	54(5)	16(5)	8(3)	14(4)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for PTTP-TEG.

	x	y	z	U(eq)
H(2)	9291	1939	-1081	40
H(3)	8546	2110	616	38
H(6)	7885	1217	2112	34
H(7)	7312	979	4057	35
H(9)	8675	-1316	6892	37
H(10)	9249	-1036	4939	35
H(11A)	8101	-305	8802	39
H(11B)	7943	-2110	8105	39
H(12A)	6935	-1661	8445	43
H(12B)	7396	-1739	10078	43
H(13A)	6685	-405	11110	45
H(13B)	6254	36	9489	45
H(14A)	6173	1885	11597	45
H(14B)	6835	2485	11560	45
H(15A)	6354	5063	11095	57
H(15B)	5695	4328	10781	57
H(16A)	5791	6869	9442	80
H(16B)	6186	5909	8387	80
H(17A)	4824	6741	6341	99
H(17B)	5128	7729	7878	99
H(17C)	5512	7206	6590	99
H(18A)	4722	5241	6075	86
H(18B)	4977	7027	6578	86
H(18C)	5361	5770	5759	86

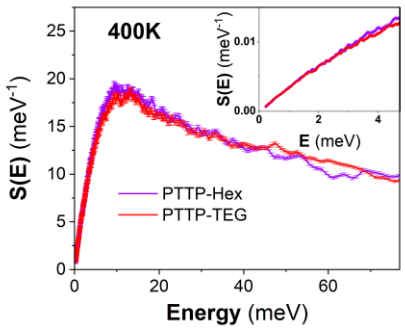

Figure S1. Comparison of the generalized density of state (GDOS) of PTTP-Hex and PTTP-TEG at 400K. The inset shows the Debye growth.

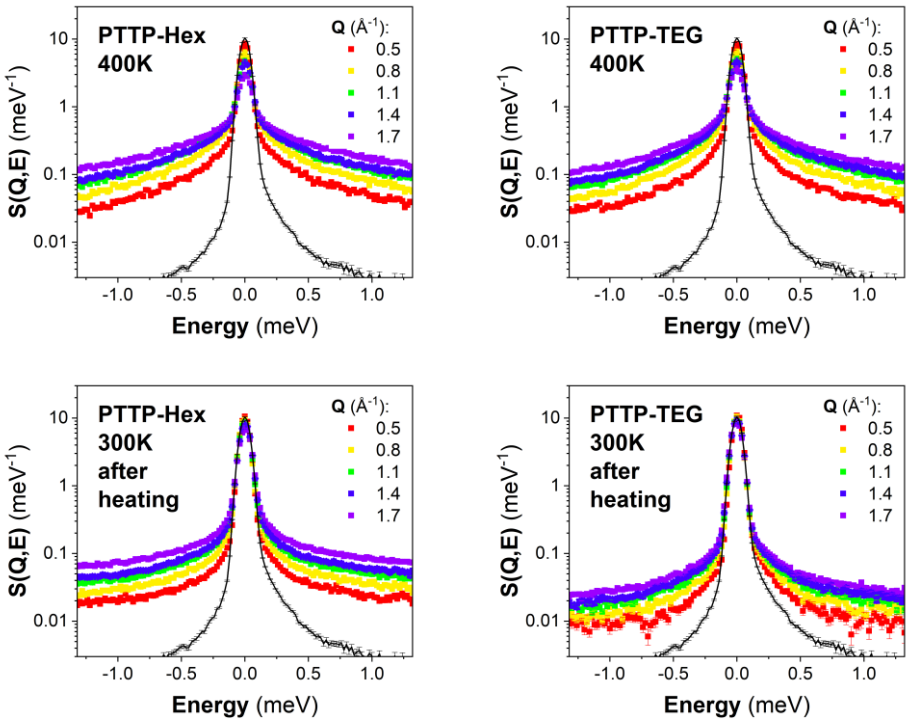

Figure S2. Q-dependent QENS spectra of (left) PTTP-Hex and (right) PTTP-TEG at (top) 400 K and (bottom) 300 K after annealing.

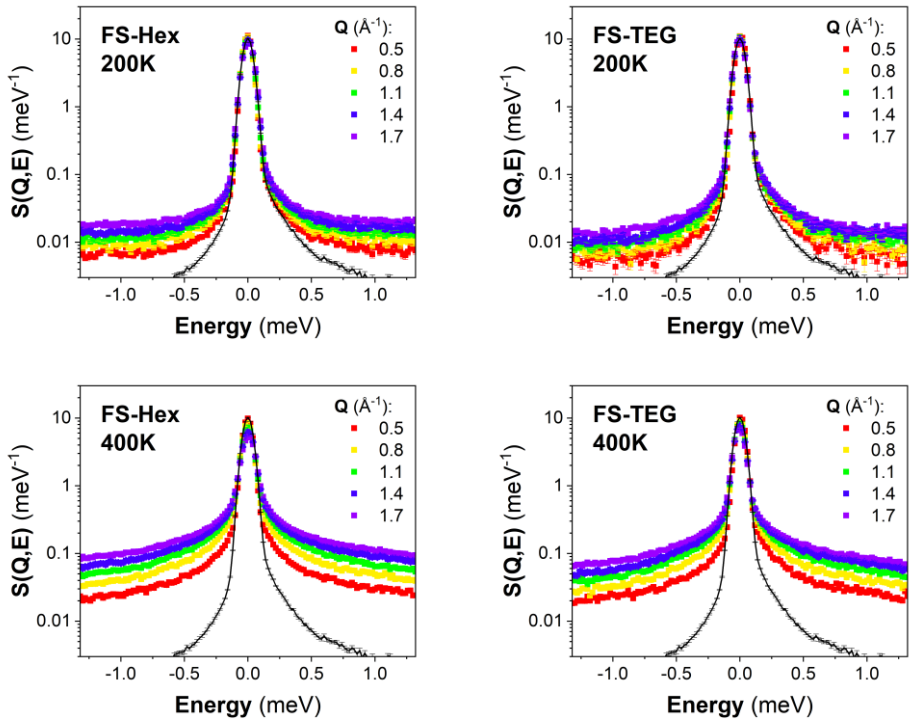

Figure S3. *Q-dependent QENS spectra of (left) FS-Hex and (right) FS-TEG at (top) 200 K and (bottom) 400 K.*