SUPPORTING INFORMATION

Effects of Side-Chain Length and Shape on Polytellurophene Molecular Order and Blend Morphology

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polymer	heteroatom	HOMO Energy (eV)	LUMO Energy (eV)	inter-unit torsion angle (degrees)
P3MT	S	-4.51	-1.91	20
P3MS	Se	-4.39	-2.11	0.16
P3MTe	Te	-4.64	-2.30	0.02

Table 1. Calculated HOMO and LUMO energy levels and average inter-unit torsion angle for oligomers of P3HT, P3HS and P3HTe after optimization in the gas phase.

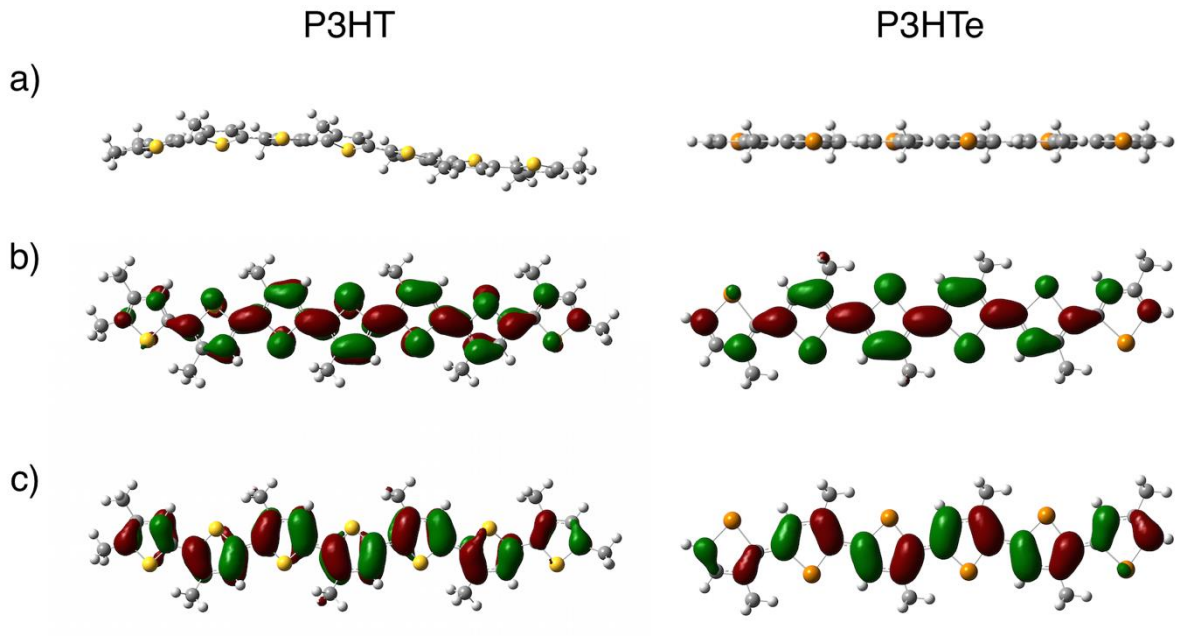

Figure S1. Optimised structures viewed edge-on (a), and distribution of LUMO (b) and HOMO (c) molecular orbitals for oligomers of P3HT and P3HTe simulated using DFT. Side-chains have been reduced to methyl groups, orbital isosurfaces were drawn for a value of 0.02.

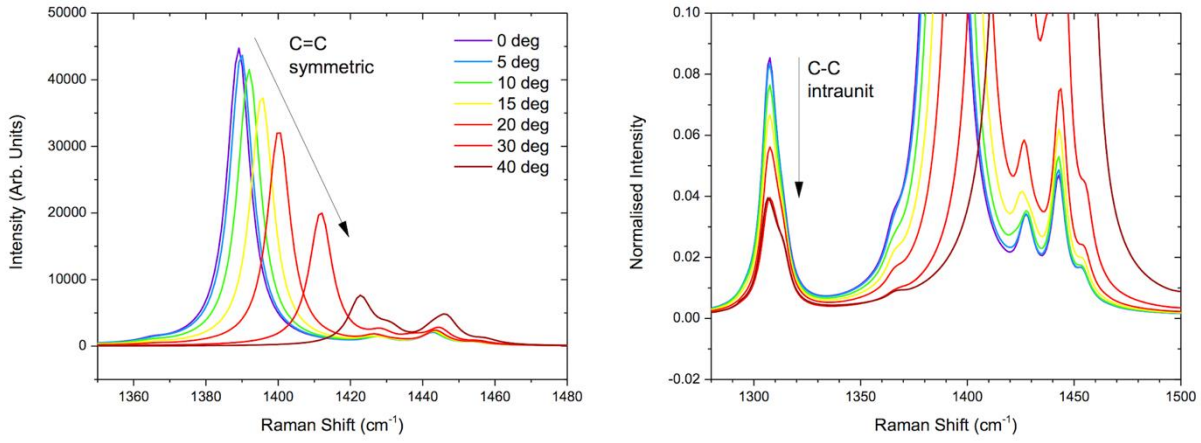

Figure S2. Evolution of the C=C and C-C modes of a hexamer of P3HTe with increasing inter-unit torsion angle, according to DFT simulations. Side-chains were reduced to methyl groups.

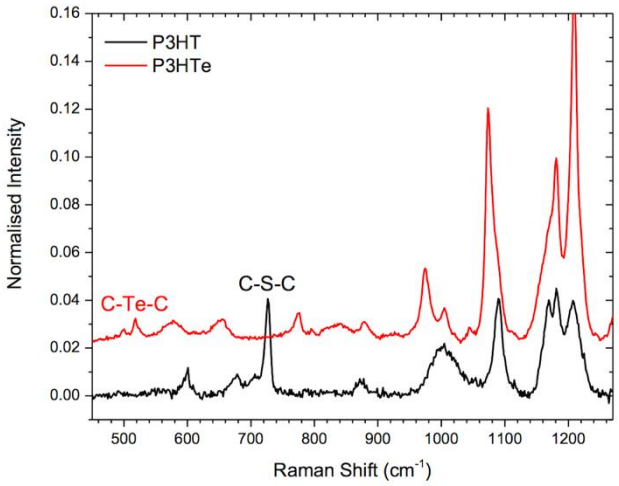

Figure S3. Normalised Raman spectra for bar-coated films of P3HT and P3HTe under 488 nm excitation; focusing on the low-intensity peaks between 450 and 1270 cm^{-1}. Labels indicate the peaks assigned to a heteroatom asymmetric stretch mode, spectra were normalised to the major C=C mode at 1390-1450 cm^{-1} (not shown) and offset by 0.02 for clarity.

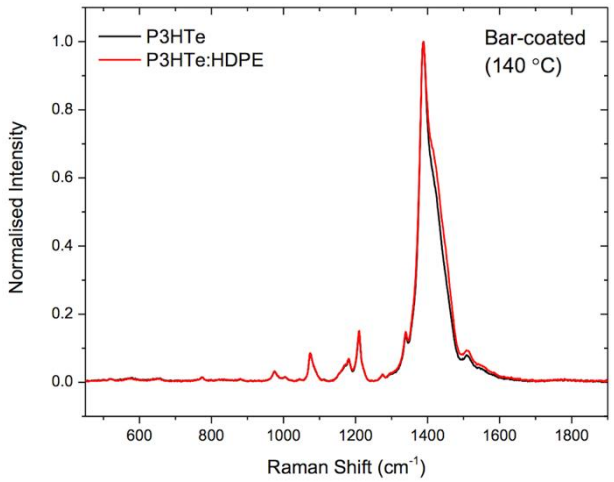

Figure S4. Normalised Raman spectra for neat P3HTe and a 2:1 blend of P3HTe:HDPE between 450 and 1900 cm^{-1}, with no new vibrational modes due to HDPE observed under 488 nm excitation. Both films were bar-coated at 140 °C.