Supporting Information for:

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Parameter free calculation of the subgap density of states in poly(3-hexylthiophene)

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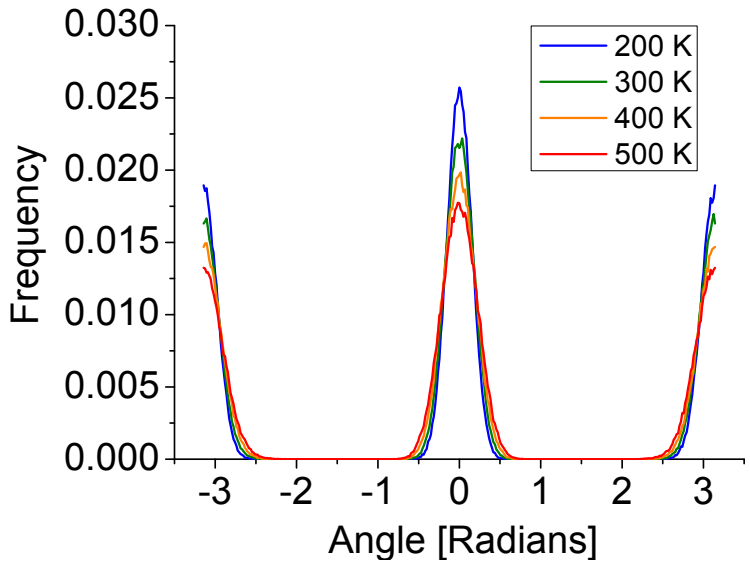
S1. Torsion angle distributions from Molecular dynamics simulations and from thermodynamic linear chain model

(a)



(b)

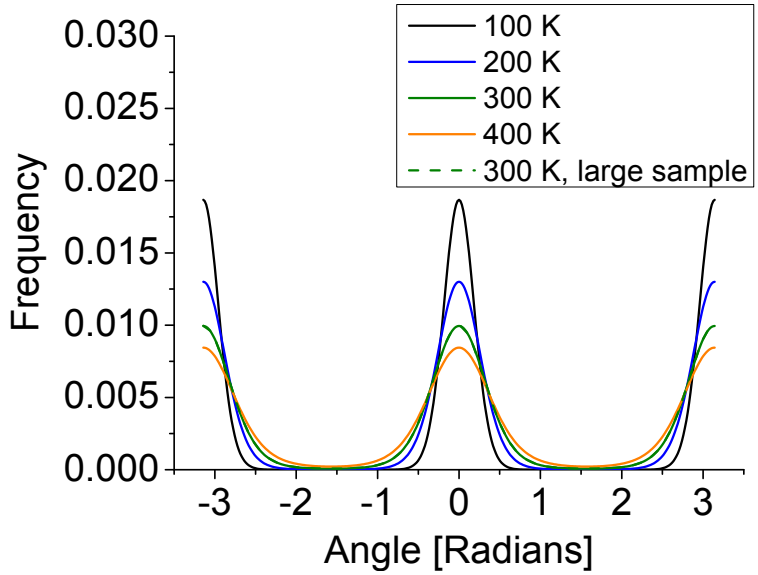


Figure S1.

(a) Distribution of torsion angles for the MD generated oligomers at different temperatures

(b) Distribution of torsion angles generated from the torsional potential (also shown) using a Boltzmann distribution, at different temperatures. For all temperatures, a chain of one million units was used and in the case of the 300 K simulation, a chain of 100 million monomers was also studied to improve statistics. The distribution resulting from the large sample is indistinguishable from that for the small sample at 300 K.

S2. Density of States extracted from interchain interactions only

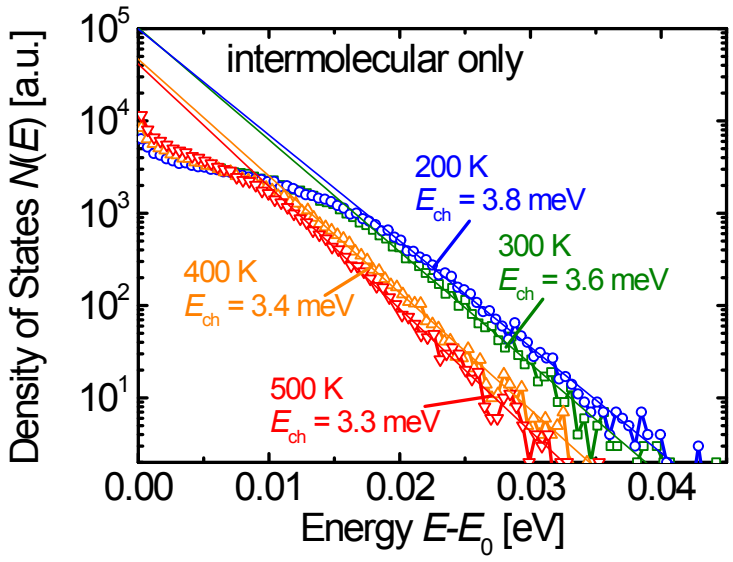


Figure S2. DoS due to coupling between different oligomers only, as a function of temperature. Energy is measured up from the energy of the thiophene HOMO used in the calculation of E_0 = -5.0 eV.

S3. Visualisation of chain conformation and dynamics

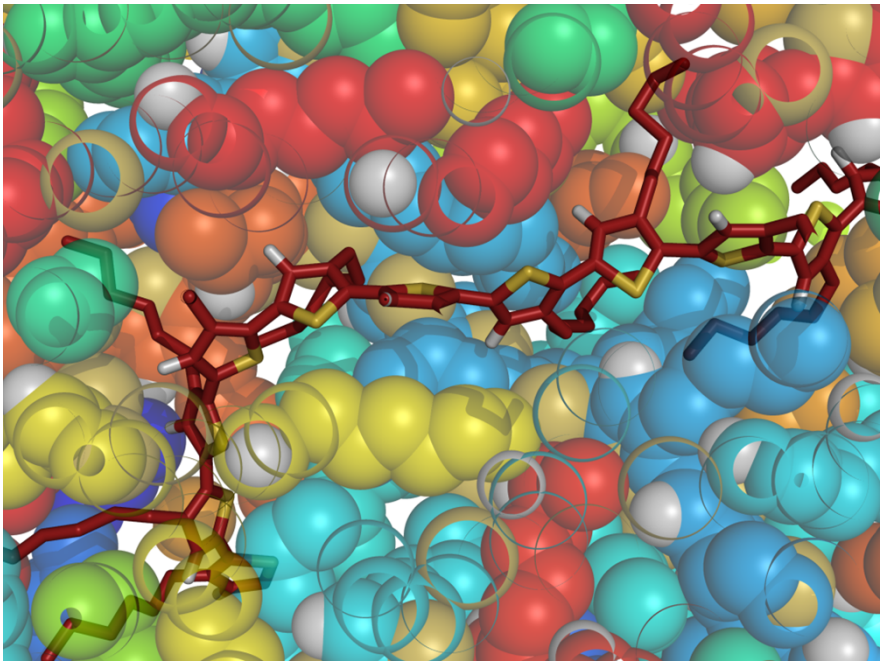


Figure S3. Visualisation of the highly constrained conformation of an oligomer within a solid film.

An accompanying movie of the molecular dynamics used in the Density of States calculation, the GROMACS format of the Moreno empirical forcefield, and other relevant data is available in a fighsare dataset. [1]

1. J. M. Frost, Parameter free calculation of the subgap density of states in poly(3-hexylthiophene). (figshare.), http://dx.doi.org/10.6084/m9.figshare.1116279, Accessed Jul 24, 2014