Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Deconstructing the Behavior of Donor-Acceptor Copolymers in Solution & the Melt: The Case of PTB7

Sean M. Ryno and Chad Risko*

Department of Chemistry &
Center for Applied Energy Research
University of Kentucky
Lexington, Kentucky 40506-0055 USA

*Corresponding author: chad.risko@uky.edu

Table of Contents

Polymer Melt Compression/Decompression Procedure

Table S1. 21 Step MD compression and decompression scheme of Larsen et al.[1]

Step	*Compression/Decompression Conditions*	*Duration (ps)*
1	NVT 600K	50
2	NVT 300K	50
3	NPT 1000 bar, 300K	50
4, 5	NVT 600K, NVT 300K	50, 100
6	NPT 30000 bar, 300K	50
7, 8	NVT 600K, NVT 300K	50, 100
9	NPT 50000 bar, 300K	50
10, 11	NVT 600K, NVT 300K	50, 100
12	NPT 25000 bar, 300K	5
13, 14	NVT 600K, NVT 300K	5, 10
15	NPT 5000 bar, 300K	5
16, 17	NVT 600K, NVT 300K	5, 10
18	NPT 500 bar, 300K	5
19, 20	NVT 600K, NVT 300K	5, 10
21	NPT 1 bar, 300K	800

Polymer Conformers

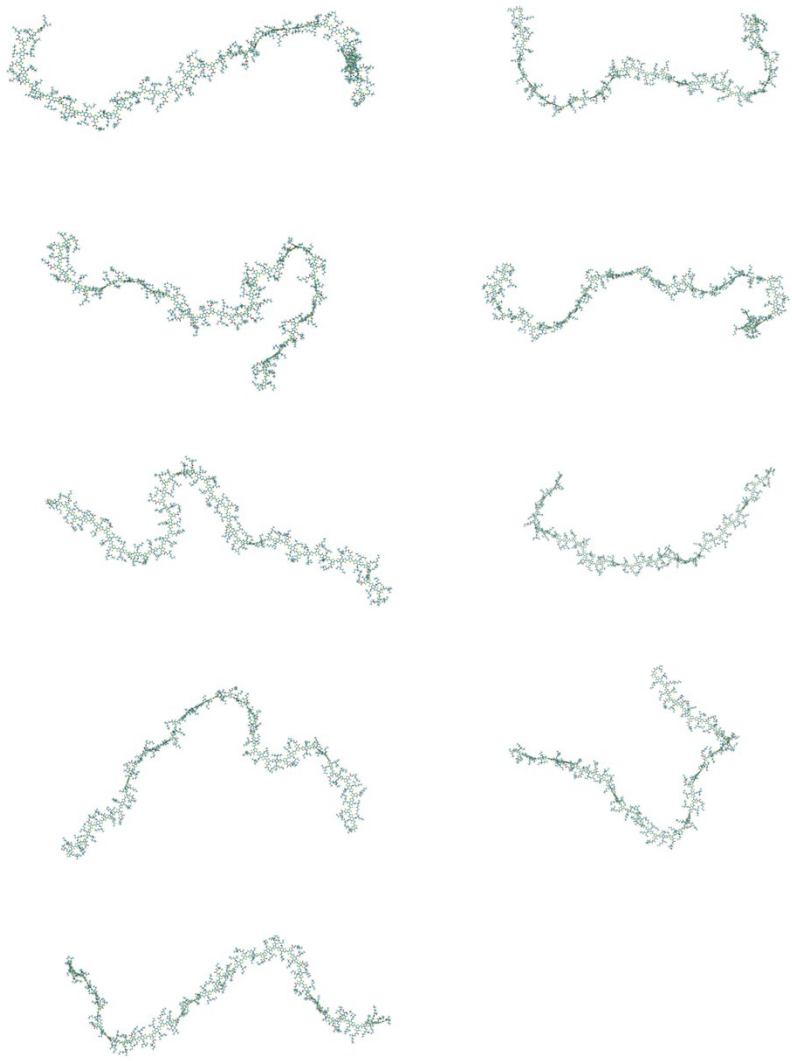

Figure S1. Rod-like conformers extracted from vacuum PTB7 MD simulations at 300 K.

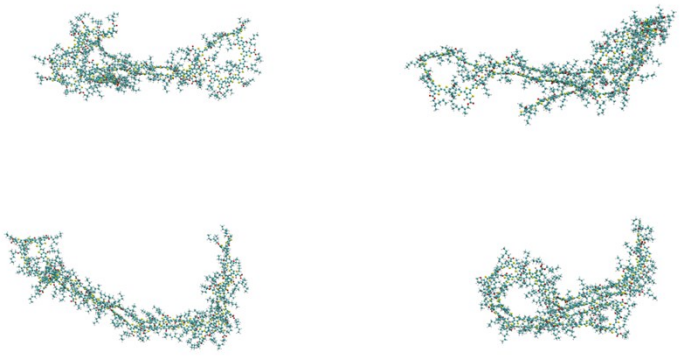

Figure S2. Stacked rod conformers extracted from vacuum PTB7 MD simulations at 300 K.

Figure S3. Toroidal conformers extracted from vacuum PTB7 MD simulations at 300 K.

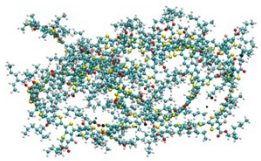

Figure S4. Globular conformer extracted from vacuum PTB7 MD simulations at 300 K.

PTB7 Persistence Length Vector Definition

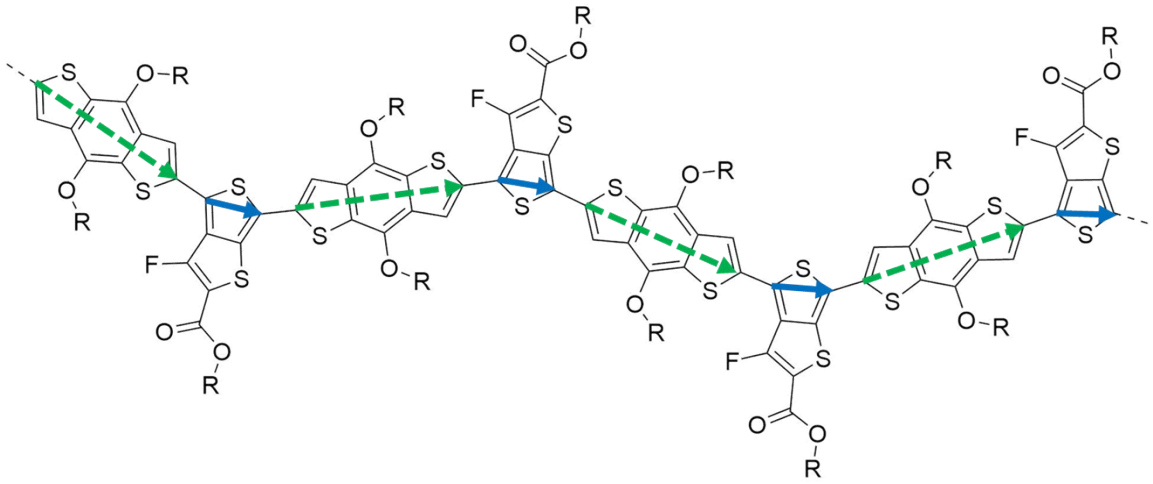

Figure S5. Schematic representation of a PTB7 segment and the vectors used in persistence length calculations. Two vectors are used per repeat unit: Following the π-conjugated pathway, the dashed (green) vector runs between the terminal carbon atoms of the benzodithiophene moiety, while the solid (blue) vector connects the terminal carbon atoms of the thienothiophene moiety.

PTB7 in Solvent: Radius of Gyrations vs. Kuhn Length

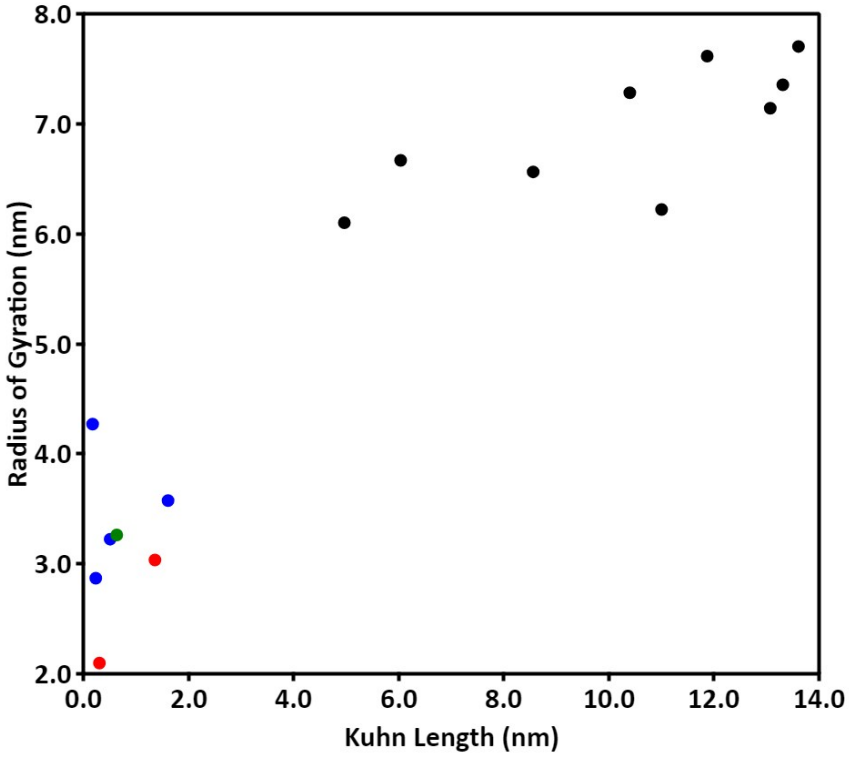

Figure S6. Radius of gyration versus Kuhn length for rod-like (black), stacked rod (blue), toroidal (red), and globular (green) conformations extracted from vacuum simulations of isolated PTB7 chains.

PTB7 Dihedral Distribution Definition

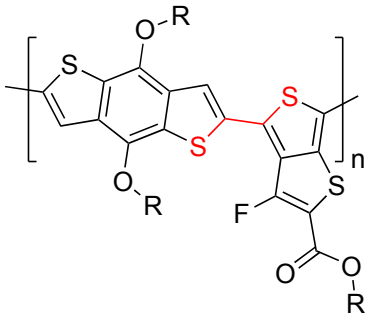

Figure S7. Schematic representation of the dihedral definition used in dihedral distribution plots. Figure is drawn in the 180 degree conformation.

References

1. G. S. Larsen, P. Lin, K. E. Hart and C. M. Colina, *Macromolecules*, 2011, **44**, 6944-6951.