Supporting Information for "Nanostructures and Electronic Properties of High-Efficiency Electron-Donating Polymer"

Ram S. Bhatta[#,*], David S. Perry[†], Mesfin Tsige[#,*]

[#]Department of Polymer Science, The University of Akron, Ohio 44325, United States

[†]Department of Chemistry, The University of Akron, Ohio 44325, United States

[*]Corresponding authors: mtsige@uakron.edu; rsb20@uakron.edu

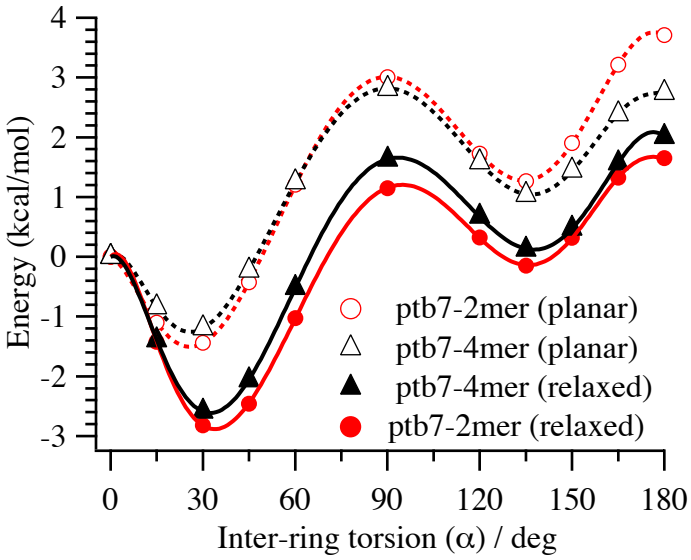

Figure S1. One-dimensional torsional potentials for planar and relaxed PTB7 oligomers as a function of inter-ring torsion angle, α. Energies were computed without the dispersion correction (B3LYP/6-31+G(d,p)). Please refer to the text (and Fig.3) for more details.

Table S1: Computed energies of PTB7 oligomers at different inter-ring torsion angles. Energies were computed with the dispersion corrected DFT (B3LYP-D/6-31+G(d,p). Please refer to Fig. 3 and text for more detail.

Torsion	Energy (kcal/mol)[a]				Energy (kcal/mol)[b]		
(deg)	2-mer	4-mer	6-mer	8-mer	2-mer	4-mer	6-mer
0	0	0	0	0	0	0	0
15	-1.29	-1.06	-1.36		-1.99	-1.96	-2.08
30	-1.48	-1.22	-1.56		-3.85	-3.71	-3.84
45	0.07	0.22			-3.28	-2.98	-3.14
60	2.05	1.99	2.03		-1.3	-0.9	-1.06
90	4.06	3.74	4.04	3.60	1.44	1.82	1.65
120	2.41	2.16	2.37		0.41	0.68	0.51
135	1.82	1.45	1.8		-0.18	-0.03	-0.18
150	2.63	1.97	2.57		0.44	0.42	0.29
165	4.1	3.04	4.06		1.59	1.52	1.42
180	4.54	3.36	4.54		1.89	1.88	1.83

[a]Energies relative to planar PTB7 oligomers
[b]Energies relative to relaxed PTB7 oligomers