Supporting Information

Effect of Chain Curvature on the Performance of Diketopyrrolopyrrole-Based Polymer Solar Cells

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Table of Contents

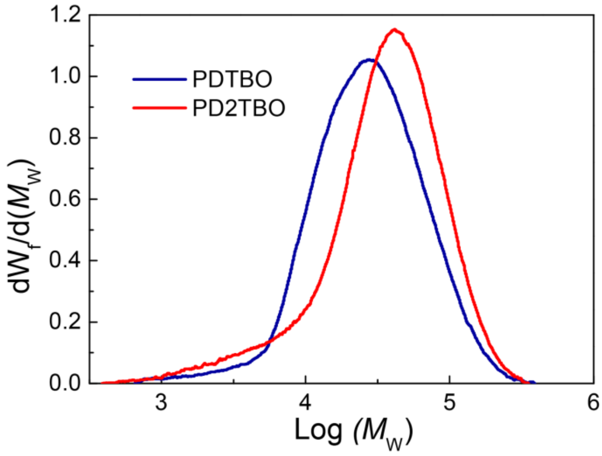

Fig. S1. Gel permeation chromatography (GPC) traces of two polymers evaluated with 1, 2, 4-trichlorobenzene as eluent at 150 ^{o}C.

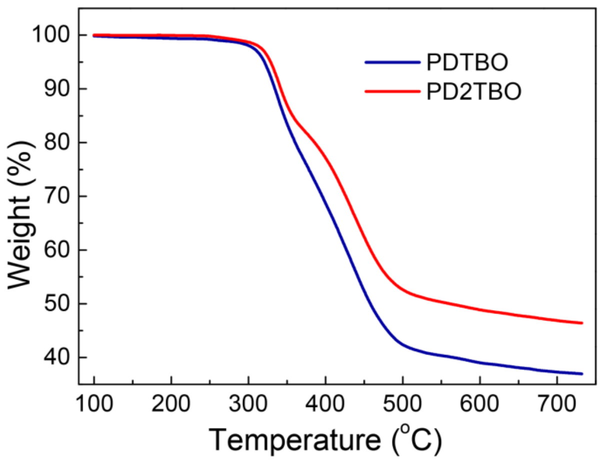

Fig. S2. Thermal gravity analysis (TGA) of two polymers.

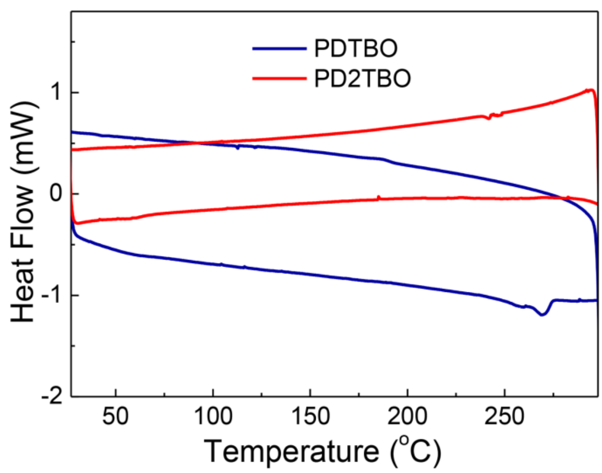

Fig. S3. Differential scanning calorimetry (DSC) thermograms of two polymers.

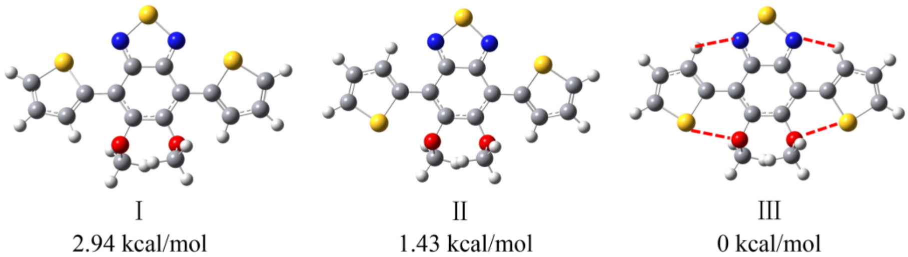

Fig. S4. Comparison of optimized geometries of thienyl-substituted BDTO using DFT B3LYP/6-31G. The energies were calculated by using geometry III as standard.

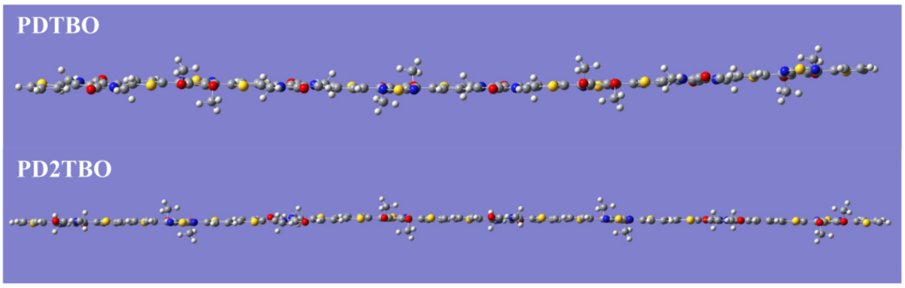

Fig. S5. The molecular conformations of two tetramers observed from side view.

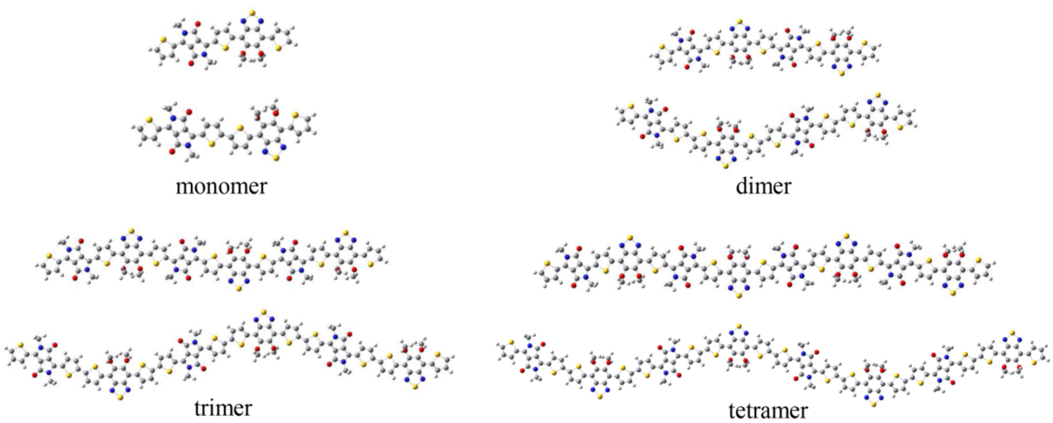

Fig. S6. The minimum-energy conformations of monomer, dimer, trimer, and tetramer for two polymers.

Table S1. Photovoltaic parameters of devices based on 1:3 weight ratio of polymer and $PC_{71}BM$ for **PDTBO** and **PD2TBO**, respectively

polymer	annealing (^{o}C)	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
PDTBO	—$^{a)}$	0.66	4.73	0.39	1.21 (1.20±0.007)
	—$^{b)}$	0.64	6.94	0.37	1.66 (1.60±0.006)
	120$^{c)}$	0.69	7.61	0.41	2.08 (2.01±0.005)
PD2TBO	—$^{a)}$	0.62	7.36	0.59	2.68 (2.50±0.021)
	—$^{b)}$	0.65	13.10	0.54	4.77 (4.75±0.014)
	110$^{c)}$	0.65	14.36	0.56	5.25 (5.23±0.006)

^{a}The blend film was spin-coated without DIO and determined without any post-treatments. ^{b}The blend film was spin-coated with 1% (v/v) DIO in chlorobenzene and determined without any post-treatments. ^{c}The blend film was spin-coated with 1% (v/v) DIO in chlorobenzene and determined after thermal annealing. The average values collected more than 8 devices are shown in parenthesis.

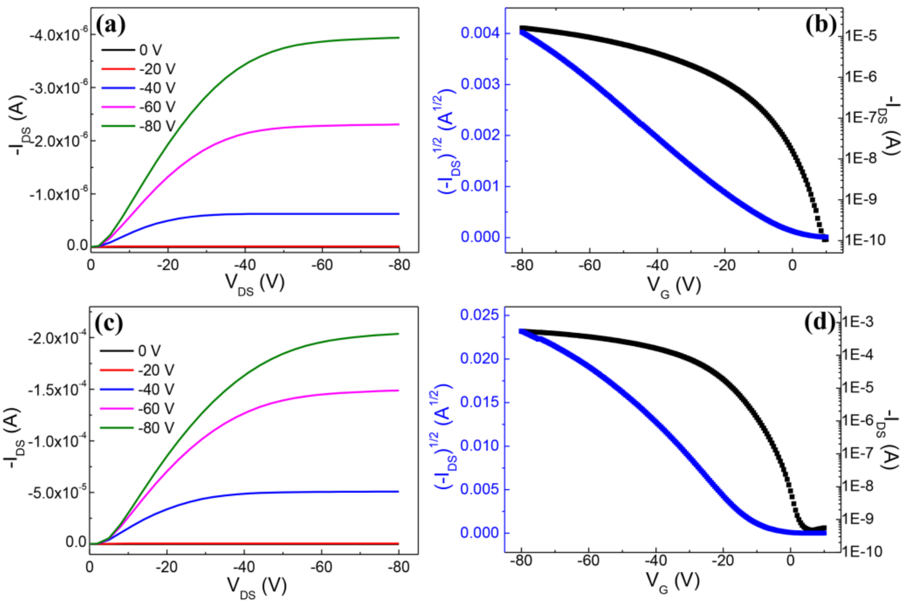

Fig. S7. Output characteristics and transfer characteristics of the typical bottom-gate/top-contact OFET devices based on **PDTBO** (a, b) and **PD2TBO** (c, d), respectively.

Table S2. Transistor properties of two polymers

polymer	$\mu_h{}^a$ ($cm^2\ V^{-1}\ s^{-1}$)		V_T (V)	$I_{on/off}$
	max	ave		
PDTBO	0.01	0.009±0.002	-4.9	10^5
PD2TBO	0.41	0.38±0.03	-8.0	10^5-10^6

[a]All of the OFETs were fabricated with channel length L = 30 μm and channel width W = 500 μm. The mobilities were collected from more than 7 devices.

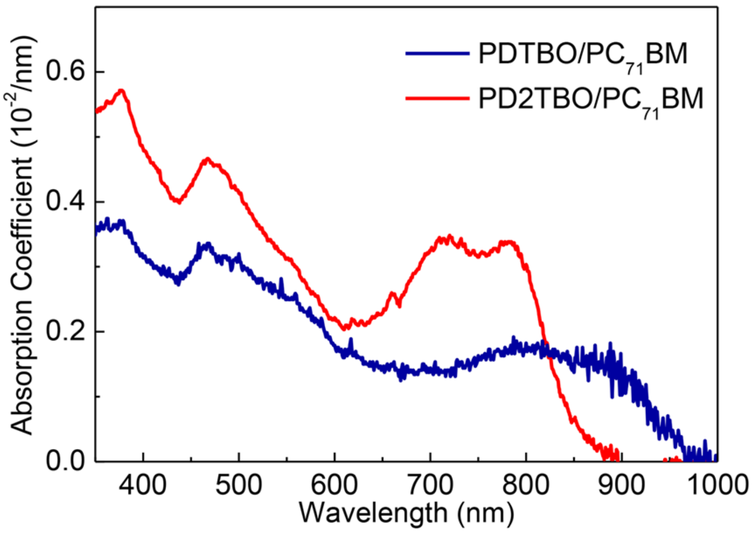

Fig. S8. UV-vis absorption of active layers in solar cells (The absorption values are divided by film thickness in 100 nm unit).

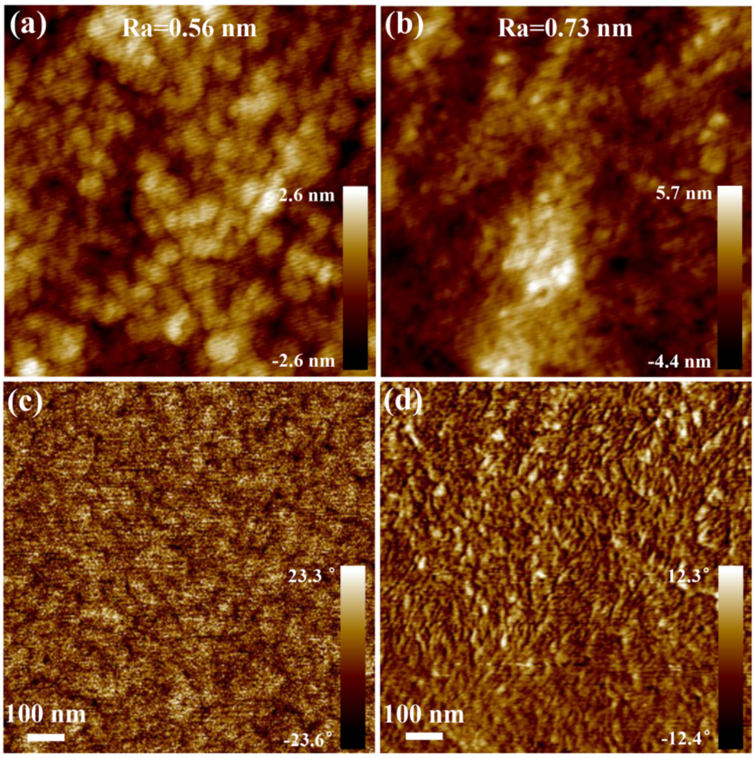

Fig. S9. Tapping mode AFM height and phase images of the optimized **PDTBO**/$PC_{71}BM$ blend film (a, c) and **PD2TBO**/$PC_{71}BM$ blend film (b, d), respectively.