Supporting Information

Dibenzopyran Based Wide Bandgap Conjugated Copolymers: Structural Design and Application for Polymer Solar Cells

Yuanyuan Zhou[a], Miao Li[a], Yijing Guo[a], Heng Lu[b], Jinsheng Song[a,*], Zhishan Bo[b,*] and Hua Wang[a,*]

[a]Engineering Research Center for Nanomaterials, Henan University, Kaifeng, 475004, China.

Email: songjs@henu.edu.cn, hwang@henu.edu

[b]Beijing Key Laboratory of Energy Conversion and Storage Materials, College of Chemistry, Beijing Normal University, Beijing 100875, China.

Email: zsbo@bnu.edu.cn

Table of Content

1. Theoretical calculations results of PDBPTBT polymers.

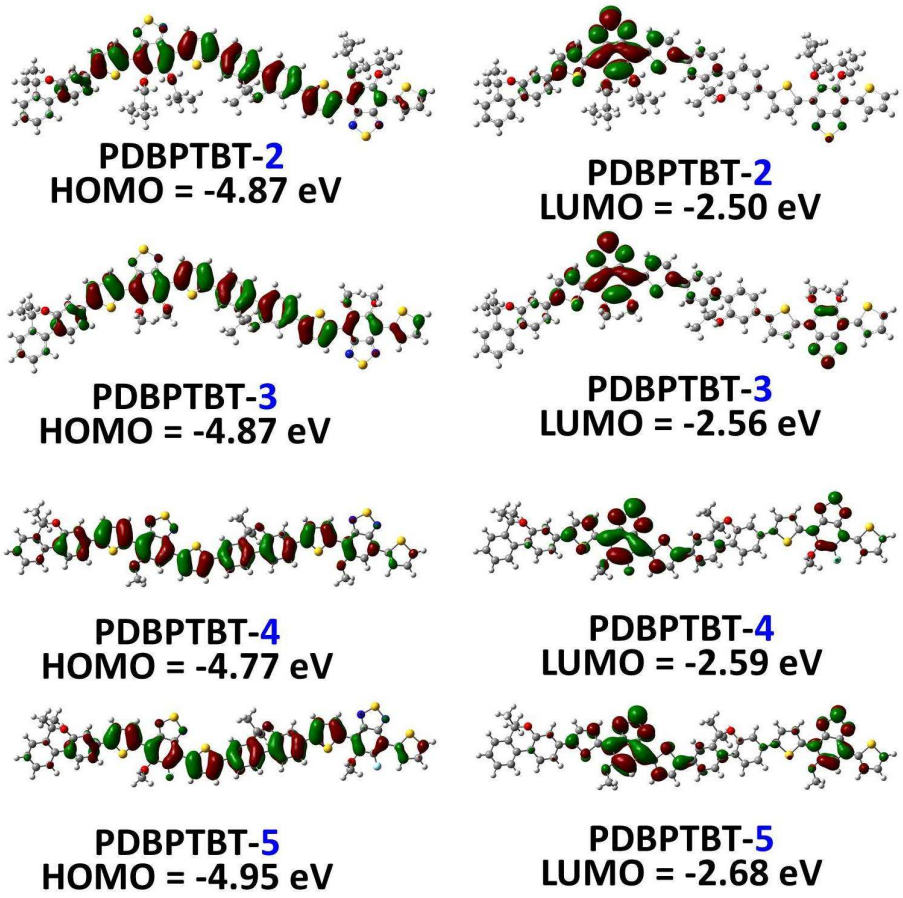

Figure S1. Frontier molecular orbitals of the optimized **PDBPTBT** dimers calculated with the DFT B3LYP/6-31G (d,p) level.

2. PSC device optimization of the PDBPTBT polymers.

Table S1. Photovoltaic properties of the PSCs based on structure of ITO/PEDOT:PSS/active layer/LiF/Al processed by DCB with different ratios of **PDBPTBT** polymers and $PC_{71}BM$ under the illumination of AM 1.5G, 100mW/cm^2.

Polymer	V_{oc} (V)	J_{sc} (mA/cm^2)	*FF*	*PCE* (%)
PDBPTBT-2:PC71BM=1:1	0.88	3.94	0.37	1.28
PDBPTBT-2:PC$_{71}$BM=1:2	0.92	4.62	0.35	1.48
PDBPTBT-2:PC$_{71}$BM=1:3	0.96	5.51	0.38	2.02
PDBPTBT-2:PC$_{71}$BM=1:4	0.93	4.72	0.36	1.56
PDBPTBT-3:PC$_{71}$BM=1:1	0.84	3.61	0.33	1.74
PDBPTBT-3:PC$_{71}$BM=1:2	0.84	6.00	0.51	2.56
PDBPTBT-3:PC$_{71}$BM=1:3	0.86	6.98	0.54	3.23
PDBPTBT-3:PC$_{71}$BM=1:4	0.85	5.55	0.52	2.46
PDBPTBT-4:PC$_{71}$BM=1:1	0.82	5.49	0.31	1.41
PDBPTBT-4:PC$_{71}$BM=1:2	0.79	7.77	0.41	2.55
PDBPTBT-4:PC$_{71}$BM=1:3	0.79	8.40	0.58	3.87
PDBPTBT-4:PC$_{71}$BM=1:4	0.77	8.22	0.55	3.47
PDBPTBT-5:PC$_{71}$BM =1:1	0.92	10.40	0.54	5.10
PDBPTBT-5:PC$_{71}$BM =1:1.5	0.90	10.60	0.56	5.32
PDBPTBT-5:PC$_{71}$BM =1:2	0.87	9.63	0.60	5.03
PDBPTBT-5:PC$_{71}$BM =1:3	0.90	9.11	0.54	4.40
PDBPTBT-5:PC$_{71}$BM =1:4	0.81	7.72	0.44	2.78

Table S2. Photovoltaic properties of the PSCs based on structure of ITO/PEDOT:PSS/ active layer/LiF/Al processed by DCB with varied ratios of DIO, CN, DPE under the illumination of AM 1.5G, 100mW/cm^2.

Polymer	Additive (v%)	V_{oc} (V)	J_{sc} (mA/cm^2)	*FF*	*PCE* (%)
PDBPTBT-5:PC$_{71}$BM=1:1.5	1.0% DIO	0.88	11.00	0.54	5.23
PDBPTBT-5:PC$_{71}$BM=1:1.5	2.0% DIO	0.91	10.80	0.58	5.66
PDBPTBT-5:PC$_{71}$BM=1:1.5	2.5% DIO	0.93	9.48	0.62	5.50
PDBPTBT-5:PC$_{71}$BM=1:1.5	3.0% DIO	0.92	9.91	0.58	5.25
PDBPTBT-5:PC$_{71}$BM=1:1.5	5.0% DIO	0.92	10.00	0.58	5.30
PDBPTBT-5:PC$_{71}$BM=1:1.5	1.0% CN	0.91	9.59	0.55	4.80
PDBPTBT-5:PC$_{71}$BM=1:1.5	2.0% CN	0.92	9.67	0.55	4.95
PDBPTBT-5:PC$_{71}$BM=1:1.5	3.0% CN	0.94	8.52	0.59	4.74
PDBPTBT-5:PC$_{71}$BM=1:1.5	5.0% CN	0.94	8.46	0.59	4.70
PDBPTBT-5:PC$_{71}$BM=1:1.5	1.0% DPE	0.86	10.40	0.58	5.17
PDBPTBT-5:PC$_{71}$BM=1:1.5	2.0% DPE	0.91	10.50	0.58	5.50
PDBPTBT-5:PC$_{71}$BM=1:1.5	3.0% DPE	0.89	9.97	0.60	5.34

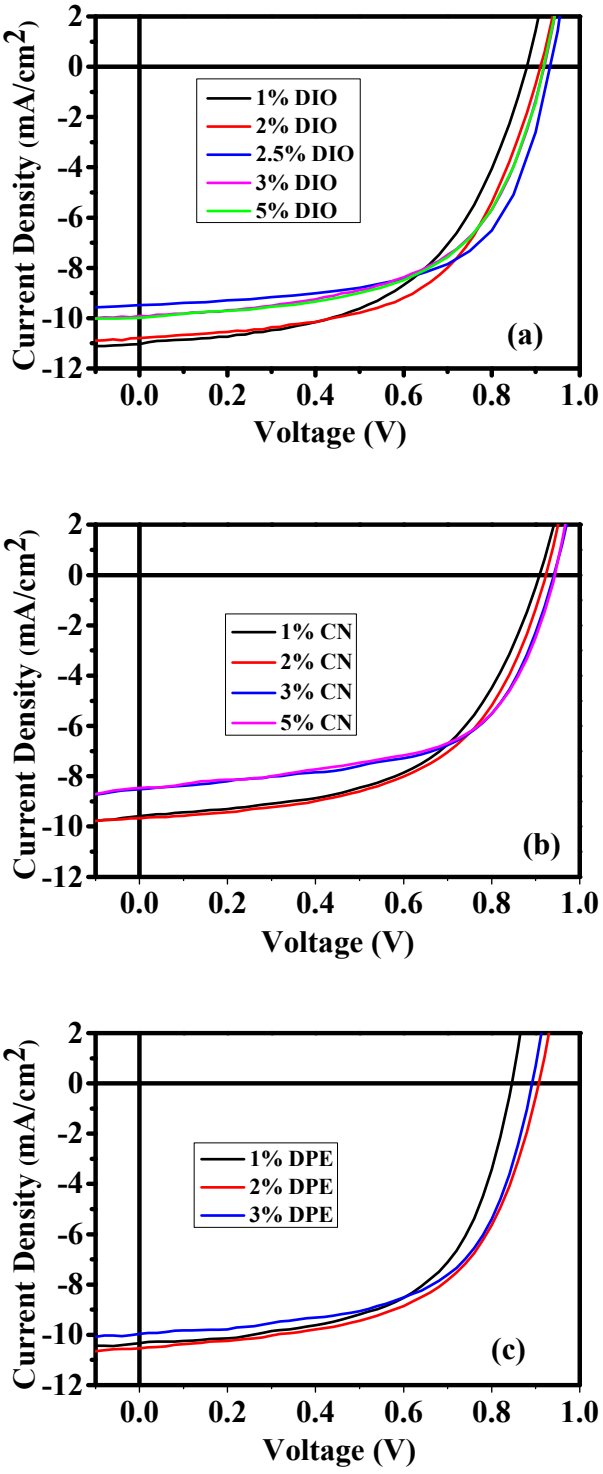

Figure S2. *J-V* curves of PSCs fabricated from the blend of **PDBPTBT-5**:$PC_{71}BM$= 1:1.5 with varied ratios of DIO **(a)**, CN **(b)**, DPE **(c)** under the illumination of AM 1.5G (100mW/cm^2).

3. SCLC mobilities of PDBPTBT:$PC_{71}BM$ blend.

Hole (μ_h) and electron (μ_e) mobilities of the **PDBPTBT:**$PC_{71}BM$ blend were investigated via the space charge limited current (SCLC) method in typical device structures of ITO/PEDOT:PSS/polymer:$PC_{71}BM$/Au and ITO/ZnO/polymer:$PC_{71}BM$/LiF/Al, respectively. Dark *J*-*V* curves of devices were fitted by using the Mott-Gurney equation: $J = 9\varepsilon_o\varepsilon_r\mu V^2/8d^3$, where J is the space charge limited current, ε_o is the vacuum permittivity, ε_r is the permittivity of the active layer, μ is the hole mobility, and d is the thickness of the active layer.

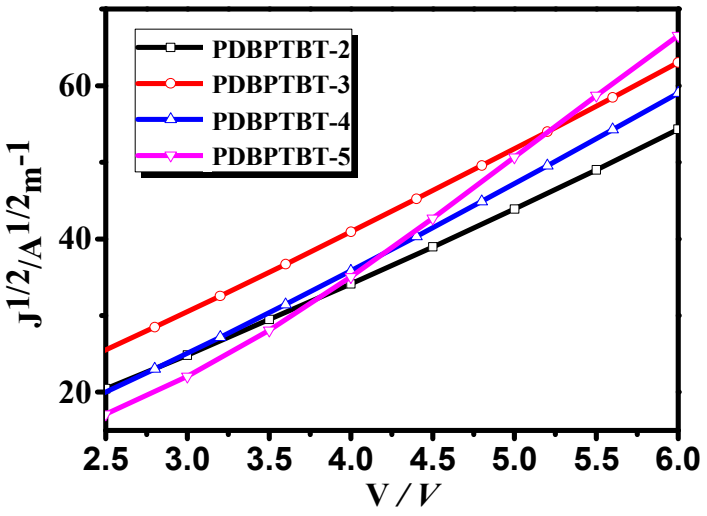

Figure S3. $J^{1/2}$–V curves of hole-only devices.

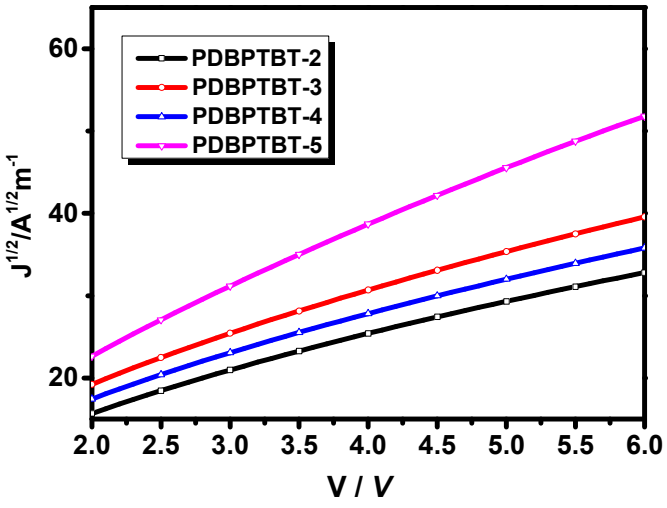

Figure S4. $J^{1/2}$–V curves of electron-only devices.