

Supporting Information

High-Efficiency Organic Solar Cells Based on Small-Molecule Donor and Low-Bandgap Polymer Acceptor with Strong Absorption

Yankang Yang,^{a,b} Beibei Qiu,^{a,b} Shanshan Chen,^c Qiuju Zhou,^d Ying Peng,^a Zhi-Guo Zhang,^{a*} Jia Yao,^a Zhenghui Luo,^a Xiaofeng Chen,^a Lingwei Xue,^a Liuliu Feng,^a Changduk Yang,^c Yongfang Li^{a,e*}

^a Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.

^b School of Chemical Science, University of Chinese Academy of Sciences, Beijing 100049, China.

^c Department of Energy Engineering, School of Energy and Chemical Engineering, Low Dimensional Carbon Materials Center, Ulsan National Institute of Science and Technology (UNIST), Ulsan 689-798, South Korea.

^d Analysis & Testing Center, Xinyang Normal University, Xinyang 464000, PR China

^e Laboratory of Advanced Optoelectronic Materials, College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou, Jiangsu 215123, China.

E-mail: liyf@iccas.ac.cn (Y. Li), zgzhangwhu@iccas.ac.cn (Z. Zhang)

Table S1. Photovoltaic performance parameters of the SM1: PZ1-based OSCs with different donor/acceptor weight ratios (with 4% NMP additive treatment).

D:A (w/w)	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE_{max} (%)	R_{sh} (KΩ cm ⁻²)	R_s (Ω cm ⁻²)
1:1	0.860	4.65	56.42	2.25	1.01	35.93
1.5:1	0.867	6.11	58.48	3.10	1.01	28.48
2:1	0.869	7.04	60.20	3.68	1.30	24.85
2.5:1	0.883	7.34	61.34	3.97	1.28	22.60
3.5:1	0.881	6.04	60.74	3.23	1.69	24.31

Table S2. Photovoltaic performance parameters of the DR3TBDTT: PZ1-based OSCs with different donor/acceptor weight ratios (with 1% CN additive treatment).

D:A (w/w)	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE_{max} (%)	R_{sh} (K Ω cm ⁻²)	R_s (Ω cm ⁻²)
1.5:1	0.861	8.20	47.07	3.32	0.46	29.79
2:1	0.862	9.53	59.90	4.92	0.96	18.47
2.5:1	0.865	11.36	59.66	5.86	0.97	16.26
3:1	0.858	9.71	60.54	5.04	1.03	19.13
4:1	0.857	9.98	55.72	4.76	0.85	25.27

Table S3. Photovoltaic performance parameters of the OSCs based on SM1: PZ1 (2.5:1, w/w) with the treatment of different NMP additive concentration.

NMP (%)	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE_{max} (%)	R_{sh} (K Ω cm ⁻²)	R_s (Ω cm ⁻²)
1	0.911	4.46	37.97	1.54	0.48	109.36
2	0.886	6.58	47.03	2.74	0.71	55.99
3	0.876	6.78	56.13	3.33	1.22	32.03
4	0.883	7.34	61.34	3.97	1.28	22.60
5	0.880	6.63	64.78	3.78	1.54	22.33

Table S4. Photovoltaic performance parameters of the OSCs based on DR3TBDTT: PZ1 (2:1, w/w) with the treatment of different CN additive concentration.

CN (%)	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE_{max} (%)	R_{sh} (K Ω cm ⁻²)	R_s (Ω cm ⁻²)
0.5	0.868	9.85	39.14	3.34	0.26	43.55
1	0.862	9.53	59.90	4.92	0.96	18.47
1.5	0.804	2.84	23.27	0.53	0.39	1048.05

Table S5. Photovoltaic performance parameters of the OSCs based on SM1: PZ1 (2:1, w/w) with the treatment of different additive (4%).

Additive	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE_{max} (%)	R_{sh} (K Ω cm ⁻²)	R_s (Ω cm ⁻²)
DIO	0.881	5.79	44.22	2.25	0.38	42.56
CN	0.876	0.14	23.99	0.03	5.34	6479.59
NMP	0.869	7.04	60.20	3.68	1.30	24.85
DPE	0.899	5.77	38.94	2.02	0.34	59.29

Table S6. Photovoltaic performance parameters of the OSCs based on DR3TBDTT: PZ1 (2.5:1, w/w) with the treatment of different additive (1%).

Additive	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE_{max} (%)	R_{sh} (K Ω cm ⁻²)	R_s (Ω cm ⁻²)
DIO	0.850	6.23	51.99	3.59	0.72	27.90
CN	0.865	11.36	59.66	5.86	0.97	16.26
NMP	0.836	4.84	51.12	2.07	1.03	45.09
DPE	0.838	8.24	51.99	3.59	0.72	27.90

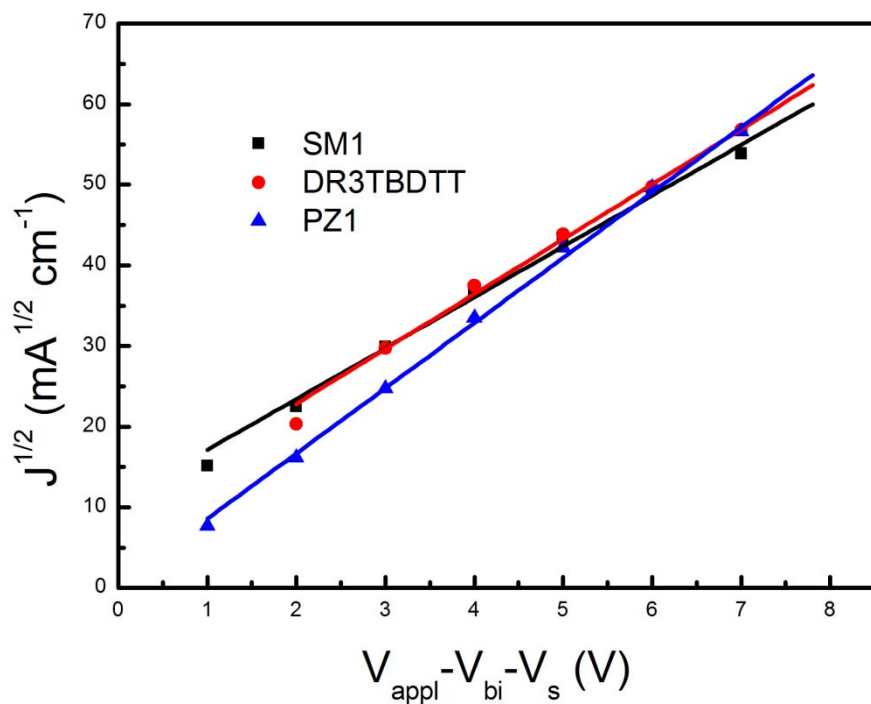


Figure S1. $J^{1/2} \sim (V_{\text{appl}} - V_{\text{bi}})$ characteristics for the SM1-based, DR3TBDTT-based hole-only device and PZ1-based electron-only device. Solid lines are the fitting lines of the data.

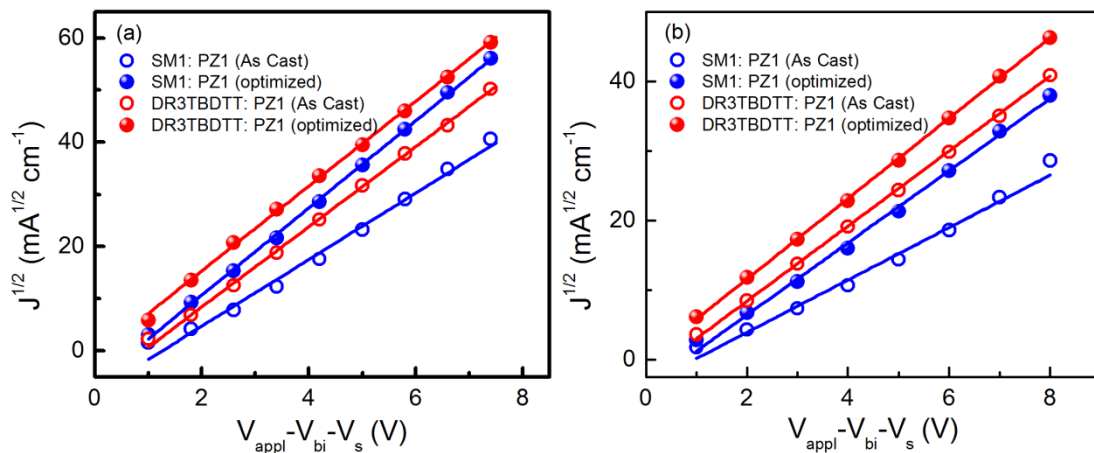


Figure S2. (a) $J^{1/2} \sim (V_{\text{appl}} - V_{\text{bi}})$ characteristics for the hole-only devices based on the blend films of SM1: PZ1 and DR3TBDTT: PZ1; (b) $J^{1/2} \sim (V_{\text{appl}} - V_{\text{bi}})$ characteristics for the electron-only devices based on the blend films of SM1: PZ1 and DR3TBDTT: PZ1.

Table S7. Charge carrier mobilities and morphology data of GIWAX of the SM1, DR3TBDTT and PZ1 neat films.

Neat films	μ_h [cm ² V ⁻¹ s ⁻¹]	μ_e [cm ² V ⁻¹ s ⁻¹]	(100) d spacing [Å]	(100) coherence length [Å]	(010) d spacing [Å]	(010) coherence length [Å]
SM1	2.21 x 10 ⁻⁵	---	22.45	91.32	3.67	41.80
DR3TBDTT	1.41 x 10 ⁻⁵	---	20.40	94.42	3.65	42.01
PZ1	---	1.34 x 10 ⁻⁵	25.52	41.27	3.86	23.27

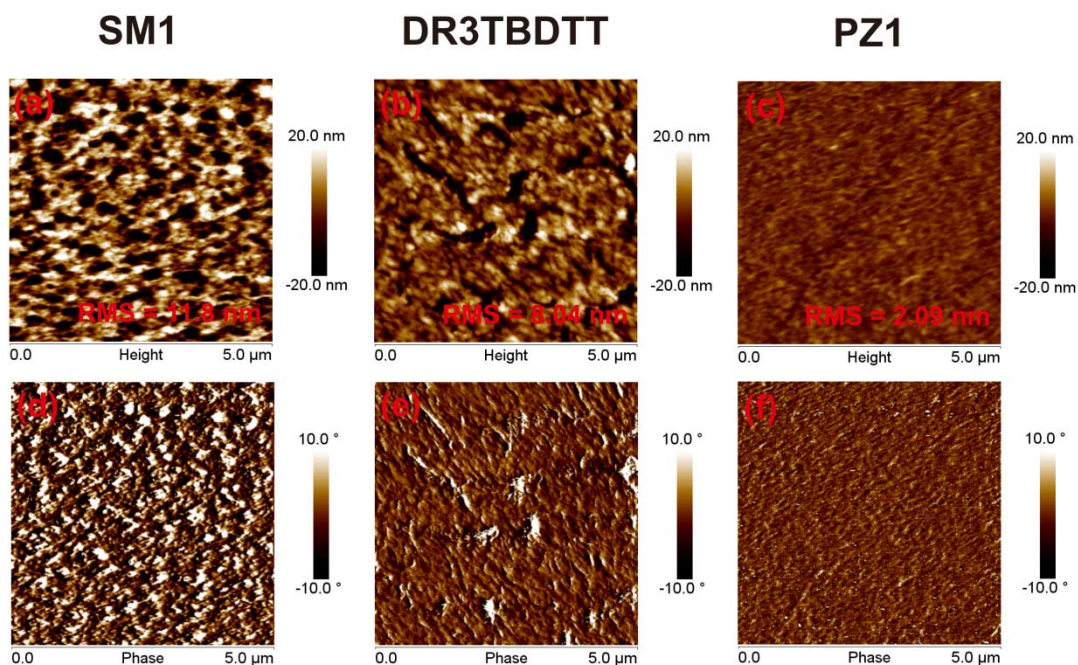


Figure 4. AFM height images of the neat films (a, b, c) and their corresponding phase images (d, e, f) for SM1, DR3TBDTT and PZ1.