

Electronic Supplementary Information

Comparison of 3D non-fullerene acceptors for organic photovoltaics based on naphthalene diimide and perylene diimide-substituted 9,9'-bifluorenylidene

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1. Optimization of devices

Table S1 Photovoltaic performance of PTB7-Th:BF-PDI₄ based solar cells. The average values are from over eight devices. The D:A ratio is 1:1.5 (w/w).

Film treat	J_{sc} (mA/cm ²)	V_{oc} (V)	FF (%)	η (%)	Best (%)
none	8.93±0.13	0.78±0.01	42.68±1.31	2.99±0.1	3.17
1% CN	9.58±0.23	0.80±0.01	40.48±0.83	3.12±0.06	3.24
2% CN	9.32±0.36	0.81±0.01	42.92±0.90	3.24±0.11	3.40
3% CN	9.35±0.26	0.82±0.01	45.55±0.80	3.50±0.06	3.64
1% DIO	8.55±0.19	0.82±0.01	45.95±0.17	3.23±0.09	3.33
2% DIO	8.31±0.16	0.82±0.00	46.17±0.61	3.14±0.06	3.23
1% DIO+1% CN	9.02±0.21	0.82±0.01	45.84±0.33	3.40±0.07	3.48
1% DIO+2% CN	8.13±0.09	0.82±0.01	45.47±0.34	3.04±0.03	3.09
1.5% DIO+1.5% CN	7.18±0.16	0.84±0.00	42.84±0.37	2.58±0.04	2.63

Table S2 Photovoltaic performance of PTB7-Th:BF-NDI₄ based solar cells. The average values are from over eight devices. The D:A ratio is 1:1.5 (w/w).

Film treat	J_{sc} (mA/cm ²)	V_{oc} (V)	FF (%)	η (%)	Best (%)
none	5.75±0.15	0.82±0.01	36.51±0.37	1.73±0.05	1.79
1% DIO	6.55±0.35	0.80±0.02	36.86±0.62	1.92±0.08	2.01
2% DIO	6.99±0.30	0.82±0.01	38.57±0.57	2.20±0.06	2.28
3% DIO	6.14±0.18	0.81±0.01	36.79±0.42	1.83±0.05	1.89
1% CN	6.42±0.16	0.81±0.01	38.68±0.57	2.02±0.07	2.12
2% CN	5.39±0.31	0.79±0.01	35.13±2.67	1.50±0.18	1.75
1% DIO+1% CN	6.43±0.21	0.80±0.01	38.02±1.78	1.94±0.13	2.09

Table S3 Photovoltaic performance of PTB7:BF-PDI₄ based solar cells. The average values are from over eight devices. The D:A ratio is 1:2 (w/w).

Film treat	J_{sc} (mA/cm ²)	V_{oc} (V)	FF (%)	η (%)	Best (%)
none	5.84±0.26	0.80±0.01	36.20±0.51	1.69±0.08	1.78
1%DIO	7.21±0.19	0.81±0.01	41.65±0.44	2.45±0.07	2.53
2%DIO	6.44±0.15	0.80±0.01	41.97±0.45	2.15±0.03	2.19
3%DIO	6.61±0.24	0.81±0.01	40.26±0.71	2.16±0.09	2.26

Table S4 Photovoltaic performance of PTB7:BF-NDI₄ based solar cells. The average values are from over eight devices. The D:A ratio is 1:1.5 (w/w).

Film treat	J_{sc} (mA/cm ²)	V_{oc} (V)	FF (%)	η (%)	Best (%)
none	2.28±0.05	0.77±0.01	33.69±0.76	0.59±0.03	0.63
1% DIO	3.26±0.11	0.70±0.02	37.27±0.97	0.85±0.04	0.89
2% DIO	3.33±0.16	0.80±0.01	37.27±0.65	0.99±0.05	1.08
3% DIO	3.09±0.10	0.70±0.03	37.08±1.07	0.81±0.03	0.83

2. Additional figures.

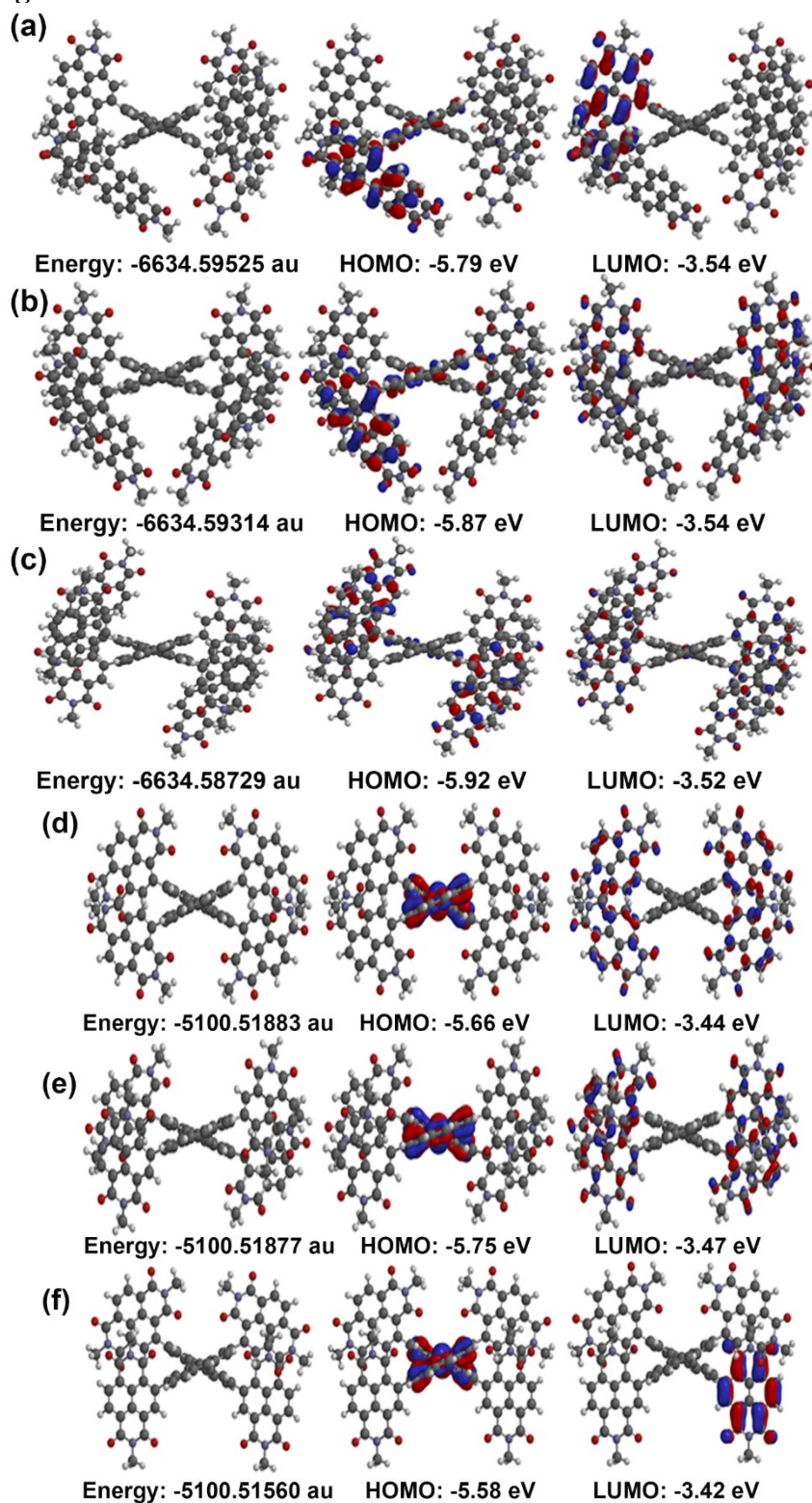


Figure S1 (a-c) Three possible structural conformations of BF-PDI₄ and their corresponding molecular orbital diagrams; (d-f) three possible structural conformations of BF-NDI₄ and their corresponding molecular orbital diagrams.

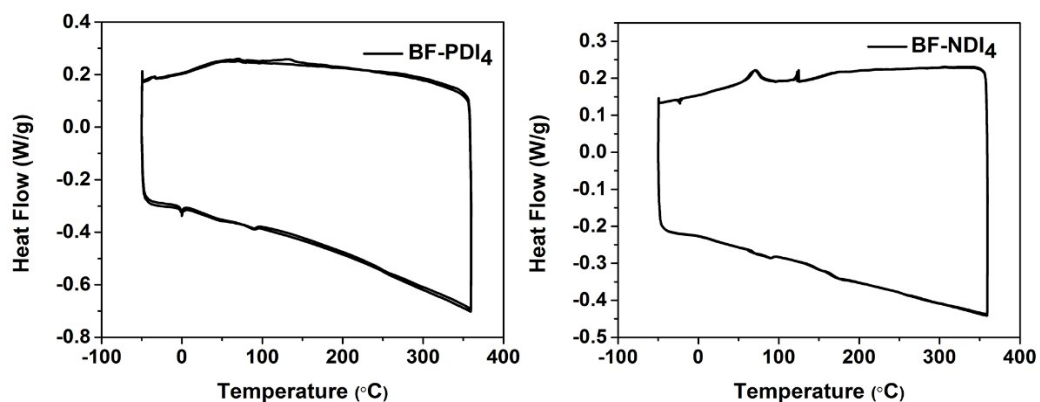


Figure S2 Differential Scanning Calorimetry curves of BF-PDI₄ and BF-NDI₄

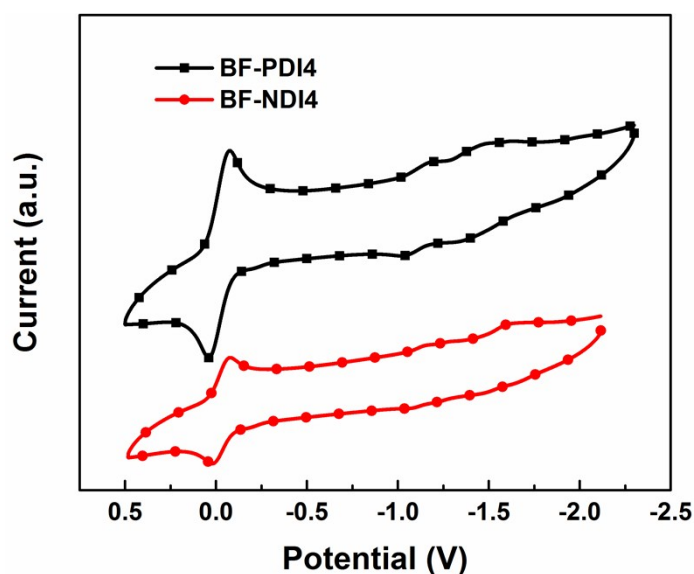


Figure S3 Cyclic voltammety of BF-PDI₄ and BF-NDI₄ (THF, 0.1 M [nBu₄N]⁺[PF₆]⁻, 50 mVs⁻¹) with FeCp₂⁺⁰ as an internal reference

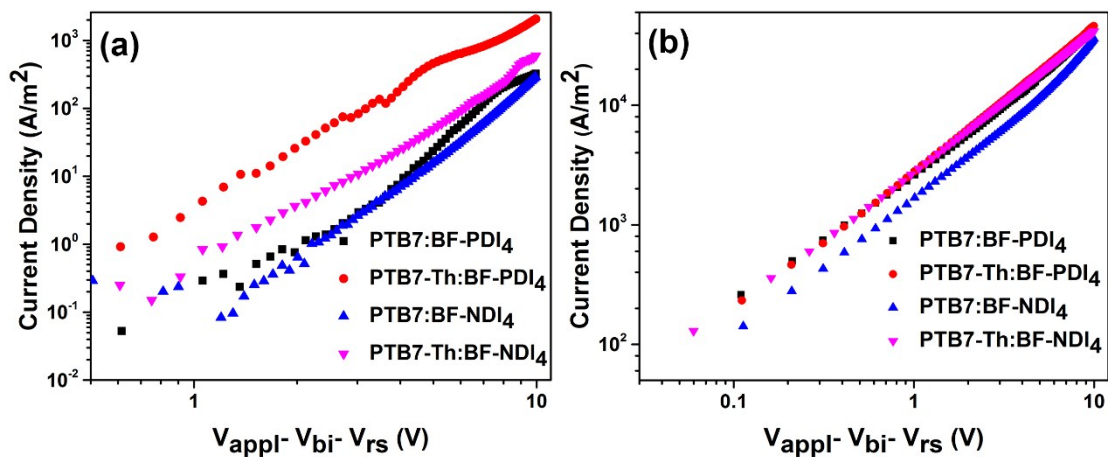


Figure S4 Current density and voltage (J–V) characteristics of (a) electron-only devices (ITO/ZnO/BHJ/Ca/Al) and (b) hole-only devices (ITO/PEDOT:PSS/BHJ/MoO₃/Ag).