

Electronic Supplementary Information (ESI)

New PDI-based small-molecule cathode interlayer material with strong electron extracting ability for polymer solar cells

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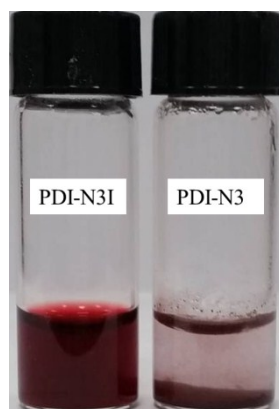


Fig. S1 The solubility of PDI-N3I and PDI-N3 in water.

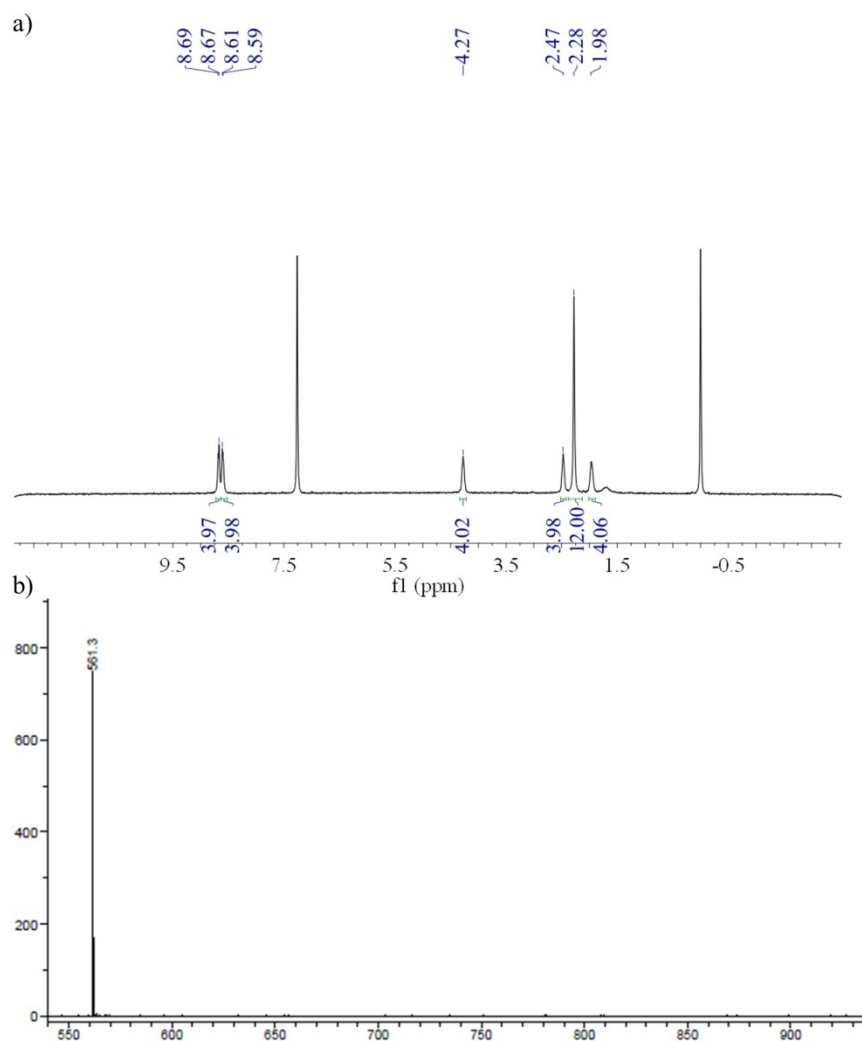


Fig. S2 ^1H NMR spectrum (a) and MALDI-TOF characterization result of PDI-N3.

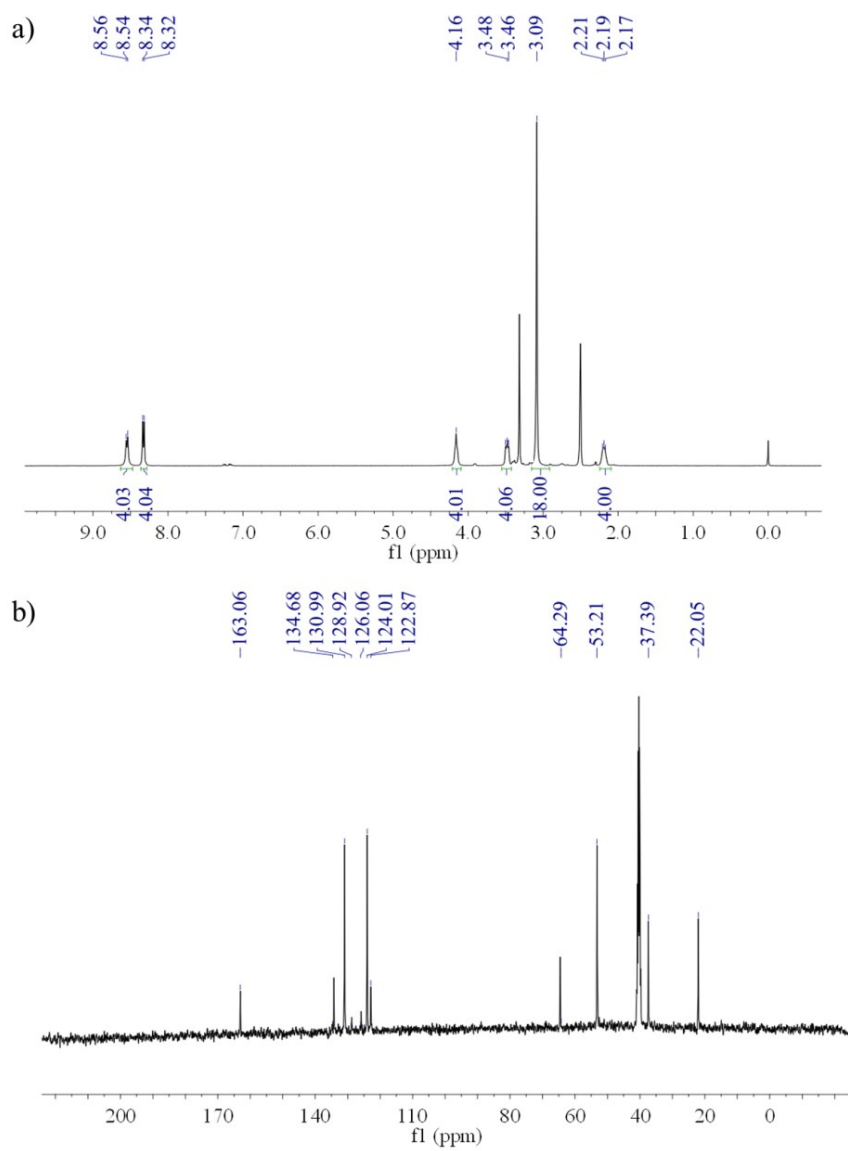


Fig. S3 ^1H NMR spectrum (a) and ^{13}C NMR spectrum (b) of PDI-N3I.

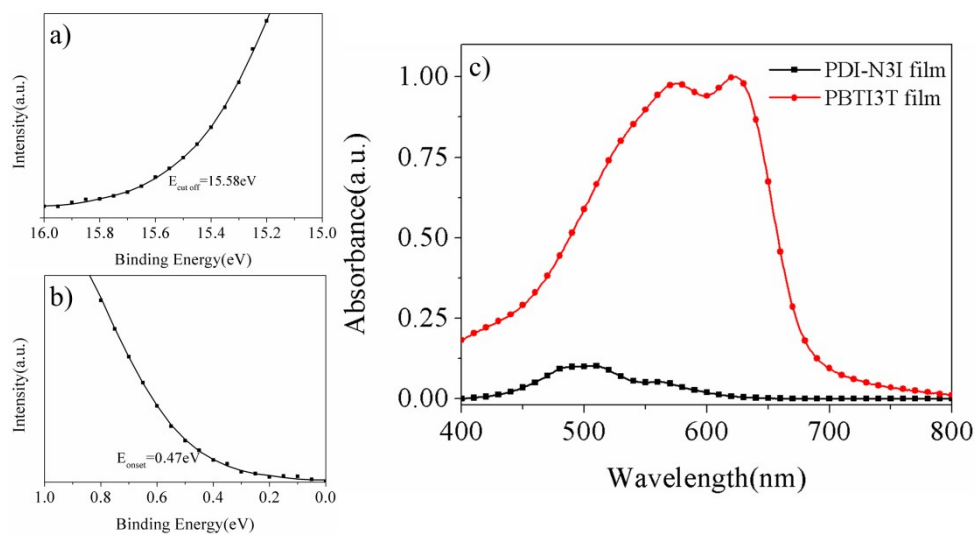


Fig. S4 (a) UPS spectra of PDI-N3I. (b) Film UV-Vis absorption spectra of PDI-N3I (30 nm) and PBTI3T (100 nm)

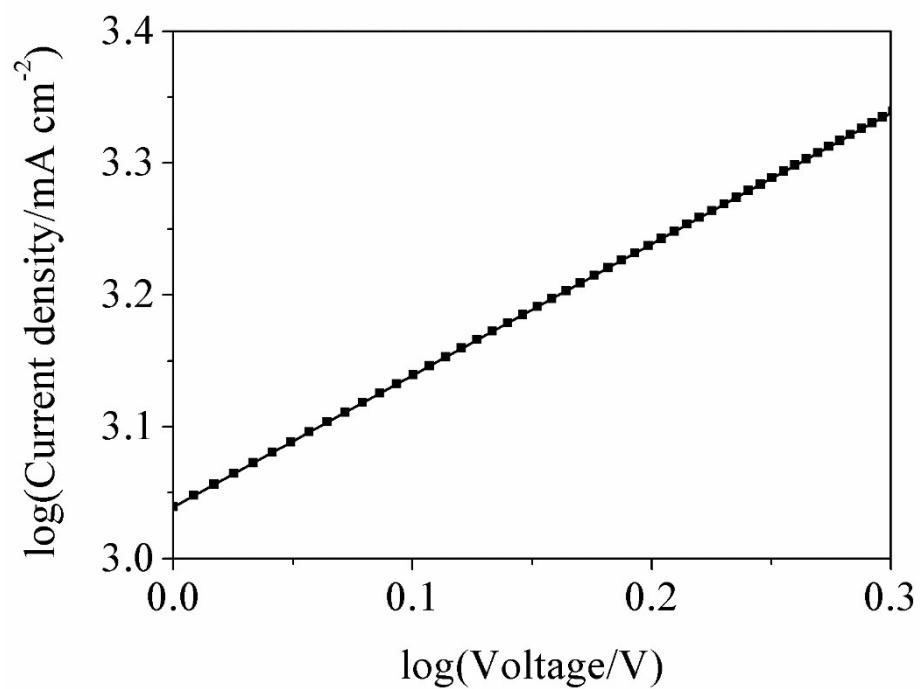


Fig. S5 J - V characteristics of electron-only device with the structure of ITO/PDI-N3I/Al on logarithmical scale.

Table S1 Statistical device parameters of PBTI3T:PC₇₁BM with different cathode interlayers under the illumination of AM 1.5G, 100 mW cm⁻².

	Thickness	V_{oc}	J_{sc}	FF	PCE	PCE ^a
Interlayer	(nm)	(V)	(mA cm ⁻²)	(%)	(%)	(%)
None	--	0.70	10.19	59.16	4.22	4.04 ± 0.18
		0.69	10.08	57.65	4.01	
		0.70	10.20	57.70	4.12	
		0.67	10.11	56.99	3.86	
		0.70	10.07	56.46	3.98	
		0.68	10.05	58.38	3.99	
		0.69	10.16	60.05	4.21	
		0.70	10.06	57.09	4.02	
LiF	0.8	0.86	10.41	73.10	6.54	6.40 ± 0.14
		0.86	10.27	70.88	6.26	
		0.84	10.38	72.37	6.31	
		0.85	10.40	73.53	6.50	
		0.86	10.43	72.58	6.51	
		0.86	10.33	72.60	6.45	
		0.85	10.27	72.17	6.30	
		0.85	10.40	72.29	6.39	
LiF*	0.8	0.86	10.33	72.15	6.41	6.26 ± 0.15
		0.86	10.28	71.03	6.28	
		0.85	10.29	73.05	6.39	
		0.86	10.09	70.53	6.12	

		0.86	10.14	70.52	6.15	
		0.85	10.18	69.79	6.11	
		0.85	10.23	72.91	6.34	
		0.86	10.26	71.40	6.30	
PDI-N3I	11	0.84	11.34	70.23	6.69	6.54 ± 0.15
		0.83	11.13	69.39	6.41	
		0.84	11.29	70.12	6.65	
		0.84	11.16	68.16	6.39	
		0.84	11.26	67.98	6.43	
		0.83	11.30	70.48	6.61	
		0.83	11.28	70.07	6.56	
		0.84	11.17	69.81	6.55	
	16	0.84	11.39	70.76	6.82	6.72 ± 0.10
		0.84	11.27	70.46	6.67	
		0.83	11.34	72.25	6.80	
		0.83	11.20	71.00	6.60	
		0.82	11.24	71.61	6.60	
		0.84	11.28	70.92	6.72	
		0.84	11.37	70.67	6.75	
		0.84	11.40	70.91	6.79	
	22	0.85	11.46	71.88	7.00	6.91 ± 0.09
		0.84	11.35	71.64	6.83	
		0.85	11.34	71.48	6.89	
		0.85	11.44	71.68	6.97	
		0.84	11.48	72.07	6.95	

	0.85	11.31	70.94	6.82	
	0.84	11.30	72.06	6.84	
	0.84	11.40	71.85	6.88	
28	0.86	11.24	69.93	6.76	6.70 ± 0.06
	0.85	11.20	70.17	6.68	
	0.84	11.16	71.15	6.67	
	0.86	11.18	69.79	6.71	
	0.86	11.09	69.62	6.64	
	0.85	11.12	70.99	6.71	
	0.85	11.21	69.69	6.64	
	0.86	11.26	69.50	6.73	

Table S2 Device parameters of PBTI3T:PC₇₁BM with PDI-N3I or PDI-N3 cathode interlayers under the illumination of AM 1.5G, 100 mW cm⁻².

	Thickness	V_{oc}	J_{sc}	FF	PCE	PCE ^a
Interlayer	(nm)	(V)	(mA cm ⁻²)	(%)	(%)	(%)
PDI-N3I	11	0.84	11.34	70.23	6.69	6.54 ± 0.15
	16	0.84	11.39	70.76	6.82	6.72 ± 0.10
	22	0.85	11.46	71.88	7.00	6.91 ± 0.09
	28	0.86	11.24	69.93	6.76	6.70 ± 0.06
PDI-N3	10	0.84	11.45	69.12	6.65	6.51 ± 0.14
	14	0.84	11.49	70.17	6.77	6.66 ± 0.11
	18	0.85	11.31	69.77	6.71	6.59 ± 0.12
	23	0.84	11.23	68.81	6.49	6.32 ± 0.17

Table S3 Statistical device parameters of the PSCs based on PBTI3T/PC₇₁BM with LiF/Al, PDI-N3I/Al, PDI-N3I/LiF/Al cathodes under the illumination of AM 1.5G, 100 mW cm⁻²

	V_{oc}	J_{sc}	FF	PCE	PCE ^a
Interlayer	(V)	(mA cm ⁻²)	(%)	(%)	(%)
LiF	0.86	10.41	73.10	6.54	6.40 ± 0.14
	0.86	10.27	70.88	6.26	
	0.84	10.38	72.37	6.31	
	0.85	10.40	73.53	6.50	
	0.86	10.43	72.58	6.51	
	0.86	10.33	72.60	6.45	
	0.85	10.27	72.17	6.30	
	0.85	10.40	72.29	6.39	
9 nm PDI-N3I	0.82	11.32	65.41	6.06	5.87 ± 0.19
	0.82	11.33	64.80	6.02	
	0.81	11.18	63.61	5.76	
	0.81	11.20	64.81	5.88	
	0.82	11.18	62.28	5.71	
	0.82	11.30	64.86	6.01	
	0.82	11.27	64.60	5.97	
	0.81	11.24	62.39	5.68	
9 nm PDI-N3I+LiF	0.86	11.22	71.12	6.86	6.76 ± 0.10
	0.86	11.17	69.85	6.71	
	0.86	11.21	70.54	6.80	
	0.86	11.20	70.70	6.81	
	0.85	11.16	70.31	6.67	
	0.86	11.13	69.58	6.66	
	0.85	11.24	71.17	6.80	

	0.86	11.25	70.70	6.84	
16 nm PDI-N3I	0.84	11.39	70.76	6.82	6.72 ± 0.12
	0.84	11.27	70.46	6.67	
	0.83	11.34	72.25	6.80	
	0.83	11.20	71.00	6.60	
	0.82	11.24	71.61	6.60	
	0.84	11.28	70.92	6.72	
	0.84	11.37	70.67	6.75	
	0.84	11.40	70.91	6.79	
16 nm PDI-N3I+LiF	0.86	11.17	74.76	7.18	7.09 ± 0.09
	0.86	11.09	73.60	7.02	
	0.86	11.05	73.66	7.00	
	0.85	11.11	75.29	7.11	
	0.86	11.13	73.97	7.08	
	0.85	11.10	74.30	7.01	
	0.85	11.18	75.45	7.17	
	0.86	11.15	74.56	7.15	
22 nm PDI-N3I	0.85	11.46	71.88	7.00	6.91 ± 0.09
	0.84	11.35	71.64	6.83	
	0.85	11.34	71.48	6.89	
	0.85	11.44	71.68	6.97	
	0.83	11.48	72.94	6.95	
	0.85	11.31	70.94	6.82	
	0.84	11.30	72.06	6.84	
	0.84	11.40	71.85	6.88	
22 nm PDI-N3I+LiF	0.86	11.02	73.96	7.01	6.93 ± 0.08
	0.86	10.98	72.97	6.89	
	0.86	10.99	74.06	7.00	
	0.85	11.04	74.70	7.01	

0.85	11.01	73.63	6.89
0.86	10.91	74.39	6.98
0.86	10.88	73.21	6.85
0.86	10.93	73.62	6.92
