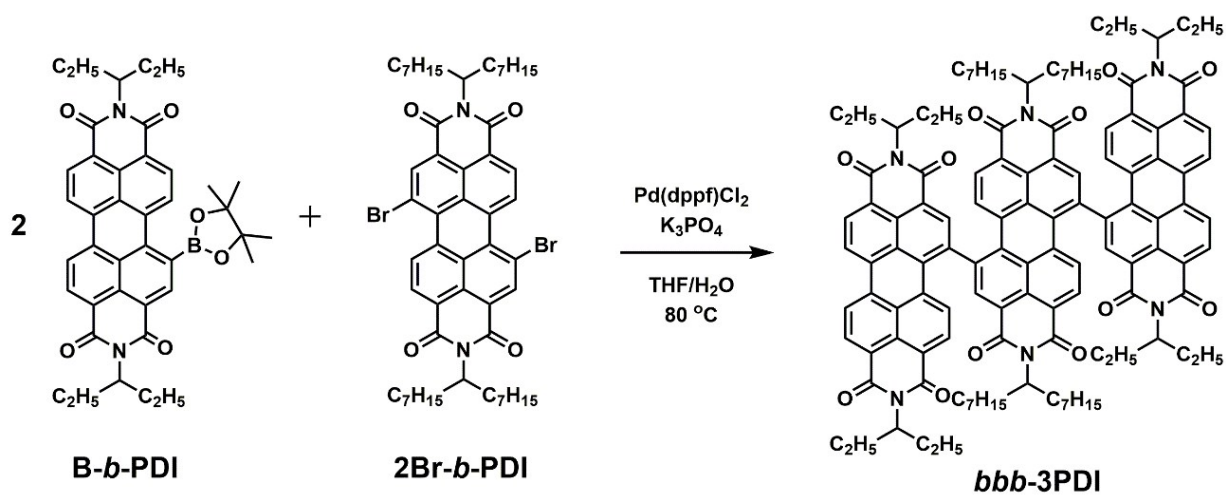


Electronic Supporting Information for

Perylene Diimides Arrays: the Promising Candidates for Non-fullerene Organic Solar Cells

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Scheme S1. Synthesis of *bbb*-3PDI.

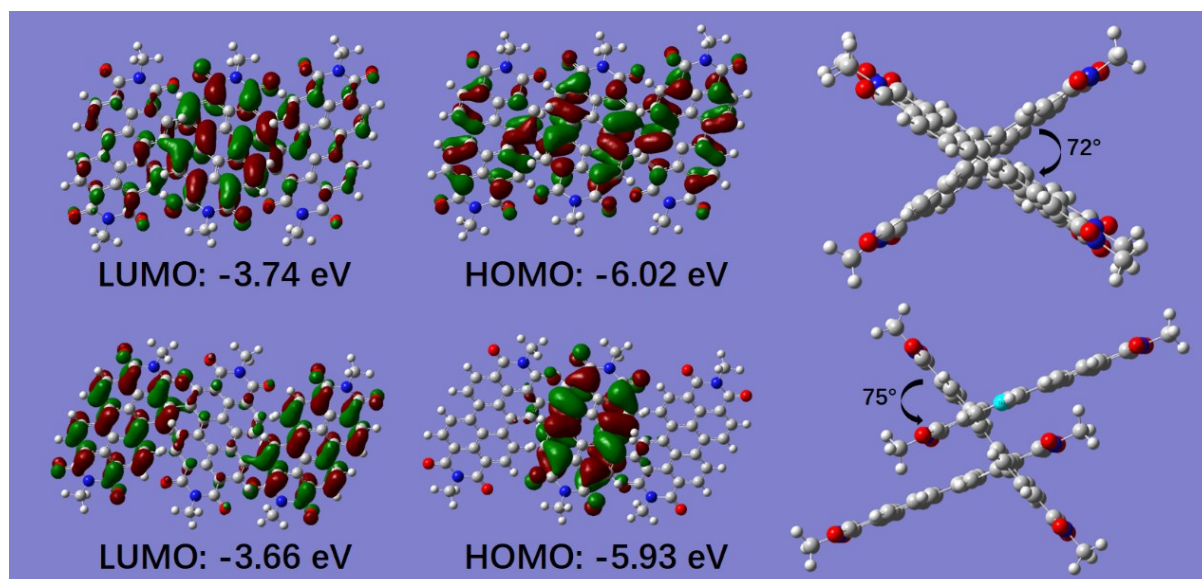


Fig. S1 Theoretical calculations of *bbb-3PDI* (upper) and *obo-3PDI* (below) using DFT calculations at the B3LYP/6-31G (d, p) level.

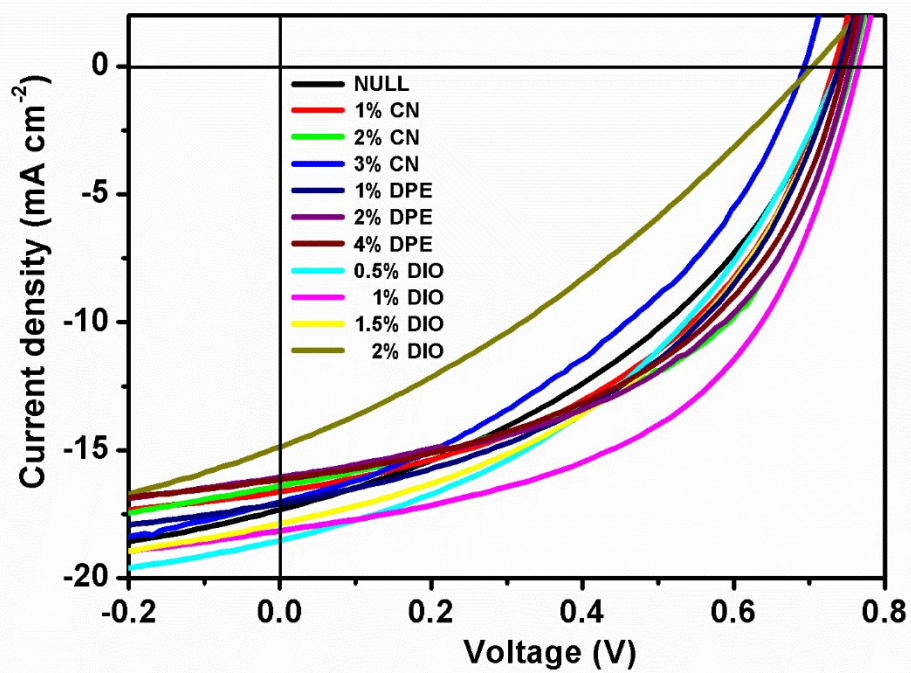


Fig. S2 J - V curves of PTB7-Th:bbb-3PDI (1:1) with different additives.

Table S1. Summary of device parameters of PTB7-Th:*bbb*-3PDI (1:1) with different additives.

Additives [volume]	J _{sc} [mA cm ⁻²]	V _{oc} [V]	FF [%]	PCE [%]
NO	17.33	0.740	40.1	5.14
1% CN	16.56	0.731	45.9	5.56
2% CN	16.39	0.755	49.1	6.08
3% CN	17.00	0.690	39.3	4.61
1% DPE	16.79	0.742	45.0	5.61
2% DPE	16.02	0.753	49.8	6.01
4% DPE	16.09	0.745	48.4	5.80
0.5% DIO	18.49	0.738	41.1	5.61
1% DIO	18.13	0.764	51.4	7.12
1.5% DIO	17.84	0.738	43.7	5.75
2% DIO	14.91	0.704	31.7	3.33

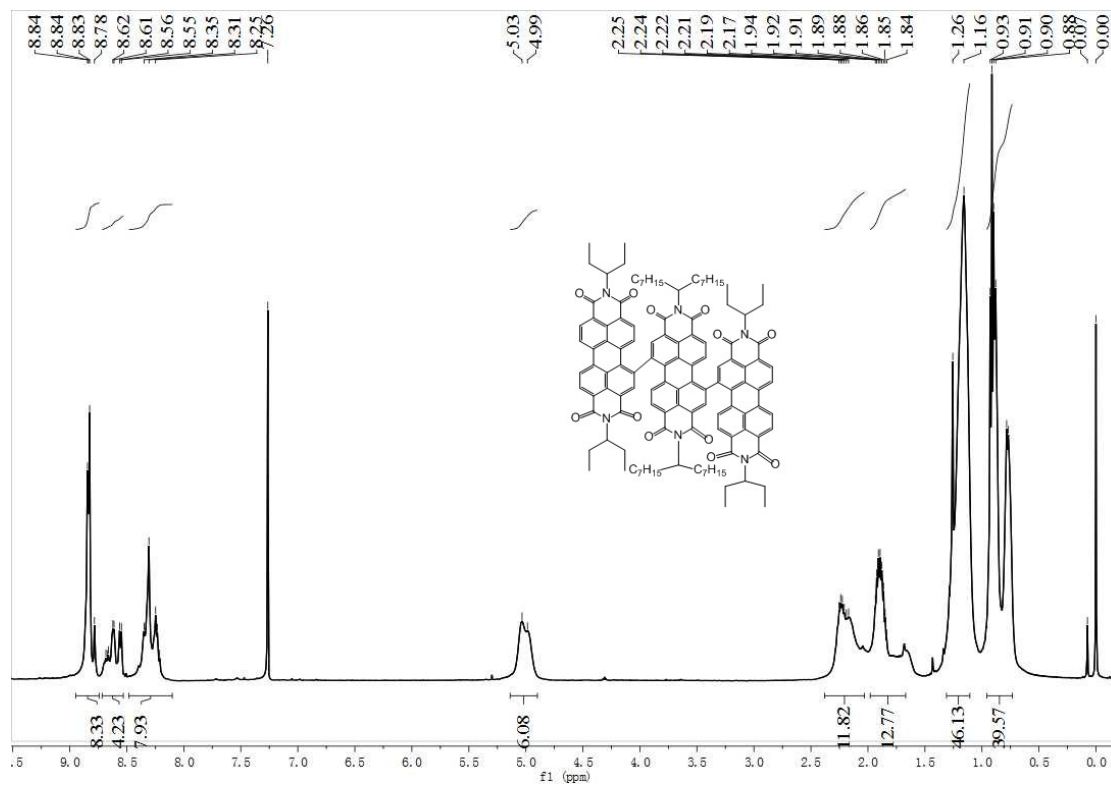


Fig. S3 ^1H NMR spectrum of *bbb*-3PDI in CDCl_3 .

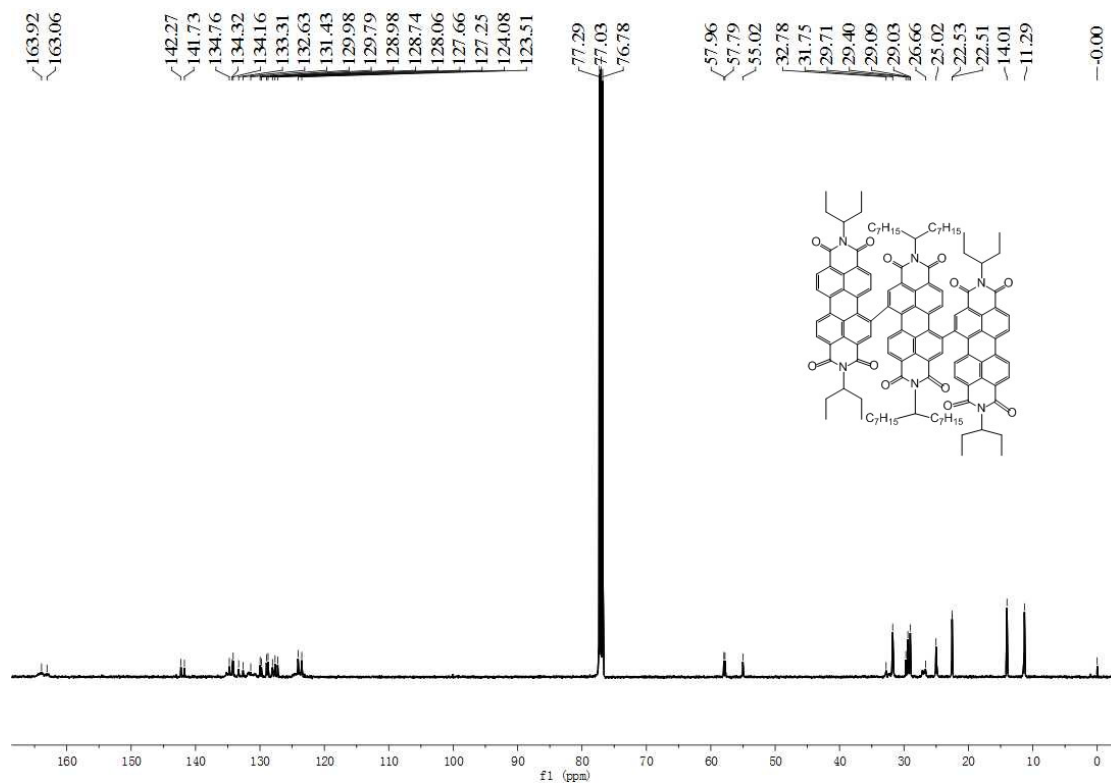


Fig. S4 ^{13}C NMR spectrum of *bbb*-3PDI in $CDCl_3$.