Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Structural Optimization of Large Acceptor–Donor–Acceptor-Type Molecules for Improved Performance of Fullerene-Free Polymer Solar Cells

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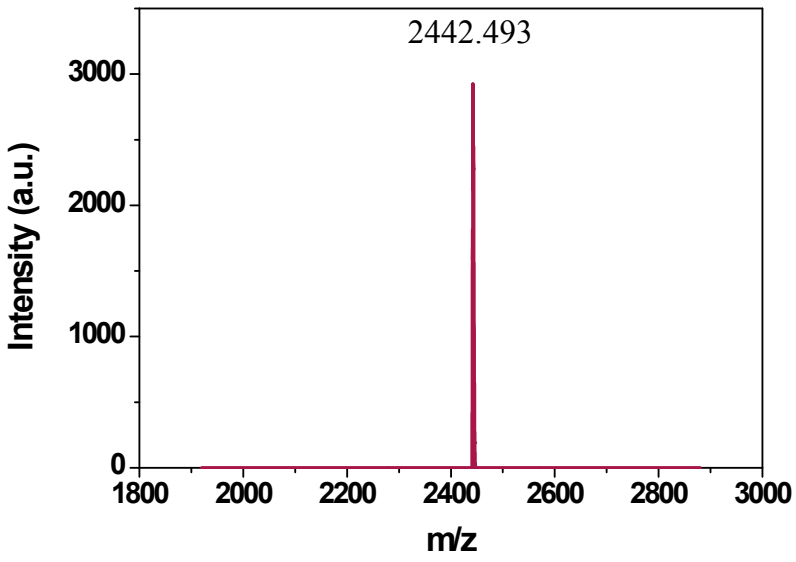

Figure S1. MALDI-TOF of compound **3**.

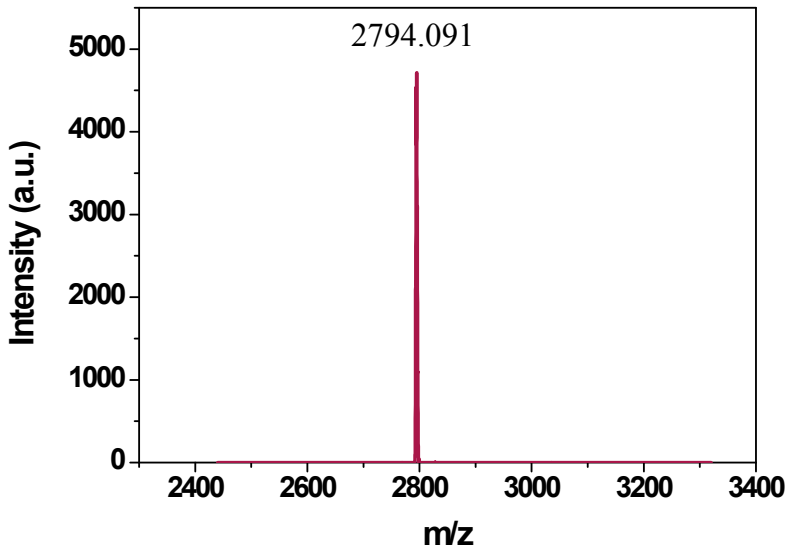

Figure S2. MALDI-TOF of IM-BDTIDT2 (**4**).

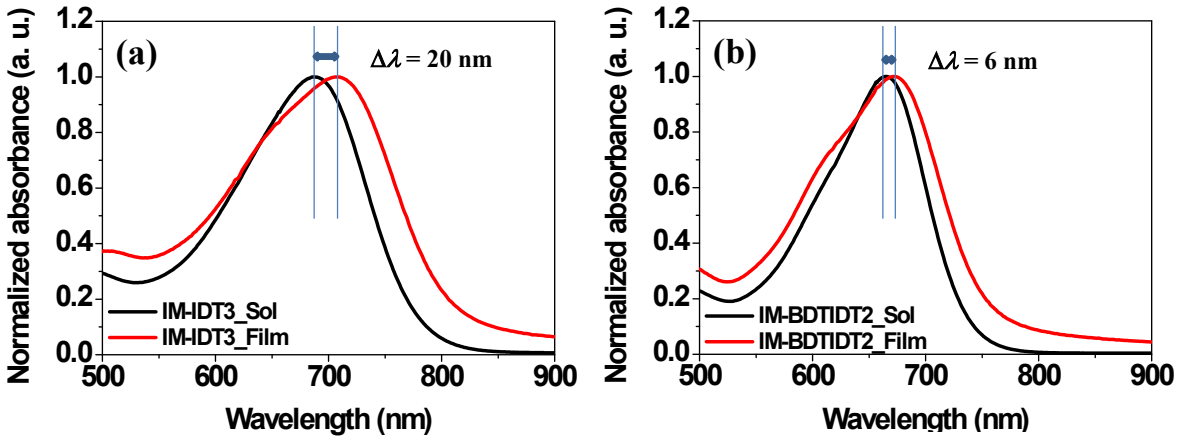

Figure S3. Bathochromic shift of UV-vis absorption spectra between solution and film. (a) IM-IDT3, (b) IM-BDTIDT2.

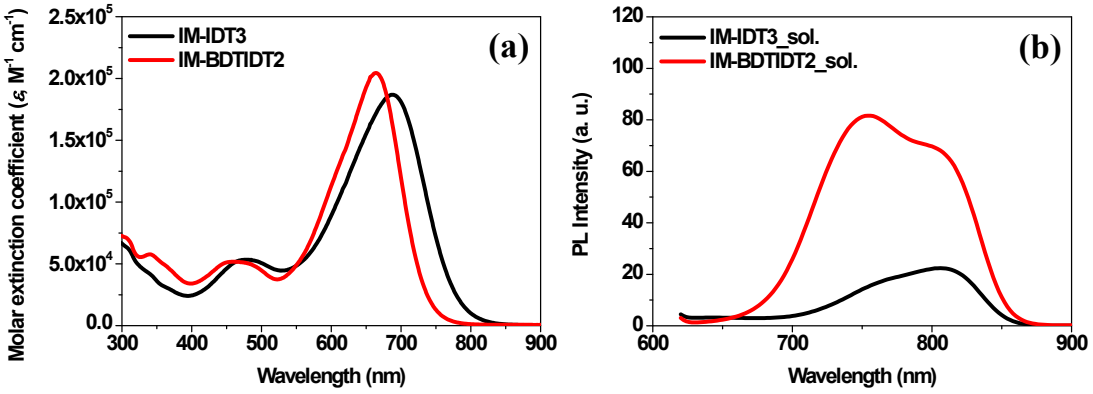

Figure S4. Molar extinction coefficient (a) and photoluminescence (PL) spectra (b) of IM-IDT3 and IM-BDTIDT2 in chloroform solution.

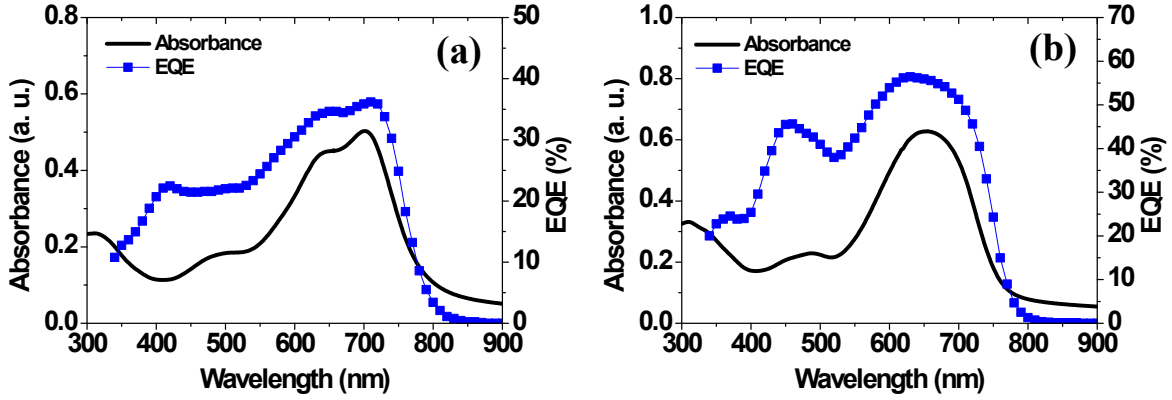

Figure S5. UV-vis absorption and EQE spectra of blend films and corresponding PSC devices. (a) PTB7-Th:IM-IDT3 (1:1) with 4 vol% DPE and (b) PTB7-Th:IM-BDTIDT2 (1:1) with 2 vol% DPE.

Table S1. Parameters of PSCs based on IM-IDT3 and IM-BDTIDT2 measured at 100 mW cm^{-2} AM 1.5 G illumination.

n-Type molecule	p/n ratio (wt%)	Solvent/ additive	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE[a] (%)
IM-IDT3	1:1	CB	0.95 (0.94±0.01)	5.72 (5.68±0.04)	49.87 (49.63±0.24)	2.70 (2.65±0.05)
	1:1	CB/ DPE 2%	0.95 (0.94±0.01)	6.66 (6.56±0.10)	49.44 (49.27±0.17)	3.13 (3.04±0.09)
	1:1	CB/ DPE 4%	0.95 (0.94±0.01)	7.15 (7.06±0.09)	47.82 (47.71±0.11)	3.25 (3.17±0.08)
	1:1.5	CB	0.95 (0.94±0.01)	6.28 (6.18±0.10)	49.08 (48.84±0.24)	2.93 (2.84±0.09)
	1:1.5	CB/ DPE 2%	0.93 (0.929±0.001)	6.13 (5.97±0.16)	48.41 (48.35±0.06)	2.76 (2.68±0.08)
IM-BDTIDT2	1:1	CB	0.96 (0.95±0.01)	9.42 (8.97±0.45)	50.79 (50.67±0.12)	4.57 (4.32±0.25)
	1:1	CB/ DPE 2%	0.97 (0.96±0.01)	11.28 (10.89±0.39)	48.72 (48.58±0.14)	5.33 (5.08±0.25)
	1:1	CB/ DPE 4%	0.97 (0.96±0.01)	10.54 (10.28±0.26)	48.30 (48.11±0.19)	4.91 (4.75±0.16)
	1:1.5	CB	0.95 (0.948±0.002)	6.31 (6.09±0.22)	50.50 (50.39±0.11)	3.00 (2.91±0.09)
	1:1.5	CB/ DPE 2%	0.97 (0.96±0.01)	10.91 (10.82±0.09)	48.69 (48.44±0.25)	5.18 (5.03±0.15)
	1:1.5	CB/ DPE 4%	0.97 (0.96±0.01)	10.97 (10.43±0.54)	49.77 (49.51±0.26)	5.12 (4.96±0.16)

[a]Average PCE values, which were obtained from more than 10 devices, are shown in parentheses.

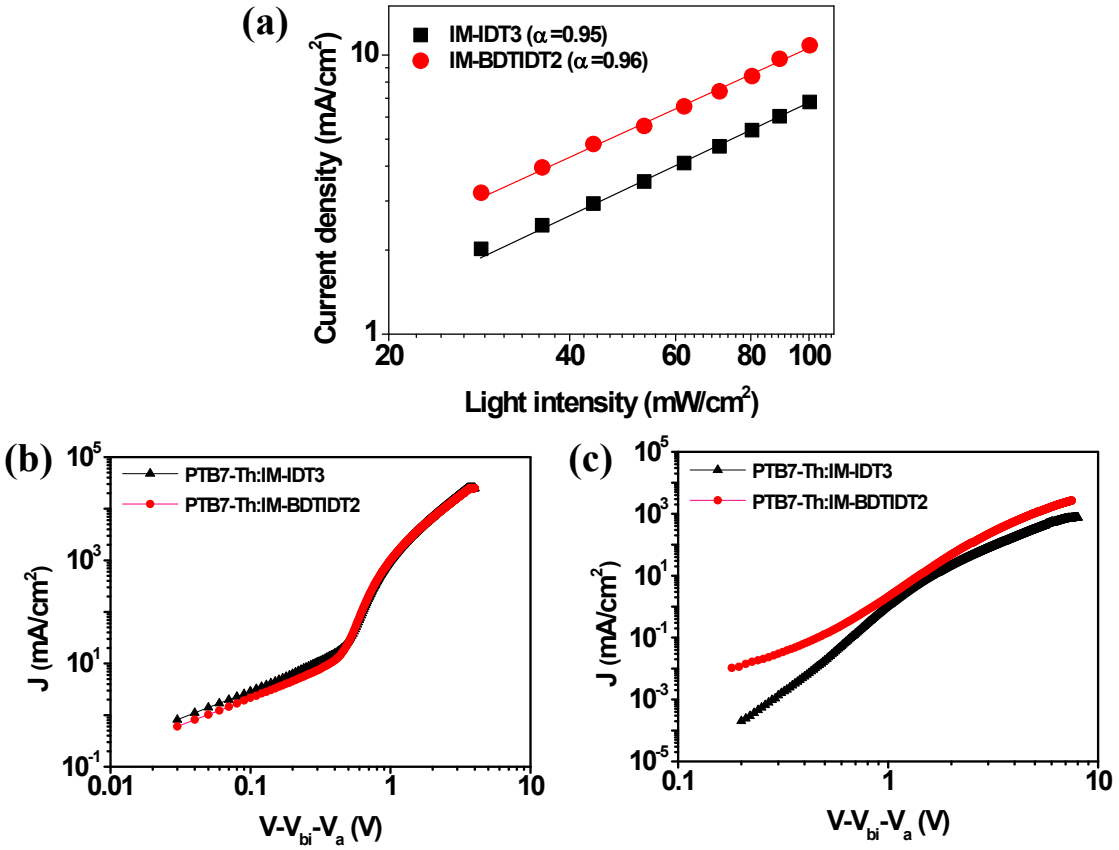

Figure S6. J_{sc} vs. light intensity curves (a) for PTB7-Th:IM-IDT3 (1:1) with 4 vol% DPE, and PTB7-Th:IM-BDTIDT2 (1:1) with 2 vol% DPE blend films. Measured space-charge-limited *J–V* characteristics for optimized PTB7-Th:IM-IDT3 and PTB7-Th:IM-BDTIDT2 blend films under dark conditions for (b) hole-only devices (HODs) and (c) electron-only devices (EODs). HOD: ITO/PEDOT:PSS/active layer/Au and EOD: ITO/ZnO/active layer/LiF/Al.

Table S2. Carrier mobilities of HODs and EODs.

n-type molecule	μ_h ($cm^2\ V^{-1}\ s^{-1}$)	μ_e ($cm^2\ V^{-1}\ s^{-1}$)	μ_h/μ_e
IM-IDT3	2.76×10^{-4}	2.59×10^{-5}	10.65
IM-BDTIDT2	5.48×10^{-4}	8.67×10^{-5}	6.32

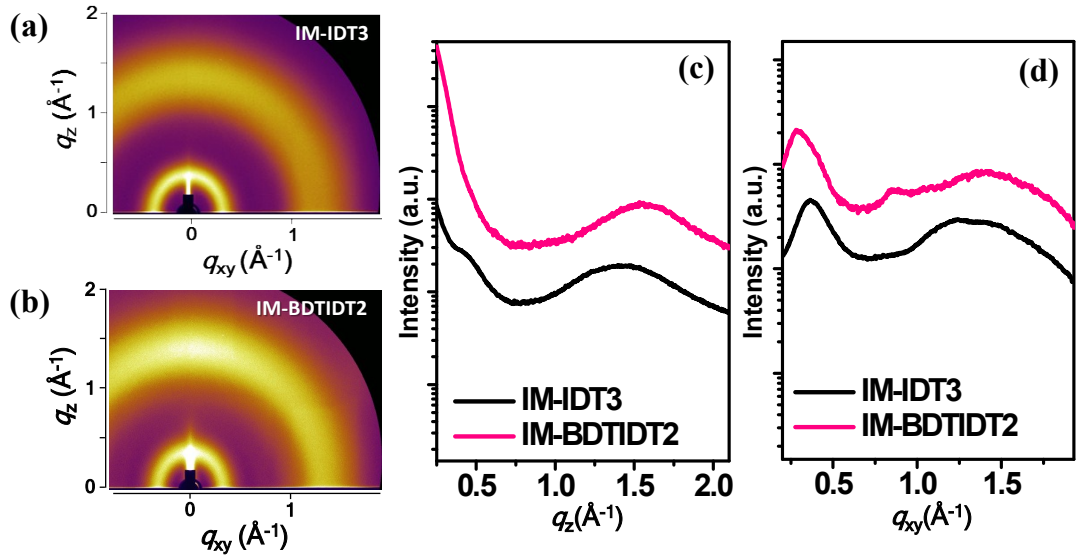

Figure S7. GIWAXS images of pure IM-IDT3 (a) and IM-BDTIDT2 (b) films. Out-of-plane (c) and in-plane profiles (d) of the pure small molecules.

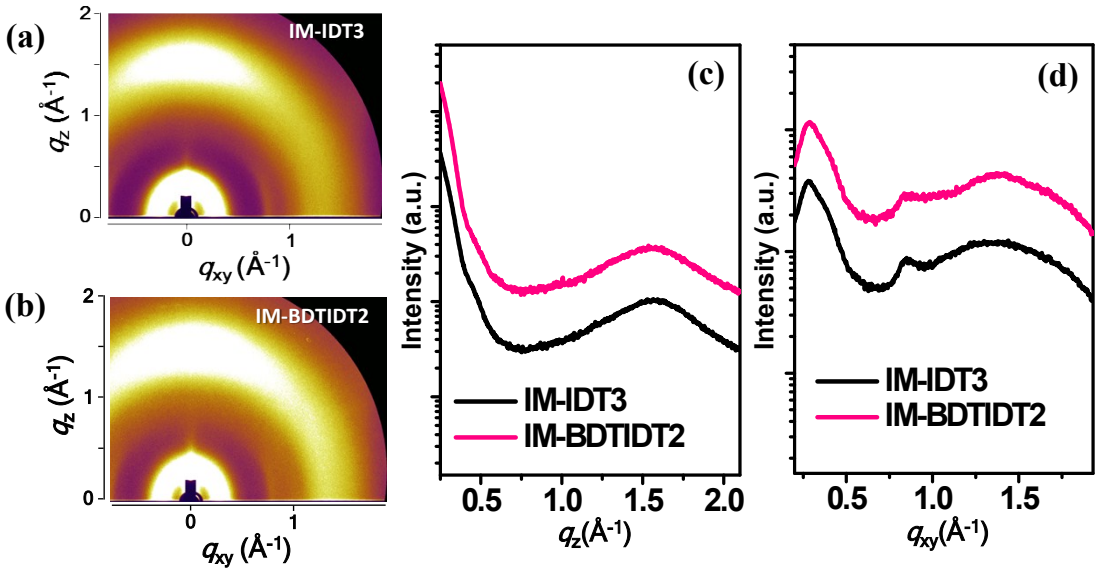

Figure S8. GIWAXS images of optimized PTB7-Th:IM-IDT3 (1:1) with 4 vol% DPE (a) and PTB7-Th:IM-BDTIDT2 (1:1) with 2 vol% DPE (b). Out-of-plane (c) and in-plane profiles (d) of the blend films.