Supporting Information

New n-type semiconducting molecule with asymmetric indenothiophene core for high-performing non-fullerene type organic solar cell

Young Un Kim, Gi Eun Park, Suna Choi, Dae Hee Lee, Min Ju Cho* and Dong Hoon Choi*

Department of Chemistry, Research Institute for Natural Sciences, Korea University, 5 Anam-dong, Sungbuk-Gu, Seoul, 136-701 Republic of Korea

KEYWORDS non-fullerene acceptor, asymmetric molecule, Indenothiophene, photovoltaic properties, polymer solar cells

Table S1 Photovoltaic properties of PSCs based on PTB7-Th:**PhITBD** with different blend ratios. Solvent : chlorobenzene with 2.0 vol % diphenylether.

n-type SM	D : A (w/w)	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	PCE (%)[a]
PhITBD	2:1	0.781 (0.777 ± 0.03)	5.60 (5.52 ± 0.06)	0.35 (0.34 ± 0.01)	1.52 (1.41 ± 0.10)
PhITBD	1:1	0.756 (0.754 ± 0.02)	12.44 (12..40 ± 0.04)	0.53 (0.52 ± 0.01)	4.99 (4.92 ± 0.07)
PhITBD	1:1.5	0.757 (0.750 ± 0.005)	14.07 (13.80 ± 0.21)	0.62 (0.60 ± 0.02)	6.57 (6.31 ± 0.23)
PhITBD	1:2	0.747 (0.743 ± 0.03)	13.73 (13.62 ± 0.07)	0.59 (0.57 ± 0.02)	6.05 (5.92 ± 0.12)

[a] The average values and their standard deviations are given in parenthesis. The parameters of V_{oc}, J_{sc}, FF, and PCE were obtained from 10 separate devices.

Table S2 Photovoltaic properties of PSCs based on PTB7-Th:**PhITBD** (1:1.5 wt. ratio) with the concentration of diphenyl ether (DPE) additive.

n-type SM	DPE (%)	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	PCE (%)[a]
PhITBD	0.0	0.770 (0.766 ± 0.004)	10.37 (10.27 ± 0.09)	0.50 (0.49 ± 0.01)	3.99 (3.86 ± 0.11)
PhITBD	2.0	0.757 (0.750 ± 0.005)	14.07 (13.80 ± 0.21)	0.62 (0.60 ± 0.02)	6.57 (6.31 ± 0.23)
PhITBD	3.0	0.729 (0.723 ± 0.005)	9.50 (9.44 ± 0.06)	0.61 (0.59 ± 0.02)	4.23 (4.11 ± 0.12)
PhITBD	4.0	0.745 (0.742 ± 0.002)	4.87 (4.85 ± 0.02)	0.49 (0.48 ± 0.01)	1.75 (1.71 ± 0.04)

[a] The average values and their standard deviations are given in parenthesis. The parameters of V_{oc}, J_{sc}, FF, and PCE were obtained from 10 separate devices.

Table S3 Photovoltaic properties of PSCs based on PTB7-Th : **PhITBD** (1:1.5 wt. ratio) with different additives.

n-type SM	Additive	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	PCE (%)[a]
PhITBD	–	0.770 (0.766 ± 0.004)	10.37 (10.27 ± 0.09)	0.50 (0.49 ± 0.01)	3.99 (3.86 ± 0.11)
PhITBD	CN 1%	0.771 (0.768 ± 0.003)	3.62 (3.56 ± 0.05)	0.52 (0.50 ± 0.02)	1.45 (1.38 ± 0.06)
PhITBD	DIO 1%	0.747 (0.766 ± 0.004)	9.03 (8.99 ± 0.004)	0.63 (0.61 ± 0.02)	4.25 (4.17 ± 0.08)
PhITBD	DPE 2%	0.757 (0.750 ± 0.005)	14.07 (13.80 ± 0.21)	0.62 (0.60 ± 0.02)	6.57 (6.31 ± 0.23)

[a] The average values and their standard deviations are given in parenthesis. The parameters of V_{oc}, J_{sc}, FF, and PCE were obtained from 10 separate devices.

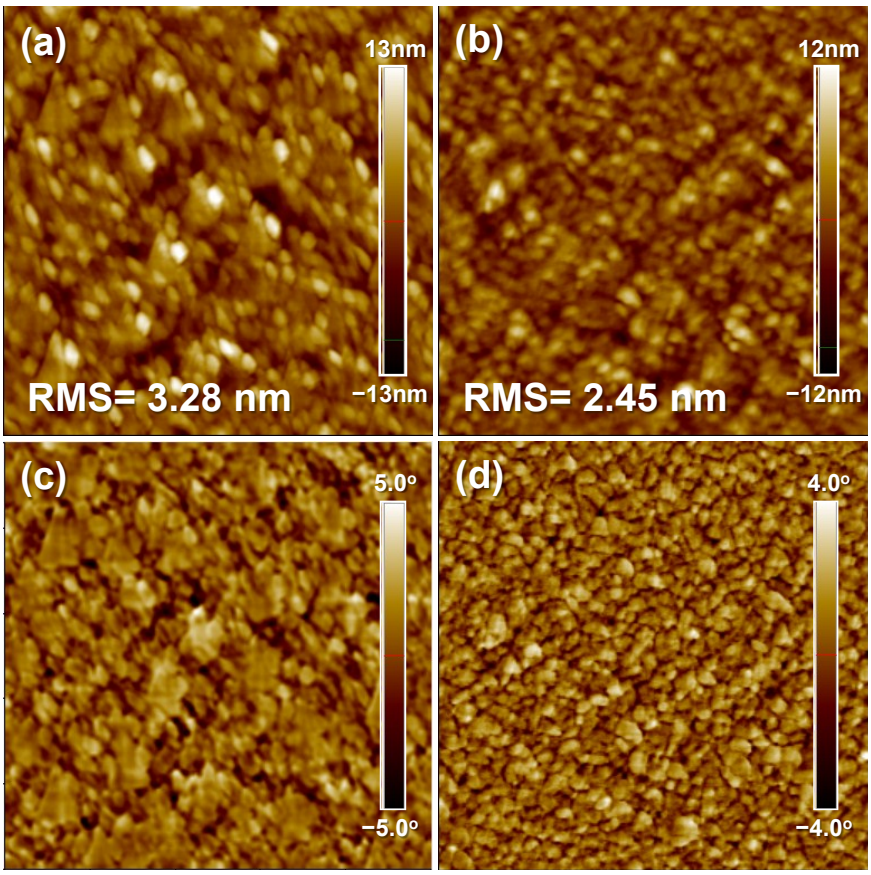

Fig. S1 AFM height (top) and phase (bottom) images (5 μm × 5 μm) of active layers. PTB7−Th: **IDT−2BM** (a, c) and PTB7−Th: **PhITBD** (b, d) films without DPE.

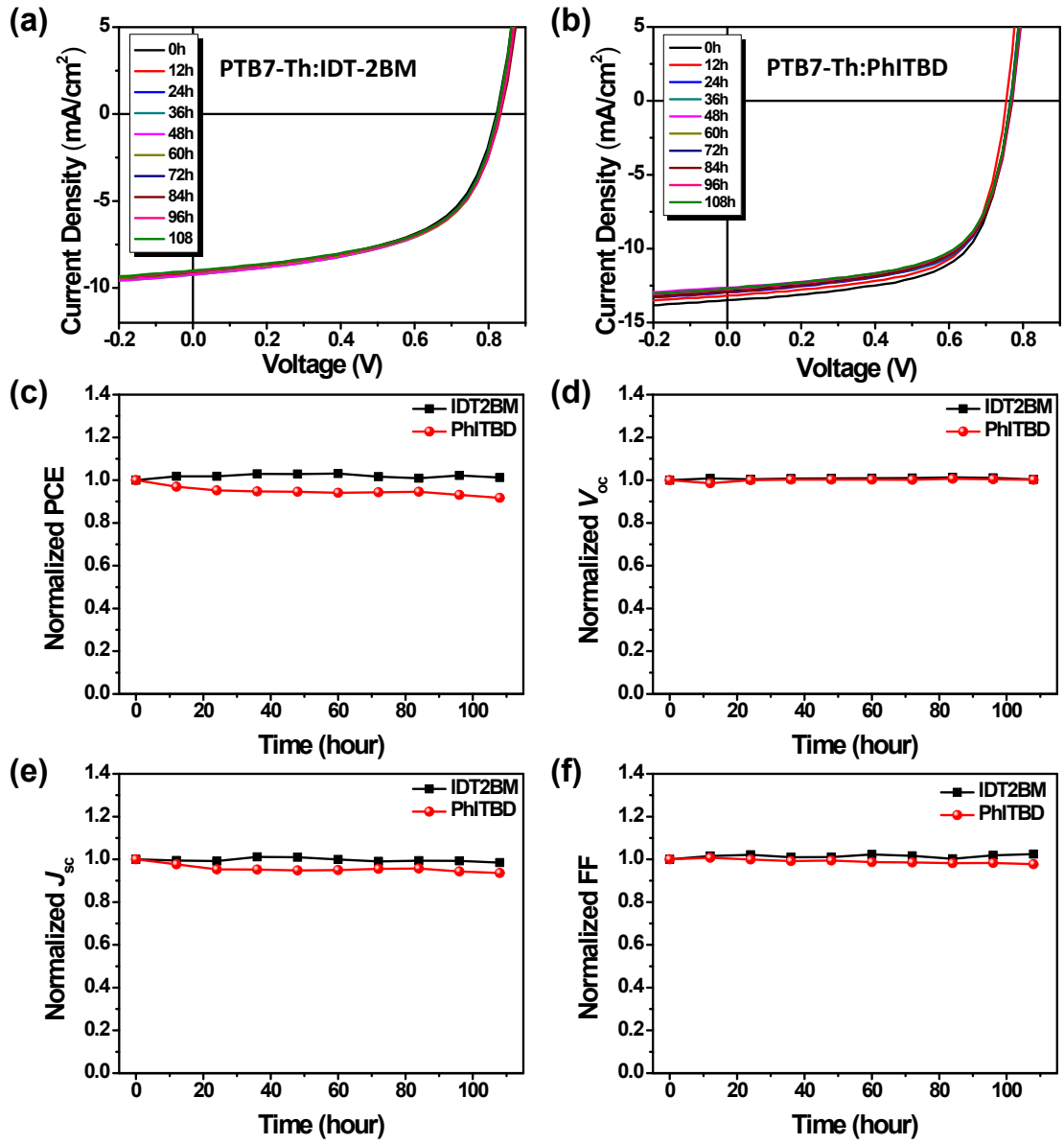

Fig. S2 Performance stability for **IDT−2BM** and **PhITBD**−based PSCs under ambient conditions for up to 108 h. Variation of *J*-*V* characteristics of BHJ PSCs based on (a) **IDT−2BM** and (b) **PhITBD**. Plots of normalized (c) PCE, (d) V_{OC}, (e) J_{SC}, and (f) FF vs. elapsed time.