Supporting Information

Energy Level-Modulated Non-Fullerene Small Molecule Acceptors for Improved V_{OC} and Efficiency of Inverted Perovskite Solar Cells

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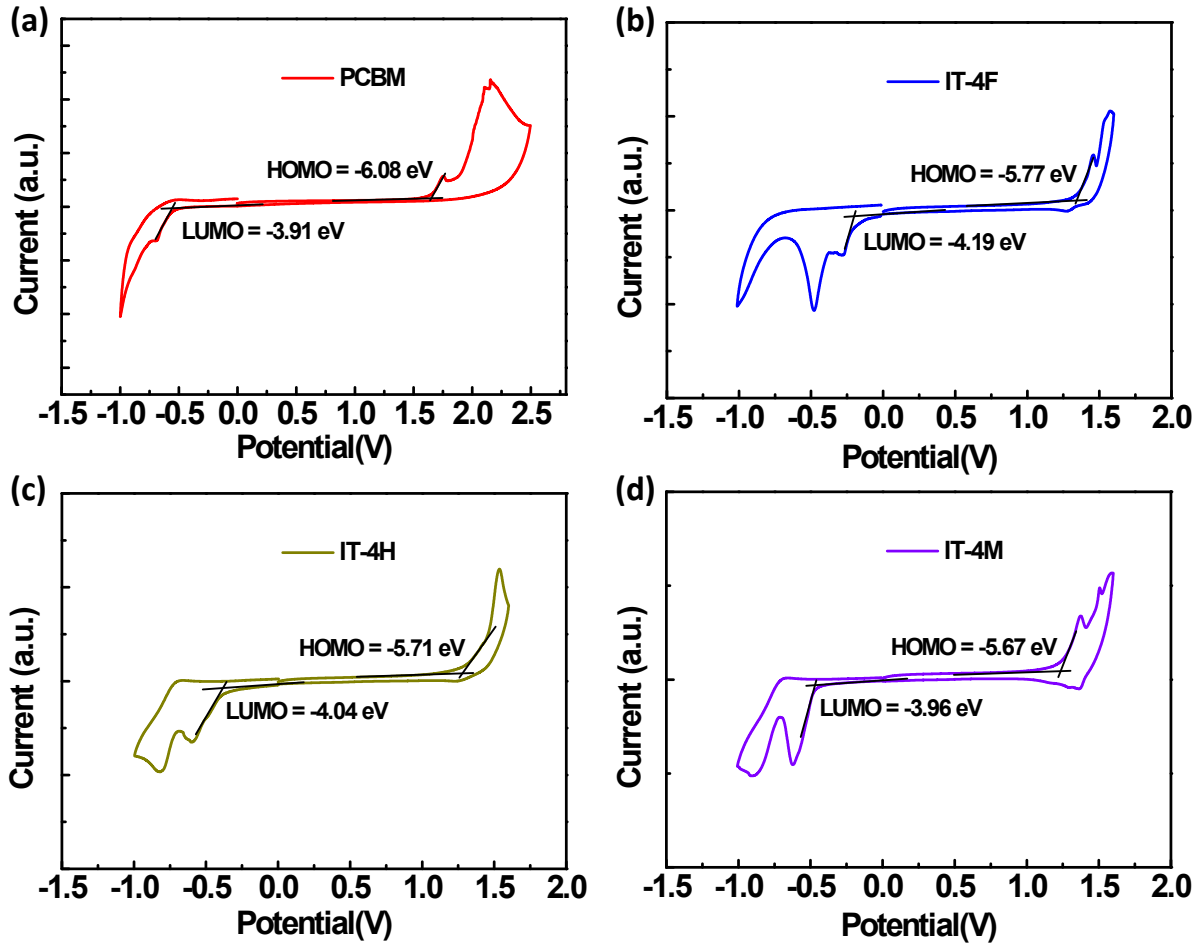

Fig. S1 Cyclic voltammetry of PCBM, IT-4F, IT-4H and IT-4M in the film measured in a 0.1 M Bu_4NPF_6-CH_3CN solutions.

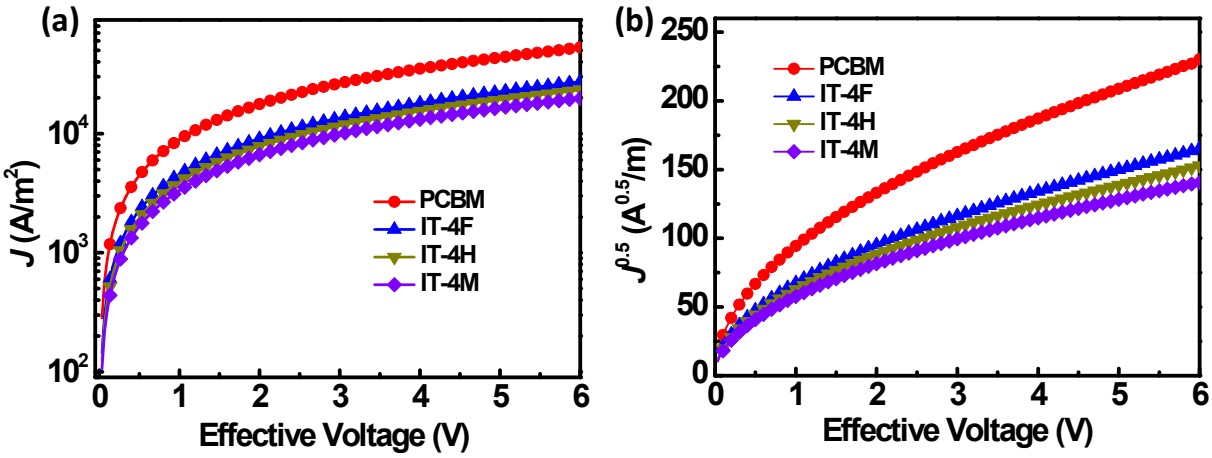

Fig. S2 (a) Dark *J*-*V* curves and (b) $J^{0.5}$-*V* characteristics of the electron-only devices based on various ETLs (IT-4F, IT-4H, IT-4M and PCBM) with ITO/ZnO/IT-4X or PCBM/ZnO/Al structure.

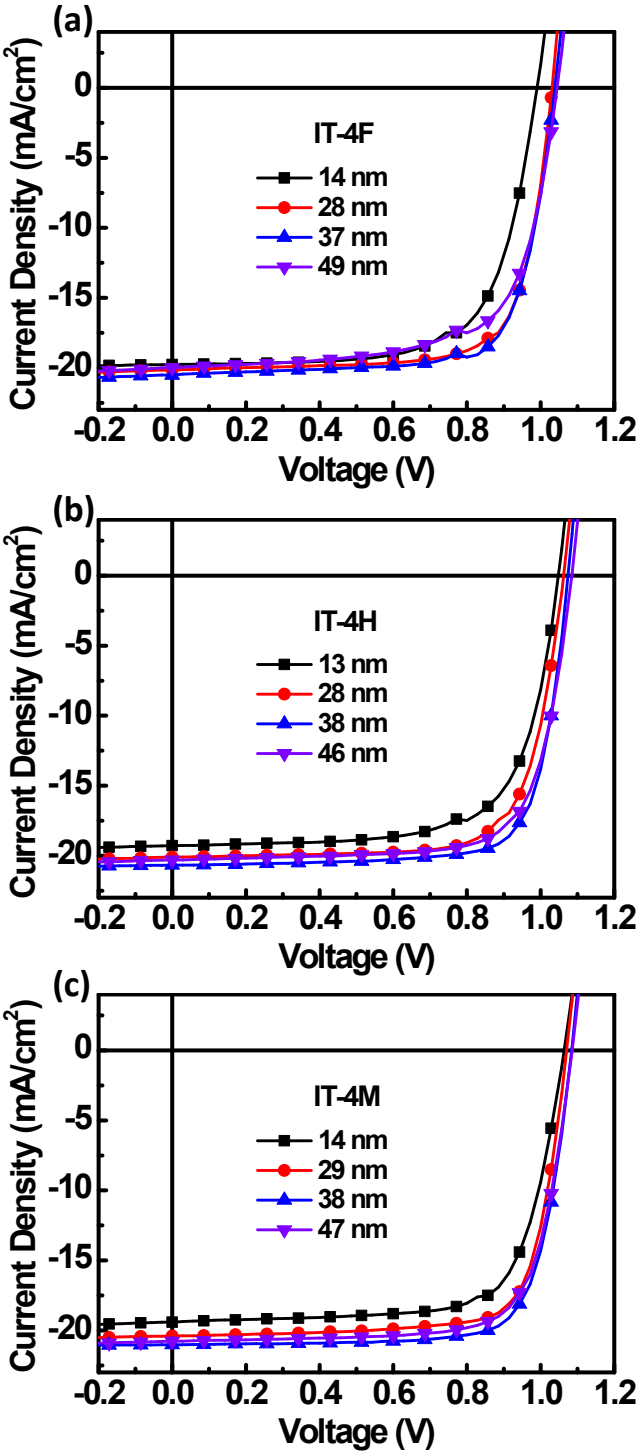

Fig. S3 *J-V* curves of PVSCs based on various ETLs (IT-4F, IT-4H and IT-4M) in different thicknesses.

Table S1. Summary of the photovoltaic performances of PVSCs based on various ETLs (IT-4F, IT-4H and IT-4M) in different thicknesses.

ETL	Thickness (nm)	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)
IT-4F	14	0.989	19.77	69.39	13.56
	28	1.029	20.15	74.46	15.44
	37	1.037	20.49	75.03	15.94
	49	1.043	19.99	68.66	14.31
IT-4H	13	1.046	19.29	70.22	14.17
	28	1.061	20.12	73.17	15.61
	38	1.072	20.68	76.83	17.04
	46	1.083	20.31	73.64	16.20
IT-4M	14	1.063	19.40	72.73	14.99
	29	1.069	20.40	76.23	16.62
	38	1.083	21.19	76.86	17.65
	47	1.085	20.78	74.71	16.84

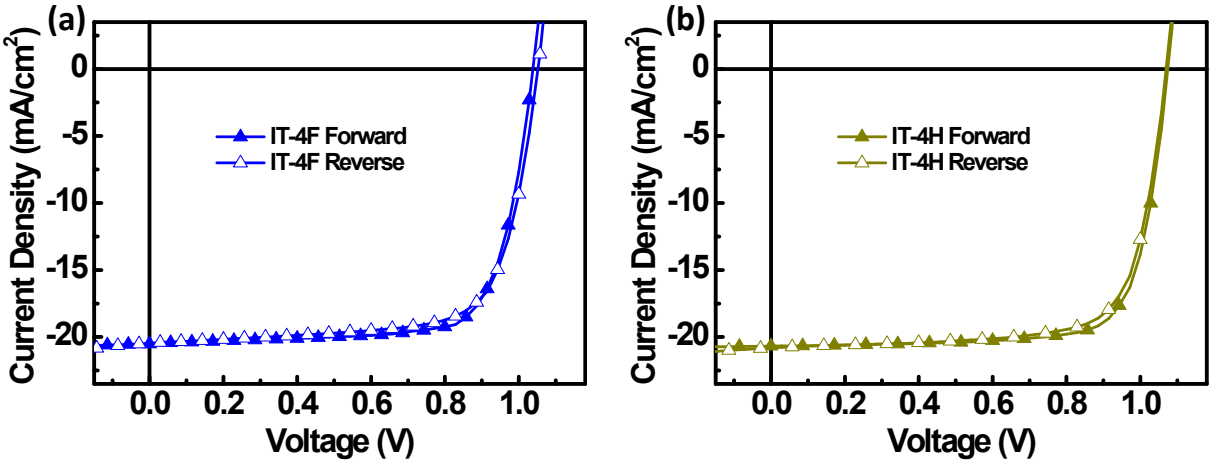

Fig. S4 *J-V* curves of PVSCs based on IT-4F and IT-4H ETLs measured under forward- and reverse-scan directions.

Table S2. Photovoltaic parameters of PVSCs with various ETLs measured under forward- and reverse-scan direction.

Interlayer	Scan direction	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)	R_S (Ω·cm^2)
w/o	Forward	1.022	11.71	38.82	4.64	43.34
	Reverse	1.021	10.70	27.63	3.02	45.10
PCBM	Forward	1.088	21.09	76.68	17.60	3.96
	Reverse	1.087	21.16	73.92	17.01	3.83
IT-4F	Forward	1.037	20.49	75.03	15.94	4.62
	Reverse	1.045	20.55	71.97	15.43	5.57
IT-4H	Forward	1.072	20.68	76.83	17.04	3.83
	Reverse	1.070	20.86	73.86	16.48	3.87
IT-4M	Forward	1.083	21.19	76.86	17.65	4.47
	Reverse	1.084	21.29	74.16	17.12	4.68

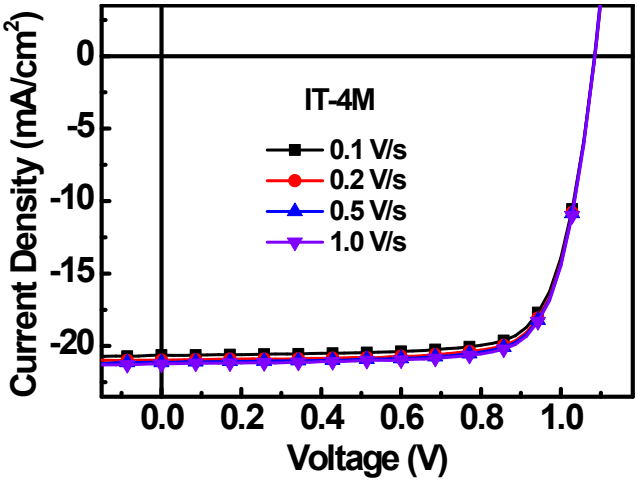

Fig. S5 *J-V* curves of inverted PVSCs using IT-4M ETL scanning at different scan speed from 0.1 to 1.0 V/s.

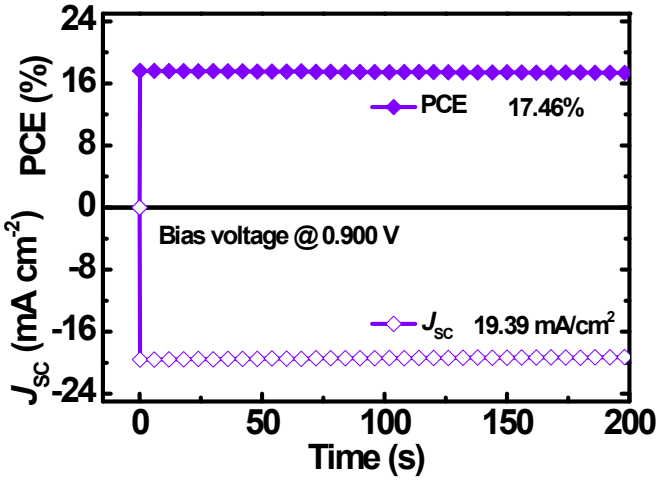

Fig. S6 Stabilized photocurrent density and PCE output of inverted PVSCs based on IT-4M ETL.

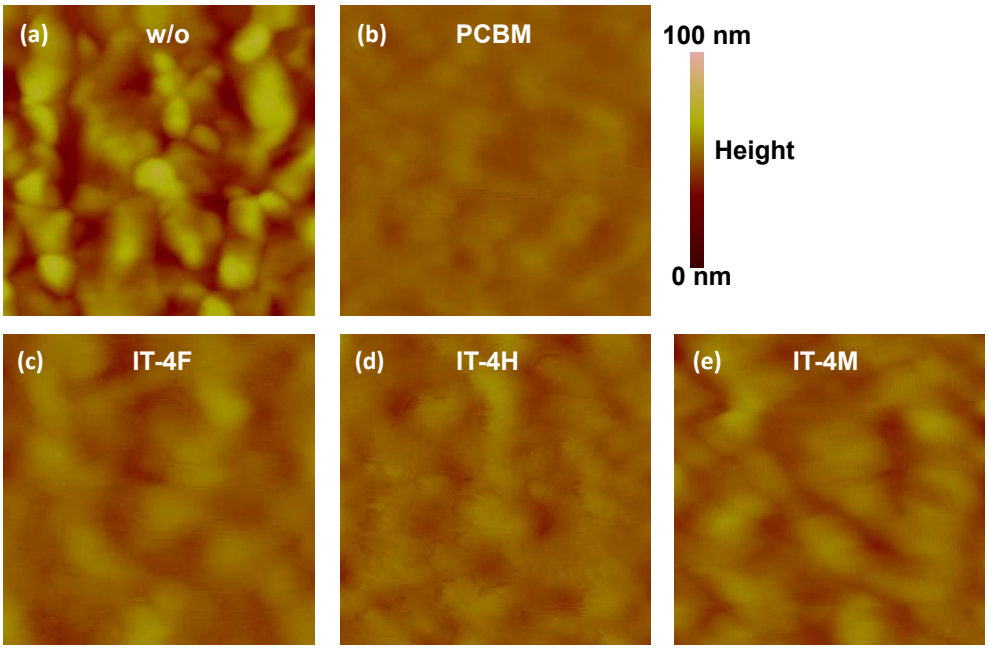

Fig. S7 AFM topography images (2 μm × 2 μm) of the perovskite films covered with different ETLs. (a) w/o, (b) PCBM, (c) IT-4F, (d) IT-4H, and (e) IT-4M.

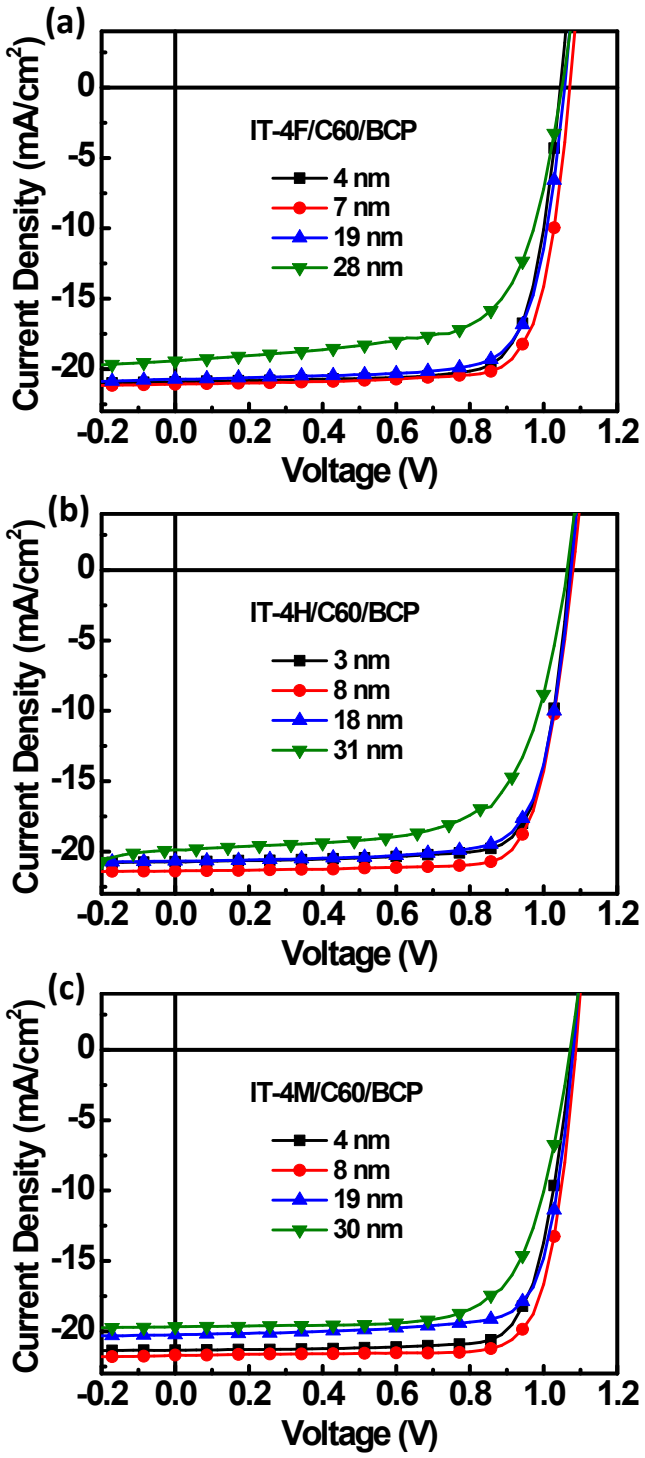

Fig. S8 *J-V* curves of PVSCs (ITO/P3CT-N/Perovskite/various interlayer/C60/BCP/Ag) based on various interlayers (IT-4F, IT-4H and IT-4M) in different thicknesses.

Table S3. Summary of the photovoltaic performances of PVSCs (ITO/P3CT-N/ Perovskite/various interlayer/C60/BCP/Ag) based on various interlayers (IT-4F, IT-4H and IT-4M) in different thicknesses.

Interlayer	Thickness (nm)	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)
IT-4F	4	1.043	20.91	77.77	16.97
	7	1.069	21.08	78.29	17.64
	19	1.055	20.74	76.28	16.69
	28	1.048	19.39	67.05	13.63
IT-4H	3	1.068	20.72	78.43	17.35
	8	1.079	21.37	78.89	18.19
	18	1.072	20.68	76.83	17.04
	31	1.064	19.99	67.17	14.28
IT-4M	4	1.076	21.34	78.14	17.95
	8	1.086	21.84	79.75	18.92
	19	1.079	20.24	77.76	16.98
	30	1.071	19.68	71.30	15.03

Table S4. Summary of the photovoltaic parameters of inverted PVSCs (ITO/P3CT-N/ Perovskite/various interlayer/C60/BCP/Ag) with different interlayers (w/o, PCBM, IT-4F, IT-4H and IT-4M).[a]

Device	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)	R_S (Ω·cm^2)
C60/BCP	1.036	20.63	76.29	16.31 (15.86±0.51)[a]	4.6
PCBM/C60/BCP	1.088	21.81	79.37	18.84 (18.35±0.44)	3.8
IT-4F/C60/BCP	1.069	21.08	78.29	17.64 (17.15±0.47)[a]	3.6
IT-4H/C60/BCP	1.079	21.37	78.89	18.19 (17.68±0.49)[a]	4.1
IT-4M/C60/BCP	1.086	21.84	79.75	18.92 (18.44±0.46)[a]	3.3

[a] The data in parentheses denote the average values based on 20 devices.