Exploiting the potential of 2-((5-(4-(diphenylamino)phenyl)thiophen-2-yl)methylene)malononitrile as an efficient donor molecule in evaporation-based organic solar cells

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Supporting information

Detail optical characterization

Refractive and extinction indexes *n* and *k* were collected by MM16 Muller-ellipsometer from Horriba Jobin-Yvon. The extracted indexed *k* of the 2-((5-(4-(diphenylamino)phenyl)thiophen-2-yl)methylene)malononitrile (DPTMM), C_{60} and DPTMM: C_{60} (60:40) have well matched with the absorption spectra respectively.

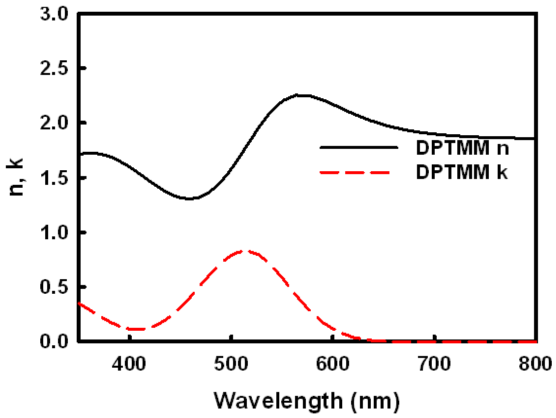

Figure S1: Refractive and extinction indexes n, k of DPTMM.

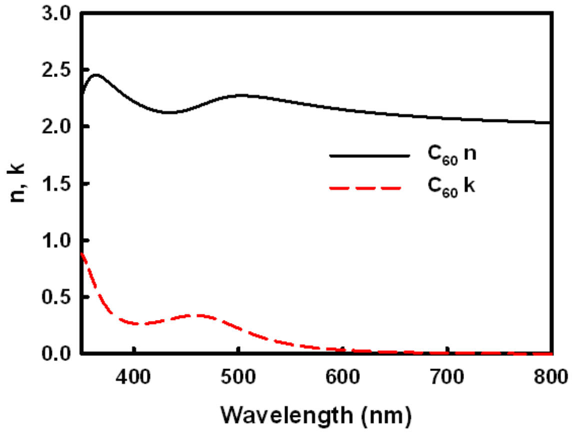

Figure S2: Refractive and extinction indexes n, k of C60.

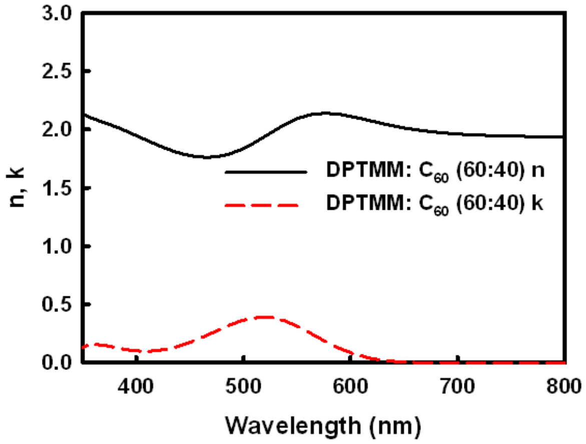

Figure S3: Refractive and extinction indexes n, k of DPTMM: C60 (60:40).

Detail device performance

The ratio of DPTMM donor material and C60 acceptor material in the active layer was changed in device D, E, and F. 4,4'-bis[N-(1-naphtyl)-N-phenylamino]biphenyl (α-NPB) layer was still introduced for all devices to prevent kink-shape at open circuit voltage (Voc). We were expected that the active layer should generate lesser amount of holes than that of electrons. In order to optimize the charge balance in the device, the DPTMM material percentage in the active layer has been decreased to reduce hole conduction path and increase electron conduction path. As a result, FF was improved from 55% to 65%. The improvement came from well-matched hole-electron balance. Power conversion efficiency (PCE) was also improved from 3.2% in the device D to 3.8% in the device F.

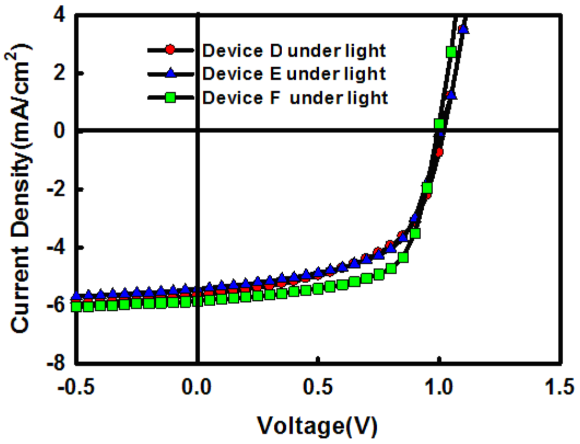

Figure S4: J-V characteristics for series of different mixed layer devices with α-NPB hole extraction layer,(ITO/ PEDOT: PSS (40 nm)/ α-NPB (5 nm)/ DPTMM (10 nm)/ DPTMM:C60 (mixed layer) (30 nm)/ C60 (30 nm)/ LiF (1.2 nm)/ Al (100 nm). J-V curves for mixed layer composition of 60 % DPTMM (circle), 55 % DPTMM (triangle) and 50 % DPTMM (square).

Device reproducibility

Reproducibility of the fabrication process was checked by using several substrates for each set of experiment. The devices show very good reproducibility.

Table 1 shows the reproducibility of the different devices.

Device	Efficiency	Open-circuit voltage (V)	Short-circuit current density (mA/cm²)	Fill Factor
A	3.0%	0.95	-6.3	50%
	3.2%	0.93	-6.7	52%
	3.2%	0.94	-5.8	55%
B	2.5%	0,94	-5,7	46%
	2.9%	0,95	-6,3	49%
C	1.7%	0.85	-3.8	53%
	2.0%	0.88	-4.0	56%
	2.0%	0.87	-4.1	56%
D	3.0%	1.05	-5.8	50%
	3.2%	1.02	-5.6	55%
	3.2%	1.00	-5.8	58%
E	3.0%	0,95	-6,3	50%
	3.2%	0,93	-6,7	52%
	3.2%	0,94	-5,8	55%
F	3.7%	1.03	-5.8	62%
	3.8%	1.00	-5.8	65%
	3.6%	0.97	-5.7	66%
G	3.9%	0.99	-6,2	63%
	4.0%	0.99	-6,3	64%
	3.9%	0.98	-6,2	65%

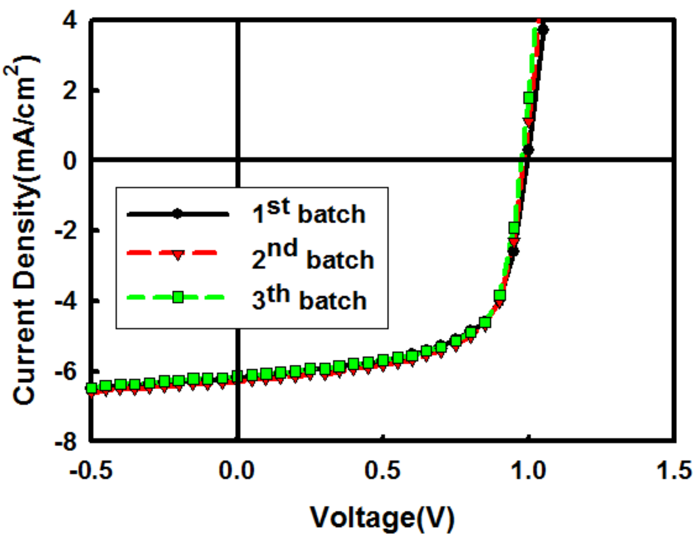

Figure S5: J-V characteristics for reproducibility test with Device G

Detail device performance

Figure S6 shows the profiles in donor and acceptor materials along the active layer in the device G. Each profile has been monitored with two separated quartz sensors during the co-evaporation of the donor and acceptor materials. One quartz sensor is located very close to the acceptor evaporation crucible and measures only C_{60} evaporation rate. The other sensor located close to the substrate measures both DPTMM and $C_{60.}$ After calibration of the quartz, the thickness and the composition of the film were calculated.

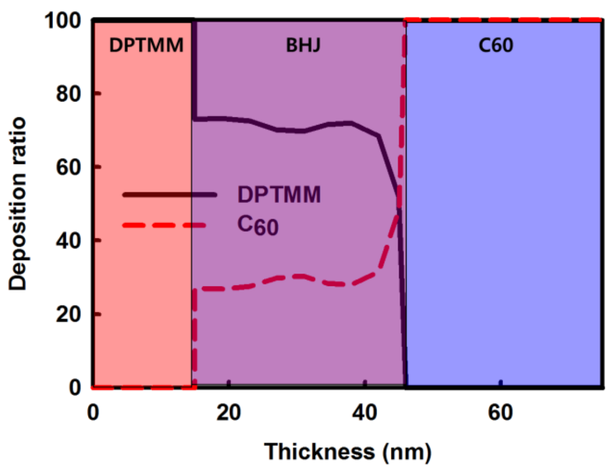

Figure S6: Donor/Acceptor Profiles of the active layer in the solar cell structure G.