Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information for

Isoindigo-Based Small Molecules for Solution-Processed Organic Photovoltaic Devices: Electron Donating Effect of Donor Group on Photo-Physical Properties and Device Performance

Walaa Elsawy[1,2,7], Chang-Lyoul Lee[3,*], Shinuk Cho[4], Seung-Hwan Oh[5], Seung-Hyeon Moon,[6] Ahmed Elbarbary [7]and Jae-Suk Lee[1,2,*]

[1]*Department of Nanobio Materials and Electronics and School of Material Science and Engineering,* [2]*Research Institute for Solar and Sustainable Energies (RISE),* [3]*Advanced Photonics Research Institute (APRI),* [6]*School of Environmental Science and Engineering, Gwangju Institute of Science and Technology (GIST), Gwangju 500-712, Republic of Korea*

[4]*Departments of Physics and EHSRC, University of Ulsan, Ulsan 680-749, Republic of Korea*

[5]*Radiation Research Division for Industry & Environment, Korea Atomic Energy Research Institute (KAERI), 580-185, Republic of Korea*

[7] *Department of Chemistry, Faculty of Science, Tanta University, Tanta 31527, Egypt*

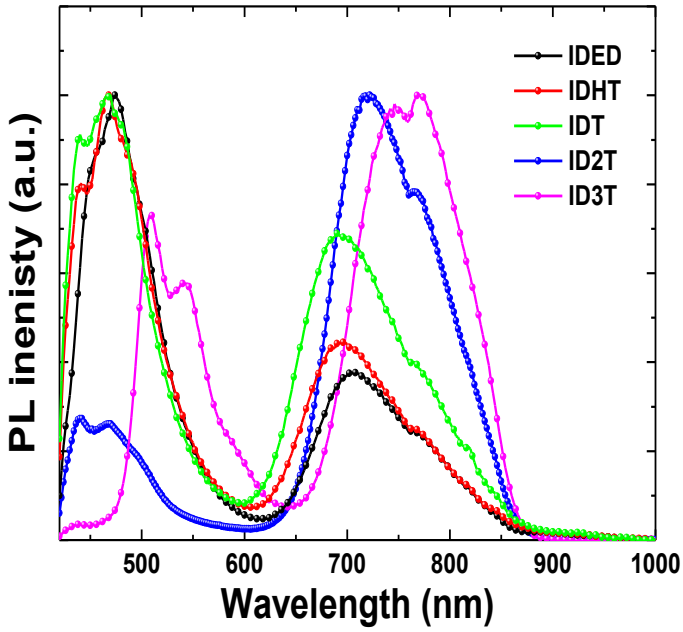


Fig. S1 PL spectra of isoindigo donor-acceptor-donor (D-A-D) small molecules in solution state. The chloroform was used as solvent. The solution concentration was 10^{-5} mol.

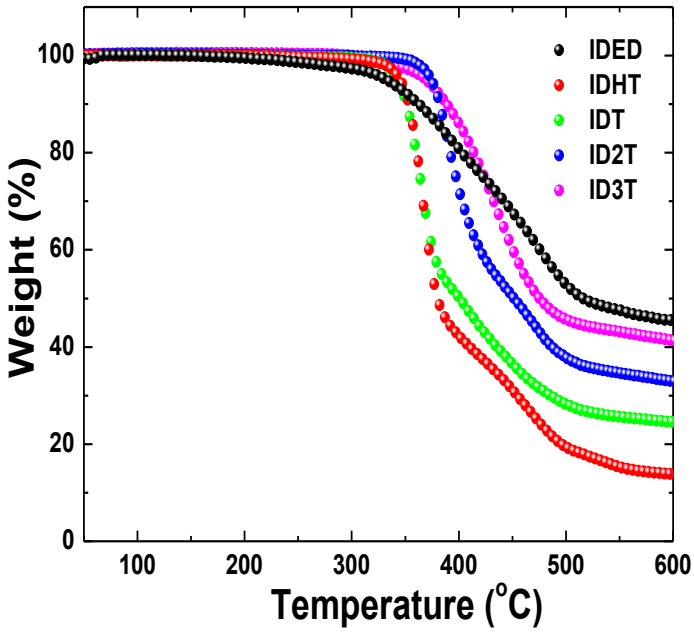


Fig. S2 Thermo Gravimetric Analysis (TGA) curves of isoindigo donor-acceptor-donor (D-A-D) small molecules.

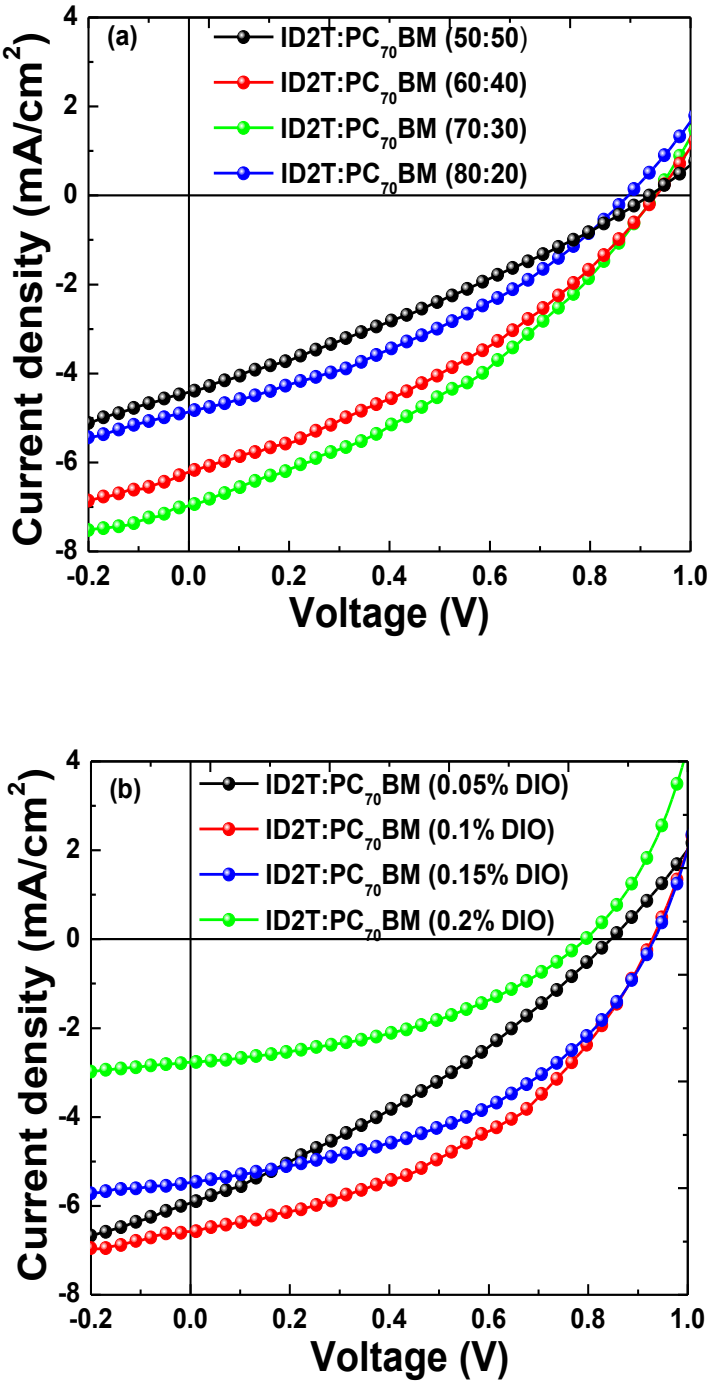


Fig. S3 (a) Current density versus voltage characteristics of ITO/PEDOT:PSS/ ID2T:$PC_{70}BM$/TiO_2/Al organic photovoltaic devices with different donor and acceptor ratio without DIO. (b) Current density versus voltage characteristics of ITO/PEDOT:PSS/ ID2T:$PC_{70}BM$(70:30)/TiO_2/Al organic photovoltaic devices with different DIO content.

Table S1 Photovoltaic performance of ITO/PEDOT:PSS/ID2T:$PC_{70}BM$/TiO_2/Al organic photovoltaic devices with different donor and acceptor ratio (without DIO) and DIO content. The ID2T and $PC_{70}BM$ ratio was fixed with 70:30 in photovoltaic devices with different DIO content.

Donor : acceptor ratio	J_{sc}**(mA/cm^2)**	V_{oc}**(V)**	**FF (%)**	**PCE (%)**
50:50	4.42	0.92	29.1	1.19
60:40	6.12	0.93	35.4	2.04
70:30	7.0	0.93	36.3	2.30
80:20	4.86	0.88	34.8	1.49
DIO content (%)				
0.05	5.93	0.85	31.7	1.59
0.1	6.58	0.93	42.8	2.60
0.15	5.48	0.93	44.6	2.26
0.2	2.77	0.80	40.9	0.90

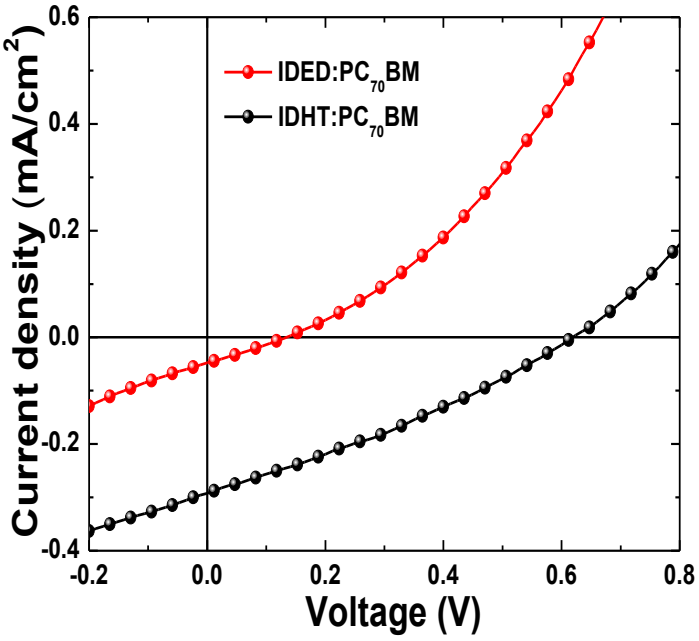
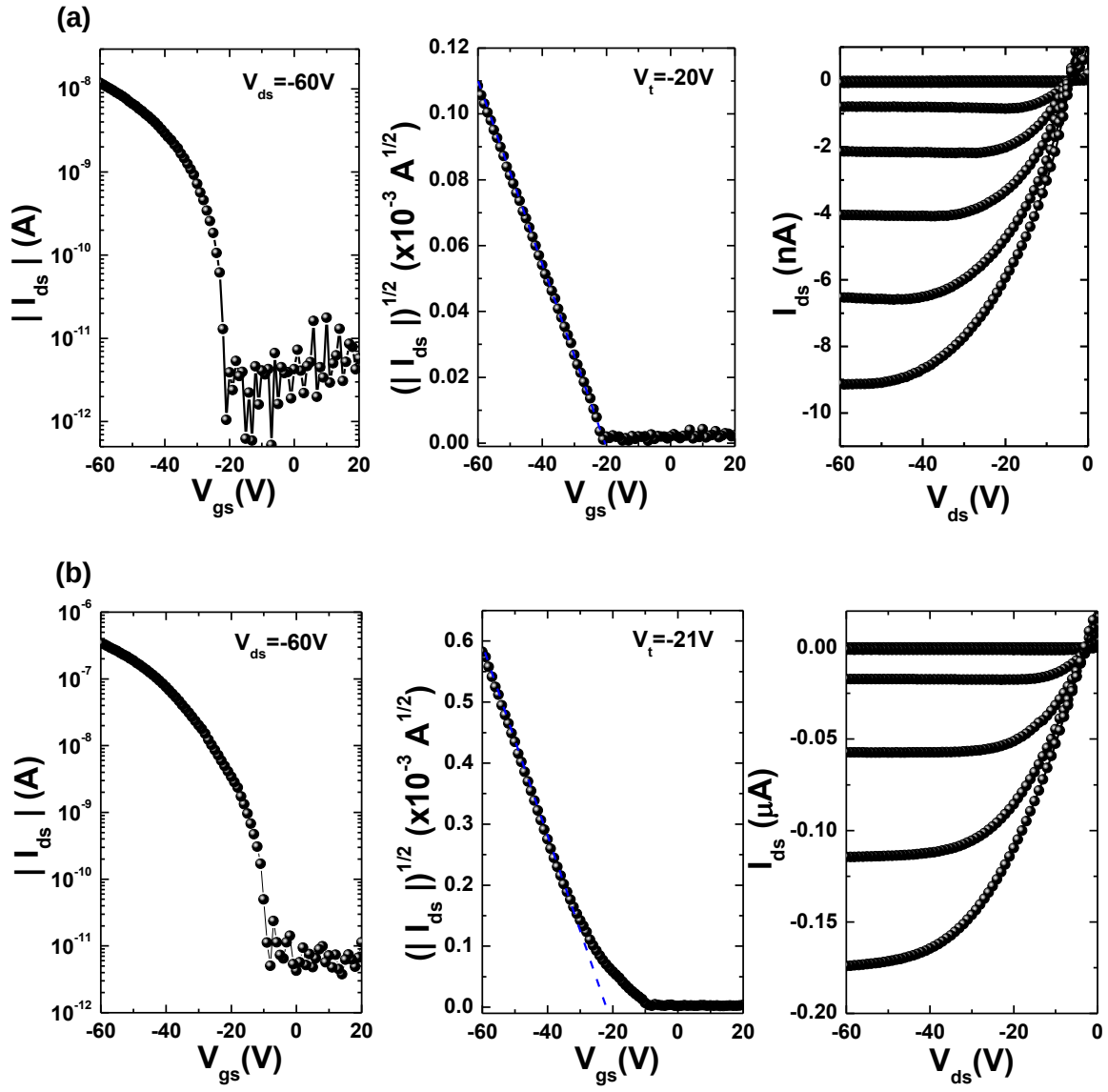


Fig. S4 (a) Current density versus voltage characteristics of ITO/PEDOT:PSS/IDHT:$PC_{70}BM$ (70:30)/TiO_2/Al and ITO/PEDOT:PSS/IDED:$PC_{70}BM$ (70:30)/TiO_2/Al organic photovoltaic devices with 0.1% DIO.

Fig. S5 Output and transfer characteristics of OTFTs based on the isoindigo donor-acceptor-donor (D-A-D) small molecules. (a) IDED, (b) IDHT, (c) IDT, (d) ID2T and (e) ID3T.



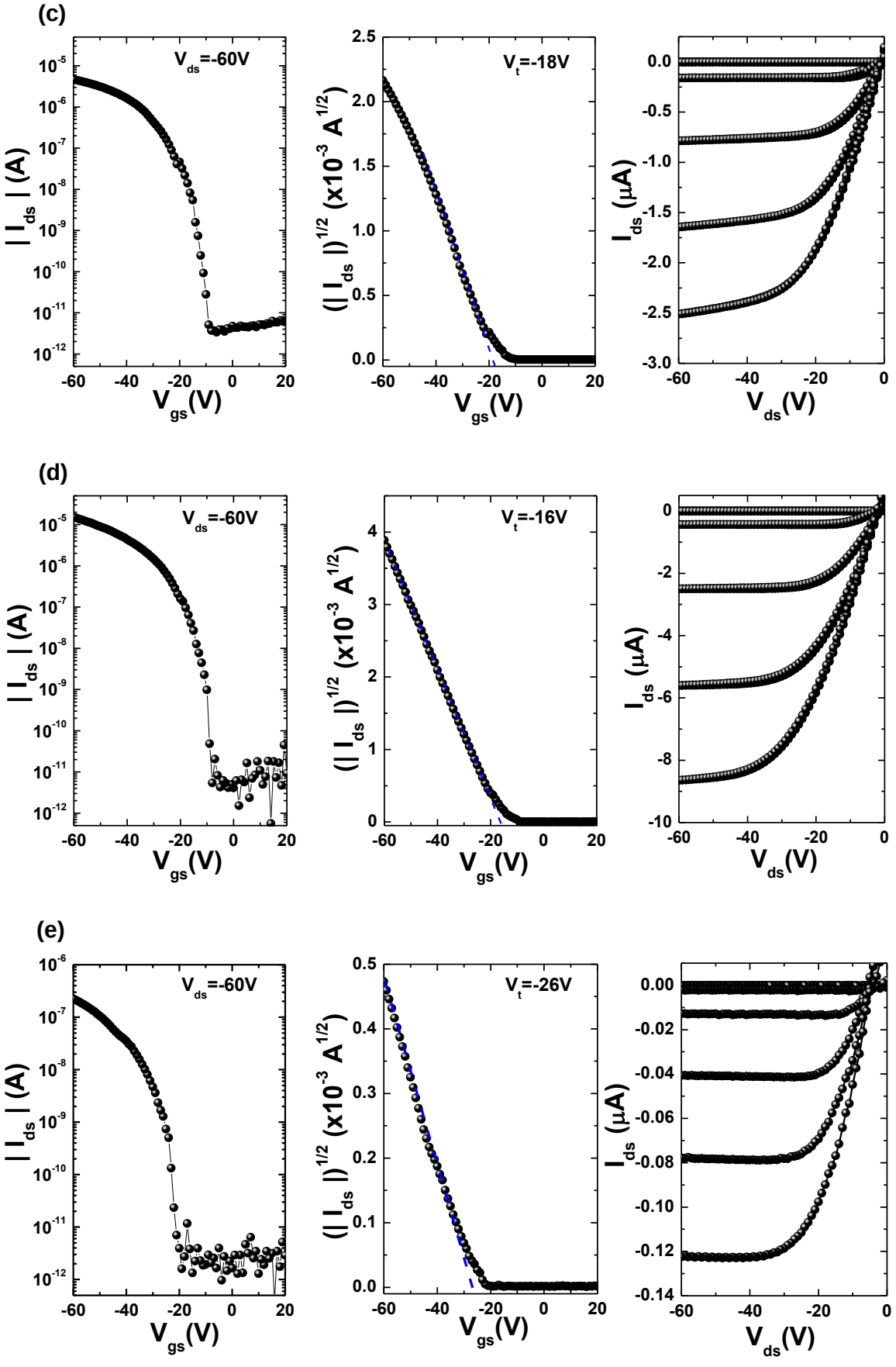

(c)
V_ds=-60V
| I_ds | (A)
V_gs(V)
V_t=-18V
(| I_ds |)^1/2 (x10^-3 A^1/2)
V_gs(V)
I_ds (μA)
V_ds(V)
(d)
V_ds=-60V
| I_ds | (A)
V_gs(V)
V_t=-16V
(| I_ds |)^1/2 (x10^-3 A^1/2)
V_gs(V)
I_ds (μA)
V_ds(V)
(e)
V_ds=-60V
| I_ds | (A)
V_gs(V)
V_t=-26V
(| I_ds |)^1/2 (x10^-3 A^1/2)
V_gs(V)
I_ds (μA)
V_ds(V)

Table S2 Field-effect charge transport properties of isoindigo donor-acceptor-donor (D-A-D) small molecules. V_{ds} is -60V.

Active layer	μ_h**(cm^2/(V·s))**	I_{on}/I_{off}	V_t **(V)**
IDED	3.2×10^{-5}	4.5×10^{3}	-20
IDHT	1.1×10^{-3}	5.7×10^{4}	-21
IDT	1.4×10^{-2}	1.3×10^{6}	-18
ID2T	3.6×10^{-2}	3.4×10^{6}	-16
ID3T	9.7×10^{-4}	1.0×10^{5}	-26

Fig. S6 Transfer curves of OTFTs based on the isoindigo donor-acceptor-donor (D-A-D) small molecules:$PC_{70}BM$ (70:30) film. (a) IDT (b) IDHT and IDED.

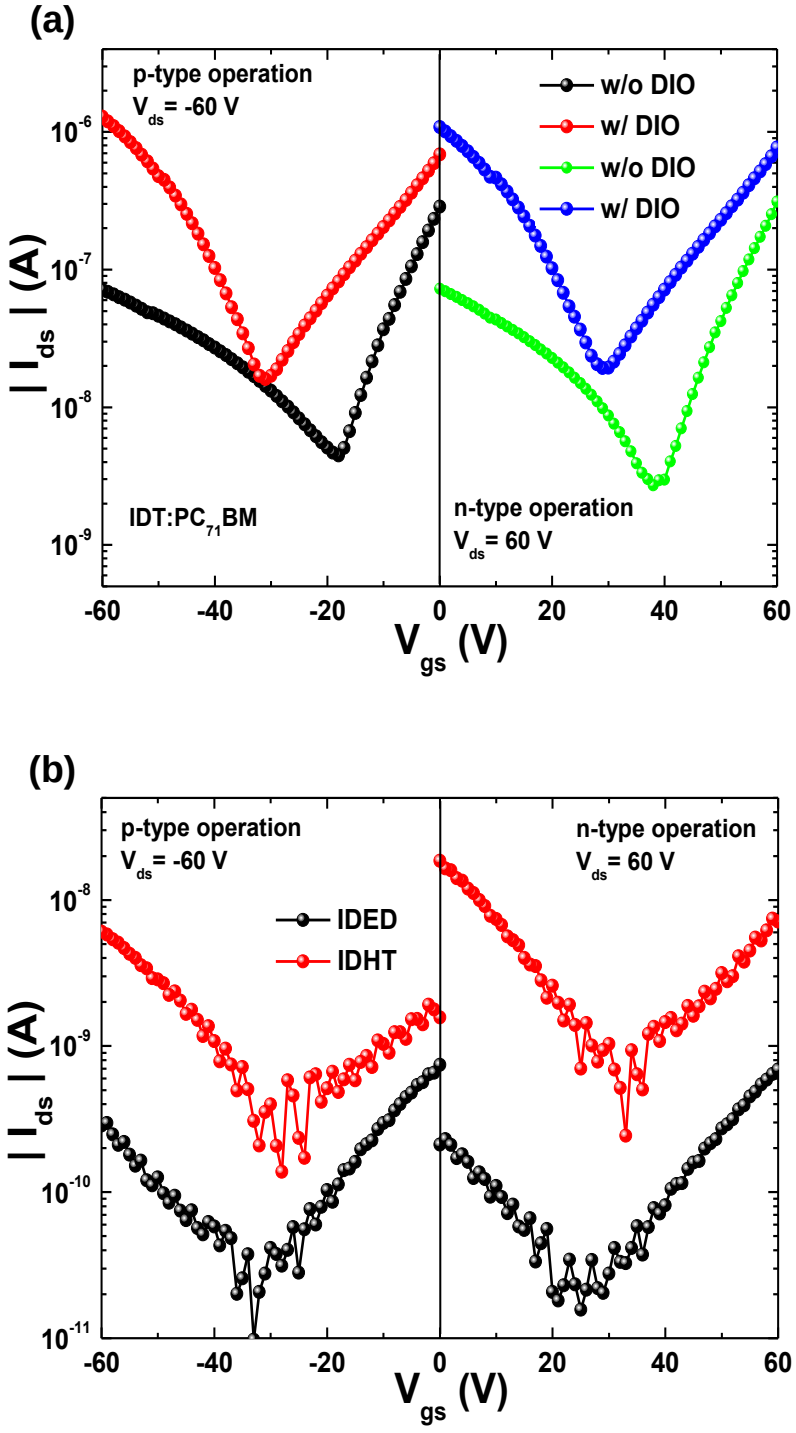


Table S3 Field-effect charge transport properties of isoindigo donor-acceptor-donor (D-A-D) small molecules:$PC_{70}BM$ (70:30). V_{ds} is ±60V.

Active layer	μ_e**(cm^2/(V·s))**[a]	μ_h**(cm^2/(V·s))**[a]	μ_e**(cm^2/(V·s))**[b]	μ_h**(cm^2/(V·s))**[b]
IDED:$PC_{70}BM$	4.62×10^{-5}	2.09×10^{-5}	N/A[c]	N/A[c]
IDHT:$PC_{70}BM$	5.19×10^{-5}	2.96×10^{-5}	N/A[c]	N/A[c]
IDT:$PC_{70}BM$	6.15×10^{-3}	1.37×10^{-4}	7.80×10^{-3}	8.76×10^{-3}

[a]Electron and hole mobility of photo-active layer without DIO, [b]Electron and hole mobility of active photo-layer with 0.1% DIO, [c]Not available, there was no additive effect on the IDED:$PC_{70}BM$ and IDHT:$PC_{70}BM$ films.

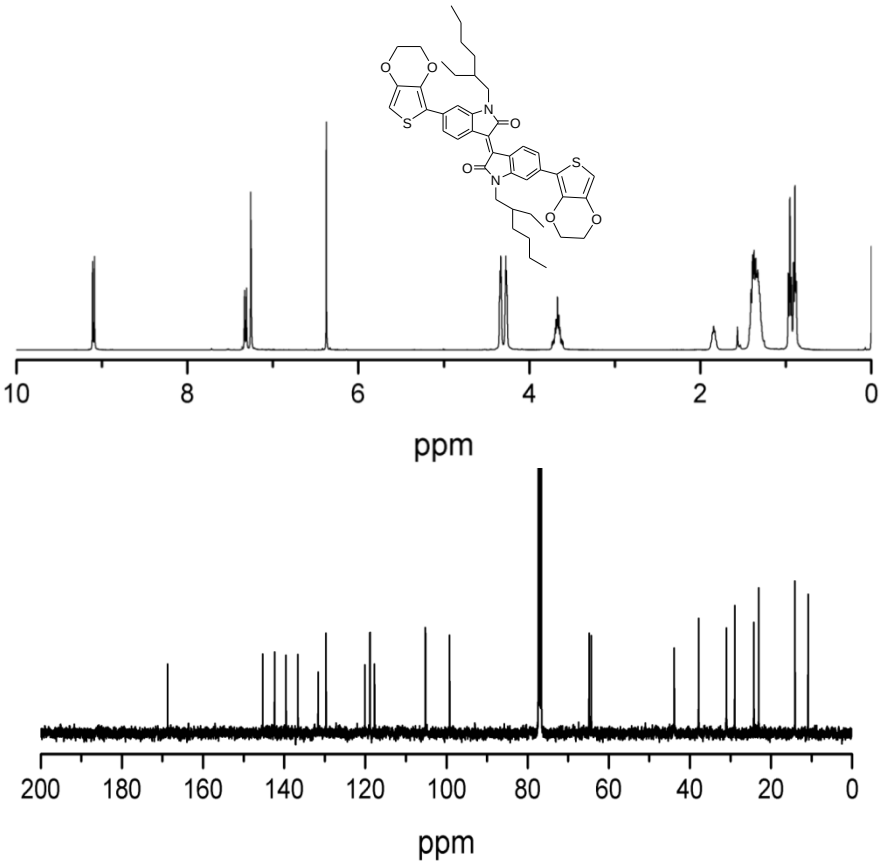


Fig. S7 ^{1}H and ^{13}C NMR spectrum of 6, 6'-dihydrothieno[3,4-b][1,4]dioxin-2-yl-N,N'-(2-ethylhexyl)-isoindigo (IDED) in $CDCl_3$.

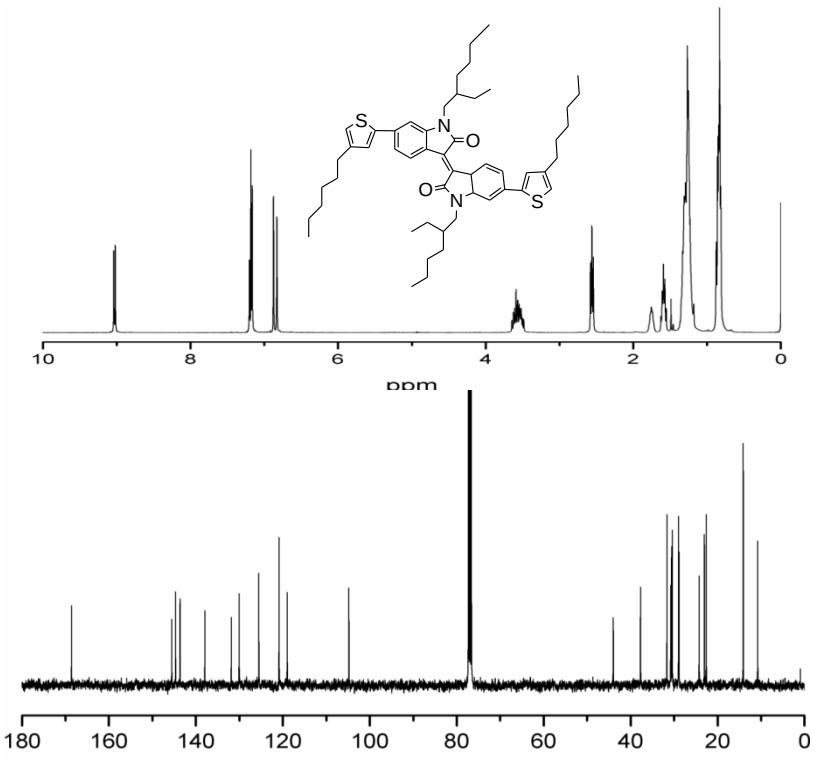


Fig. S8 ^{1}H and ^{13}C NMR spectrum of 6,6'-dihexylthiophen-2-yl-N,N'-(2-ethylhexyl)-isoindigo (IDHT) in $CDCl_3$.

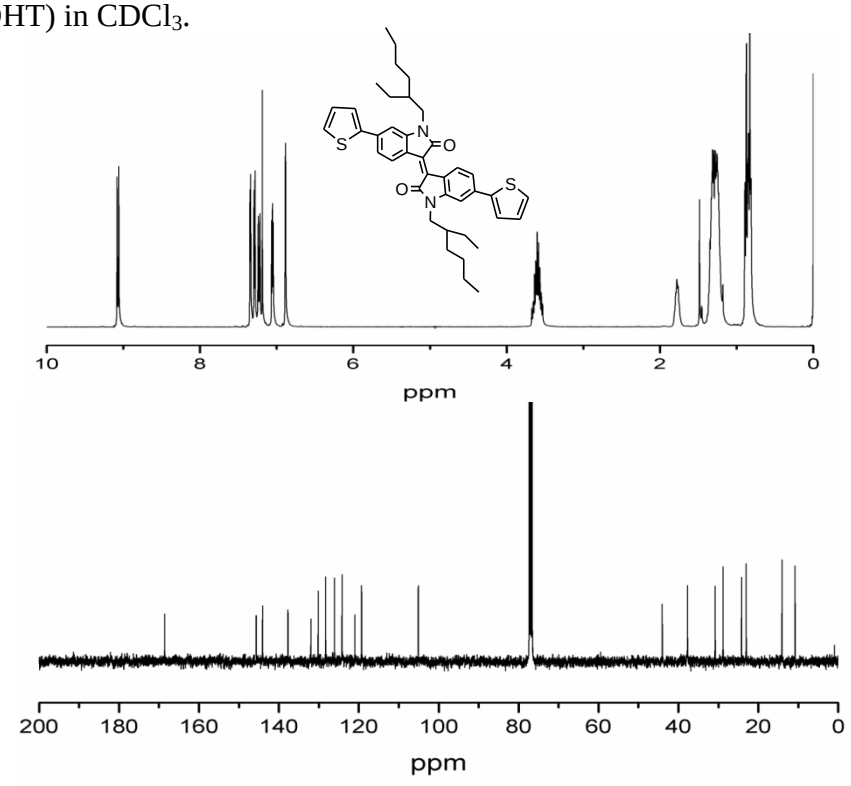


Fig. S9 ^{1}H and ^{13}C NMR of spectrum of 6, 6'-thiophen-2-yl-N,N'-(2-ethylhexyl)-isoindigo (IDT) in $CDCl_3$.

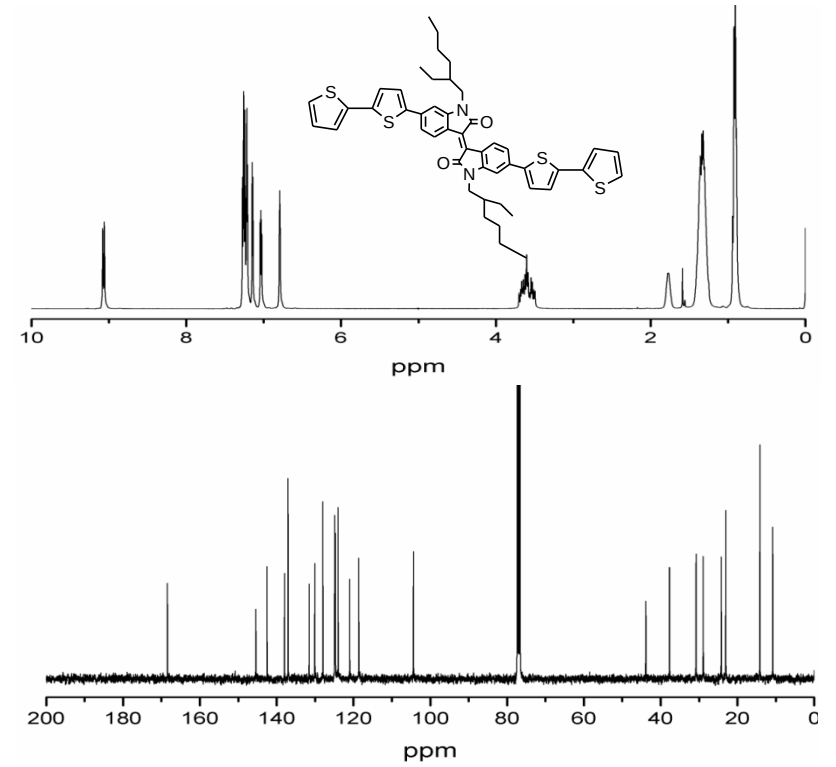


Fig. S10 ^{1}H and ^{13}C NMR spectrum of 6, 6'-bithiophen-2-yl-N,N'-(2-ethylhexyl)-isoindigo (ID2T) in $CDCl_3$.

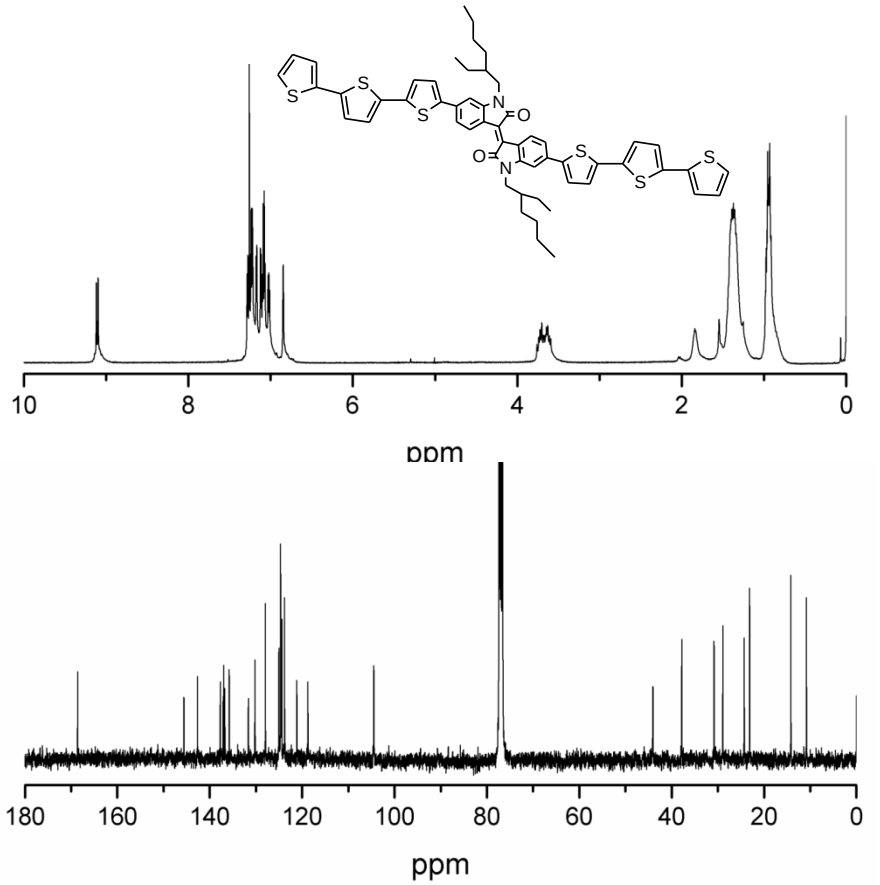


Fig. S11 ^{1}H and ^{13}C NMR spectrum of 6, 6'-terthiophen-2-yl-N,N'-(2-ethylhexyl)-isoindigo (ID3T) in $CDCl_3$.