Electronic Supplementary Information (ESI)

A Perylene Diimide Dimer-Based Electron Transporting Material with A-D-A Type for Efficient Inverted Perovskite Solar Cell

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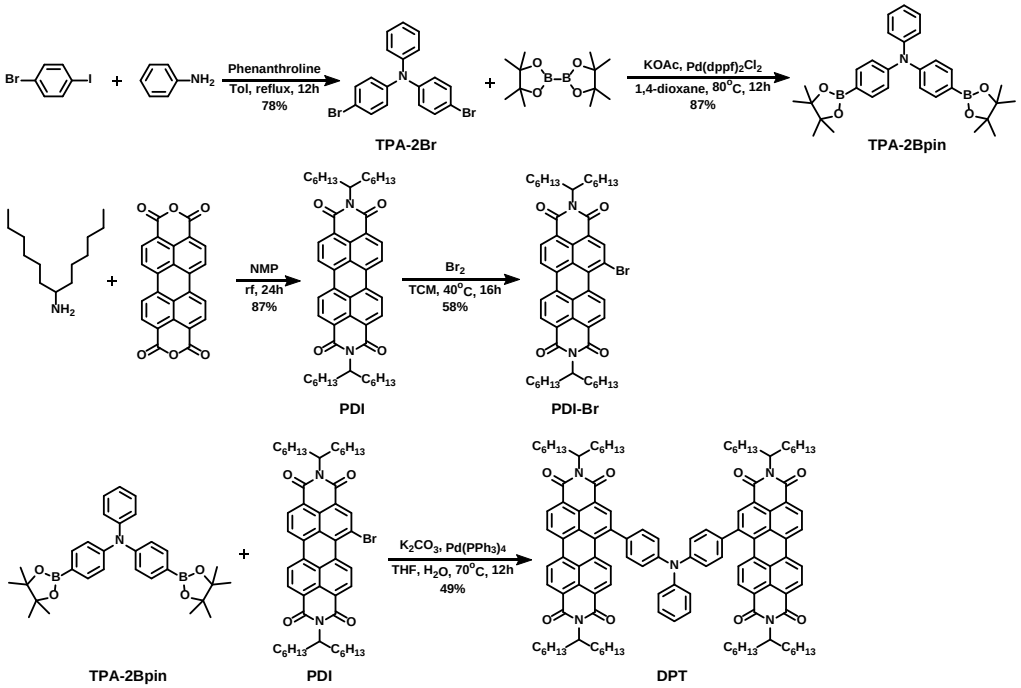

Scheme S1 Synthetic routes of target molecule DPT

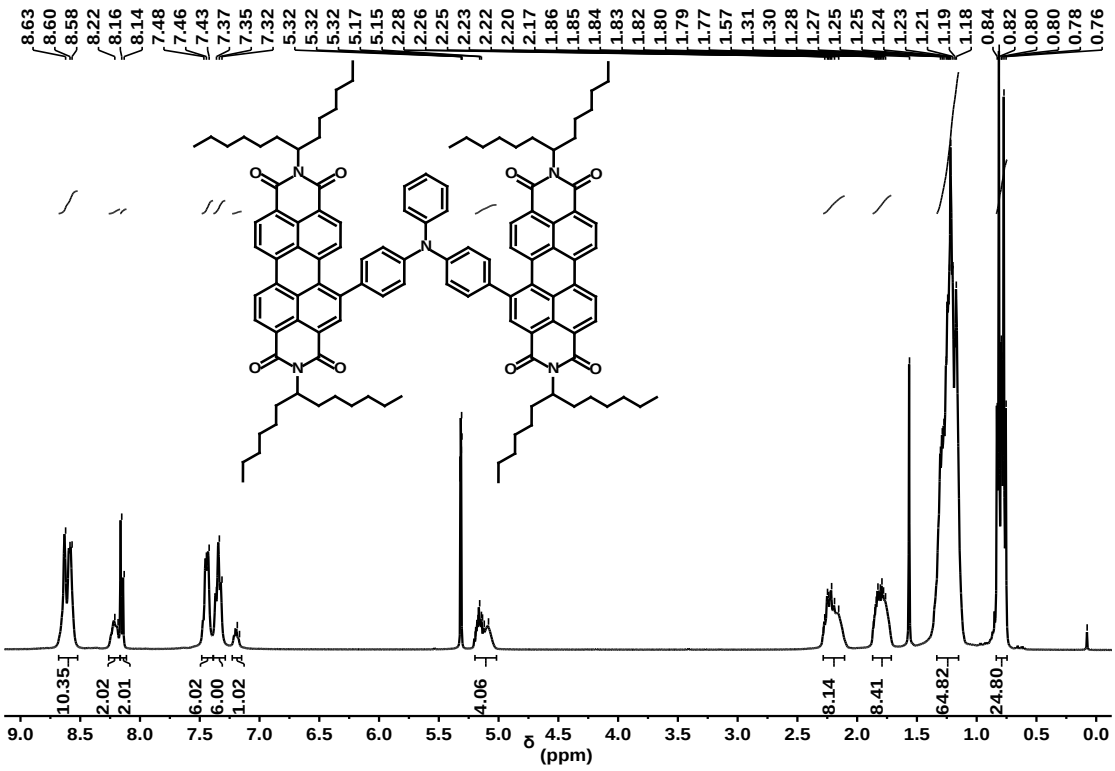

Figure S1 ^{1}H NMR spectrum of DPT with dichloromethane-d_2 as solvent

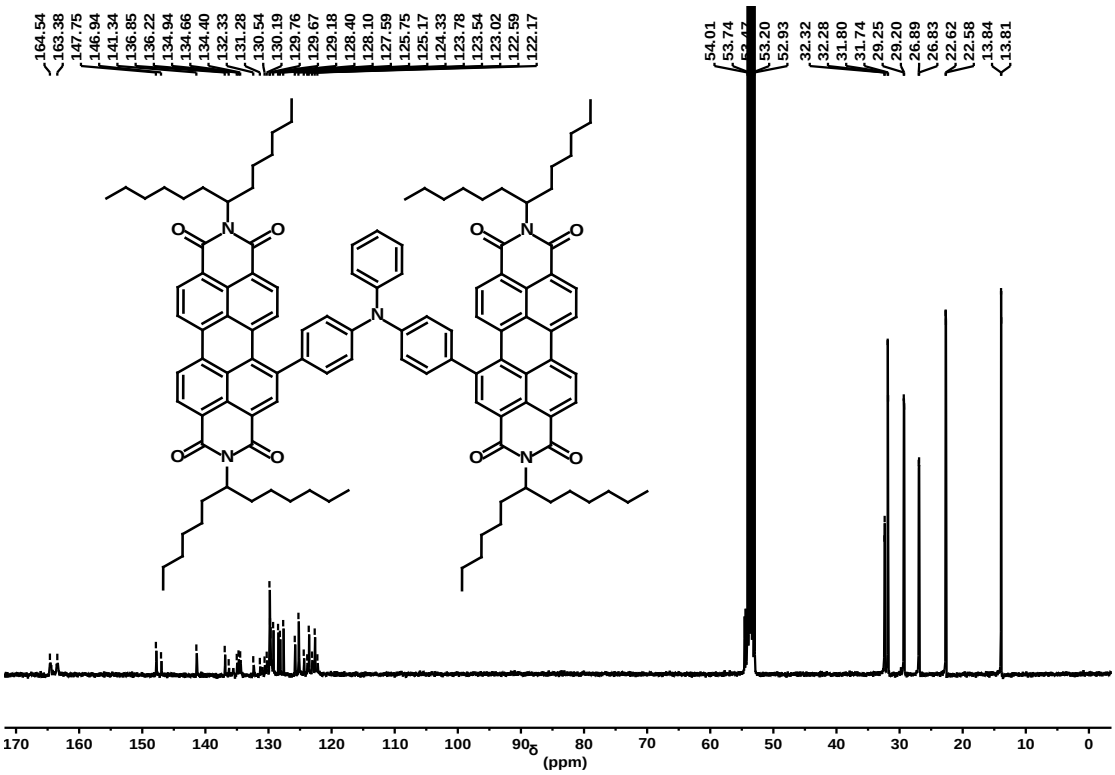

Figure S2 ^{13}C NMR spectrum of DPT with dichloromethane-d_2 as solvent

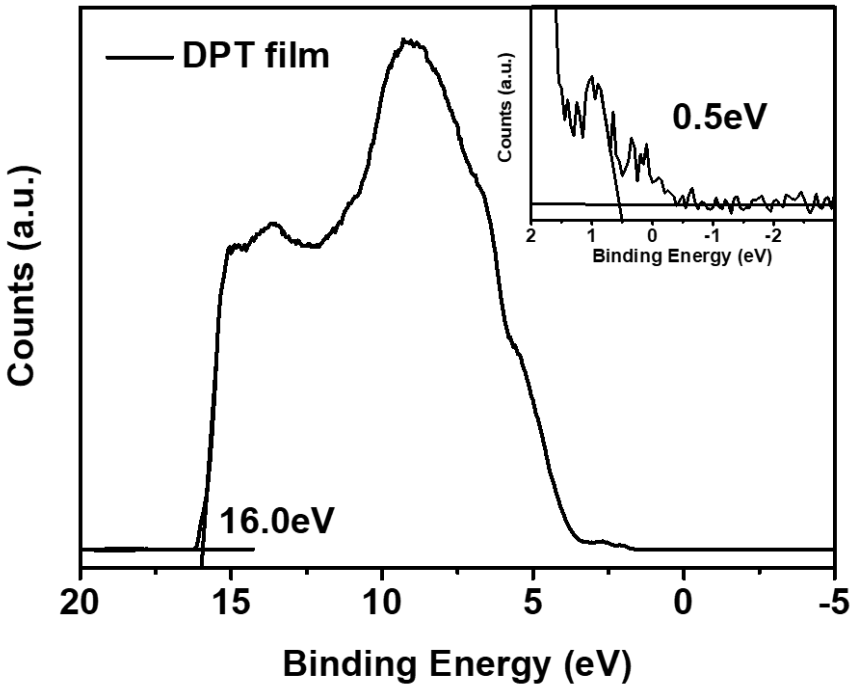

Fig S3 UPS spectrum of DPT film. HOMO energy level is calculated according to the following equation: HOMO (*vs.* vacuum conditions) = - (E_{photon} - width of UPS spectra), where E_{photon} denotes the excitation energy of He I (21.22 eV)

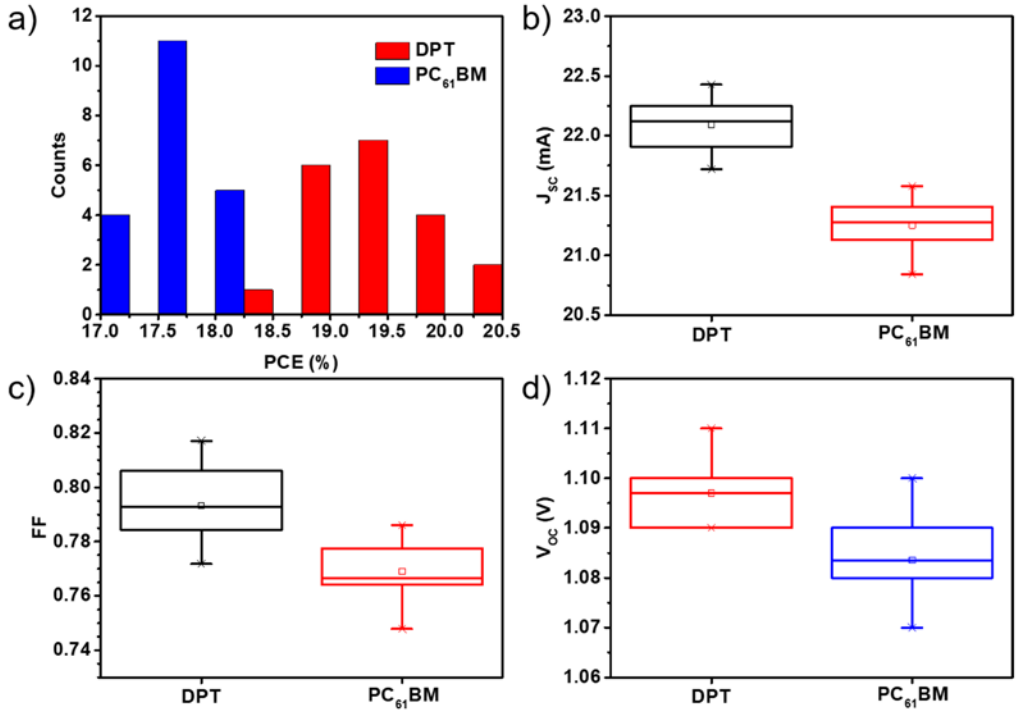

Fig. S4 a) The PCE distributions of perovskite solar cells with $PC_{61}BM$ and DPT as ETMs. b-d) The corresponding photovoltaic parameters statistic

Table S1. Photovoltaic parameters of inverted PSCs

Sample	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)
DPT	1.10 (1.10±0.01)	22.33 (22.09±0.21)	81.7 (79.3±1.4)	20.07 (19.23±0.52)
$PC_{61}BM$	1.09 (1.08±0.01)	21.45 (21.25±0.19)	78.6 (76.9±1.1)	18.38 (17.71±0.36)

The data in parentheses are the average values based on 20 devices.

Table S2 Summary of photovoltaic parameters of PSCs based on DPT with different concentrations and corresponding thickness

Sample	Thickness (nm)	V_{OC} (V)	J_{SC} (mA/cm^2)	*FF* (%)	PCE (%)
DPT (8 mg/mL)	28.7	1.03	20.75	72.0	15.38
DPT (10 mg/mL)	35.1	1.09	21.97	77.1	18.47
DPT (12 mg/mL)	44.6	1.10	22.33	81.7	20.07
DPT (15 mg/mL)	53.2	1.10	22.21	80.0	19.54

Table S3 Photovoltaic parameters of PSCs based on PDI derivative as ETMs

ETL	Electron mobility (cm^2 V^{-1} s^{-1})	Fabrication	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)	Published year	Ref
SFX-PDI4	1.80×10^{-4}	Inverted	1.08	19.9	71.4	15.3	2017	[1]
hPDI2-Pyr-hPDI2	——	Inverted	0.93	21.17	79	14.9	2017	[2]
hPDI3-Pyr-hPDI3	——	Inverted	0.93	22.68	78	15.9	2017	[2]
TPE-PDI4	1×10^{-3}	Inverted	1.01	21.68	74	16.29	2018	[3]
PDI-C_{60}	8.76×10^{-4}	Inverted	1.06	22.1	79.2	18.6	2019	[4]
TCl-PDI	2.75×10^{-5}	Conventional	1.07	17.86	76.77	14.73	2019	[5]
Tr-PDI_3	1.21×10^{-3}	Inverted	1.03	21.47	79	17.45	2019	[6]
Tr-PDI_3-C	1.00×10^{-3}		1.05	20.92	77	16.9	2019	[6]
Bis-PDI-T-EG	——	Inverted	0.96	20.84	74.45	14.96	2020	[7]

ClPDI-C4	1.3×10^{-3}	Inverted	0.98	23.6	75	17.3	2020	[8]
ClPDI-C8	2.1×10^{-4}	Inverted	1.00	23.4	70	16.4	2020	[8]
ClPDI-EH	1.5×10^{-4}	Inverted	0.96	23.0	71	15.7	2020	[8]
PDI-Ph	1.69×10^{-1}	Inverted	0.91	21.7	67.7	15.0	2020	[9]
PDI-PhCN	2.12×10^{-1}	Inverted	1.02	22.4	73.4	18.8	2020	[9]
PDI-PhCN-2Br	1.19×10^{-1}	Inverted	0.88	21.9	70.2	16.0	2020	[9]
PDI-PhCN-4Br	3.88×10^{-3}	Inverted	0.92	20.6	49.6	10.8	2020	[9]
PDO-PDI2	9.60×10^{-4}	Inverted	1.02	21.85	72.79	16.22	2021	[10]
PDO-PDI3	9.37×10^{-4}	Inverted	1.10	22.64	75.19	18.72	2021	[10]
PDI-LP	——	Conventional	1.08	22.57	72.81	17.83	2021	[11]
PDI-LAS	——	Conventional	1.11	22.88	73.98	18.77	2021	[11]
DPT	8.23×10^{-4}	Inverted	1.10	22.33	81.7	20.07	This work	

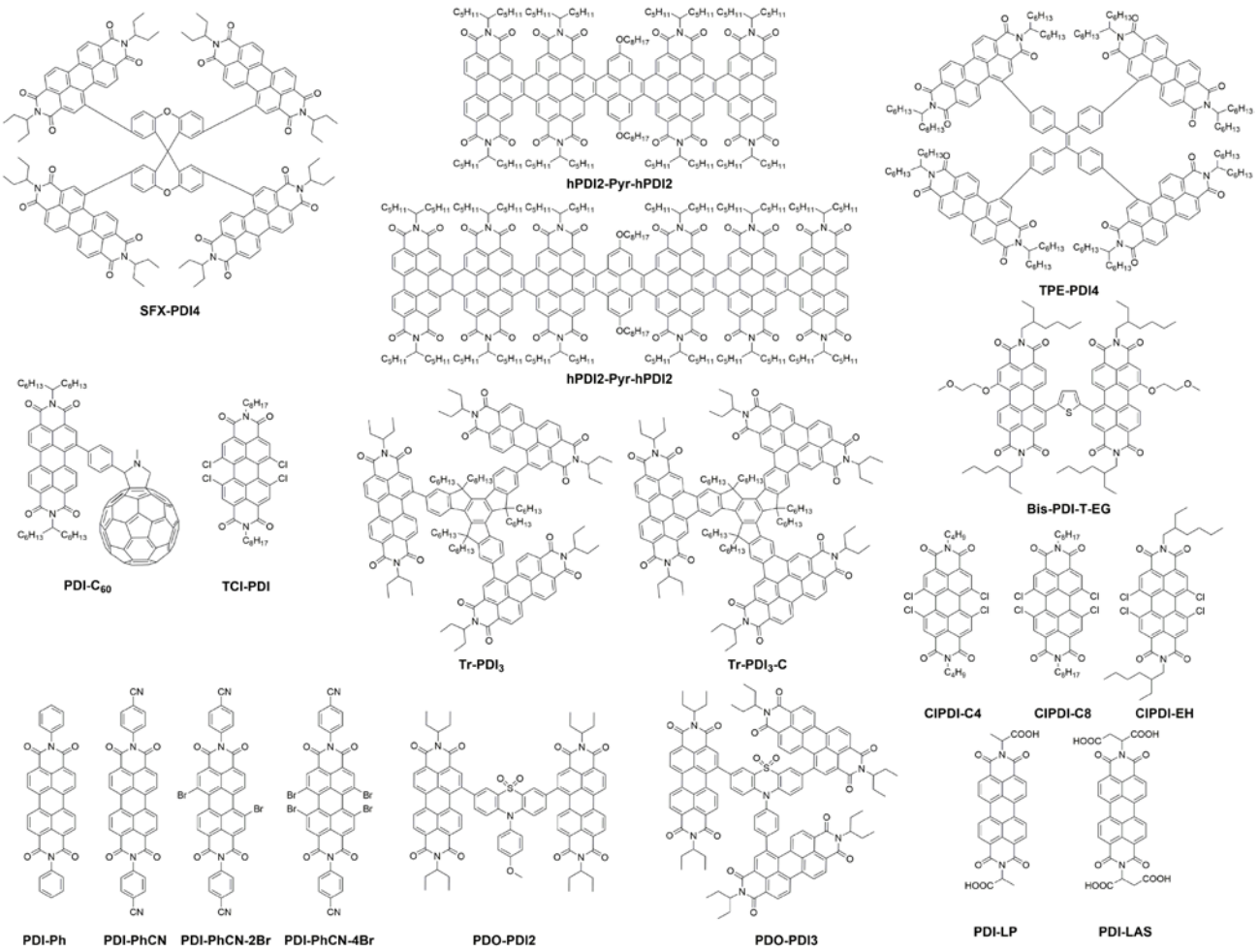

Fig S5 Molecular structures of PDI derivatives as ETMs in PSCs

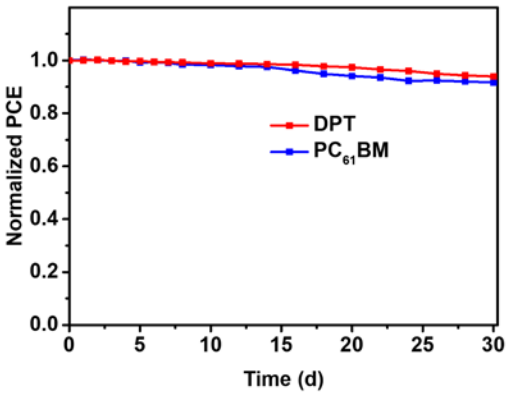

Fig S6 Storage stability of devices under an atmosphere of nitrogen with DPT or $PC_{61}BM$ as the electron transporting material

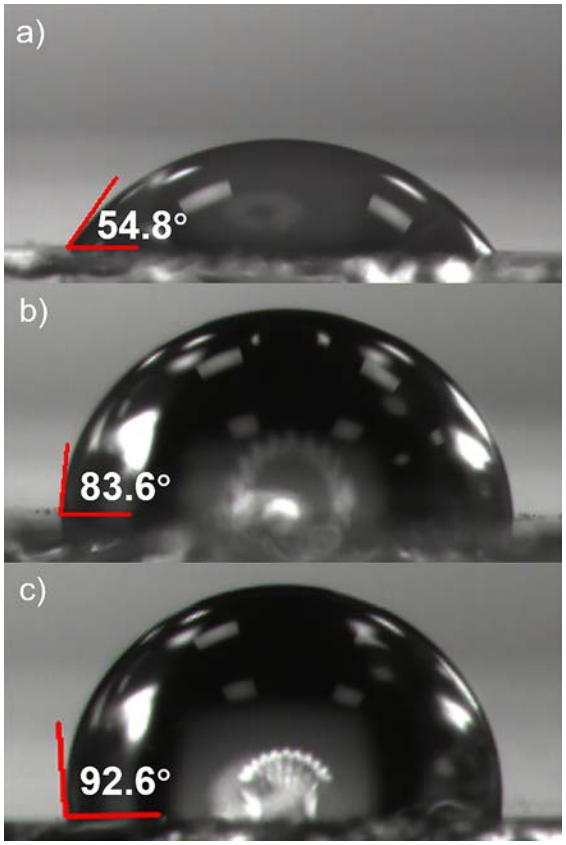

Fig S7 Water contact angles of (a) perovskite film, (b) $PC_{61}BM$ covered perovskite film, and (c) DPT covered perovskite film, respectively

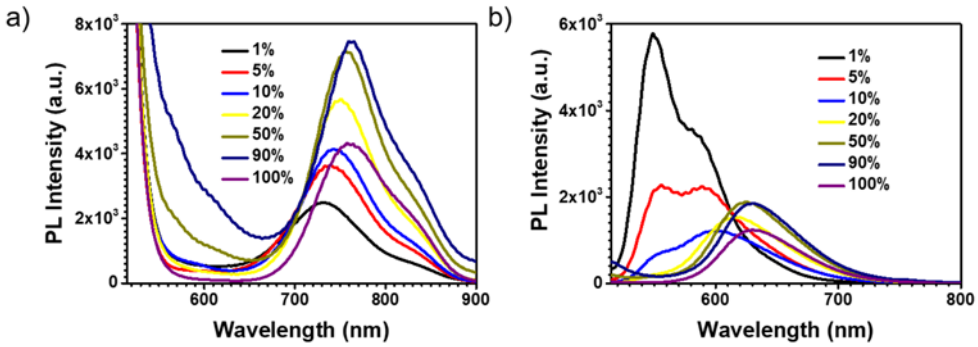

Fig S8 Photoluminescence of PMMA film doped with a) DPT or b) PDI with different mass fraction.

References

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