Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

"Like-Likes-Like" strategy for the design of electron transport materials and emitters with facilitated interlayer electron transport and improved efficiency

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1. The equation of Lippert-Matage

$$v_f = \frac{2\mu_e(\mu_e - \mu_g)}{4\pi\varepsilon_0 hca^3}\Delta f + C \qquad (1)$$

$$\Delta f = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{0.5(n^2 - 1)}{2n^2 + 1} \qquad (2)$$

$$a = \left(\frac{3M}{4N\pi d}\right)^{\frac{1}{3}} \qquad (3)$$

where μ_g is the ground-state dipole moment, *a* is the solvent cavity (Onsager) radius, which was derived from Avogadro's number (N), molecular weight (M), and density (d = 1), and ε, ε_0, and n are the solvent dielectric constant, vacuum permittivity, and solvent refractive index, respectively.

2. Electron-only device study

Electron-only devices were fabricated for the studies of electron mobility by using space charge limited current (SCLC) method. The device structure is ITO/Al (100 nm)/PTB7:$PC_{71}BM$ (100 nm)/Ca (20 nm) /Al and ITO/ Al/PTB7:PC71BM (100 nm)/ MSAPBS (x nm) /Al.

The SCLC is described by modified Mott-Gurney's law[3]:

$J=(9/8)\varepsilon_0\varepsilon_r\mu(V^2/d^3)exp[0.89\beta(V/d)^{0.5}]$

We can get the following formula:

$ln(Jd^3/V^2)\approx 0.89\beta(V/d)^{0.5}+ln(9\varepsilon_0\varepsilon_r\mu/8)$

The results are plotted as $ln(Jd^3/V^2)$ versus $(V/d)^{0.5}$, as shown in Figure S8. *J* stands for current density, *d* is the thickness of the active layer, V is the applied potential, ε_r is the relative dielectric constant of the blend (assuming that 3.5), ε_0 is the permittivity of free space (8.85×10^{-12} C V^{-1} s^{-1}), β is the field activation factor and m the electron mobility.

3. hotophysical Equation

The rate constants were determined using the following basic photophysical functions

$$\phi_{PF} = \phi_{PL}\ R_{prompt} \qquad \text{(S1)}$$

$$\phi_{DF} = \phi_{PL}\, \mathrm{R}_{delayed} \qquad \text{(S2)}$$

$$\mathrm{k}_r^s = \phi_{PF} / \tau_{PF} \qquad \text{(S3)}$$

$$\phi_{PL} = k_r^s / (k_r^s + k_{nr}^s) \qquad \text{(S4)}$$

$$\phi_{PF} = k_r^s / (k_r^s + k_{nr}^s + k_{ISC}) \qquad \text{(S5)}$$

$$\phi_{ISC} = k_{ISC} / (k_r^s + k_{nr}^s + k_{ISC}) \qquad \text{(S6)}$$

$$\phi_{hRISC} = \phi_{DF} / \phi_{ISC} \qquad \text{(S7)}$$

$$k_{hISC} = \phi_{hRISC}\,(k_{hRISC} + k_{IC}^{Tn}) \qquad \text{(S8)}$$

$$k_{PF} = 1/\tau_{PF} \qquad \text{(S9)}$$

$$k_{DF} = 1/\tau_{DF} \qquad \text{(S10)}$$

here ϕ_{PL} is the photoluminescence quantum yield (PLQY). ϕ_{PF} and ϕ_{DF} are the prompt and delayed fluorescence efficiencies, respectively. ϕ_{ISC} and ϕ_{hRISC} are the ISC and hRISC efficiencies, respectively. τ_{PF} and τ_{DF} are the prompt and delayed fluorescent lifetimes, respectively. k_r^s, k_{nr}^s, k_{ISC} , k_{hRISC} , k_{IC}^{Tn}, k_{PF} and k_{DF} are the rates of singlet radiation, singlet non-radiation, ISC, hRISC, IC from T_n to T1, prompt fluorescence and decay fluorescence processes, respectively. R_{prompt} and $R_{delayed}$ are the component ratios of prompt and delayed fluorescence, respectively.

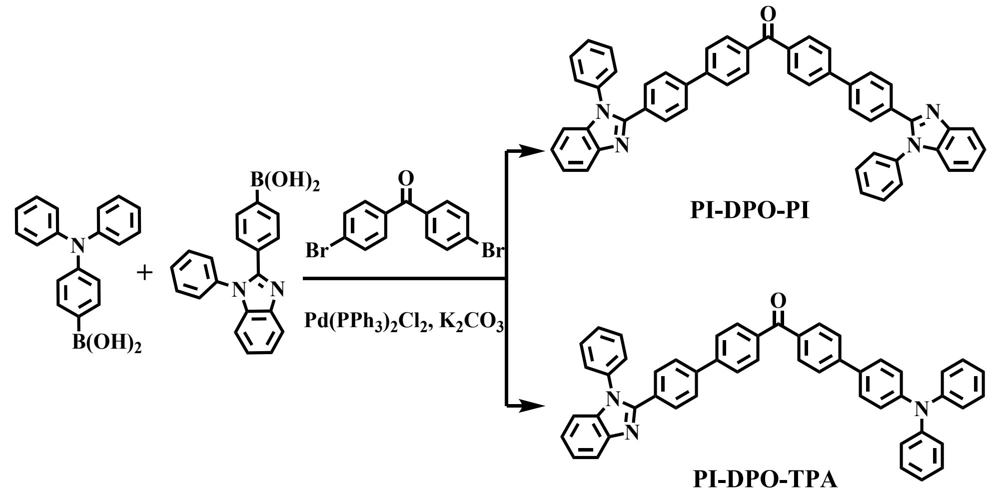

Figure S1 The synthetic route of PI-DPO-TPA and PI-DPO-PI

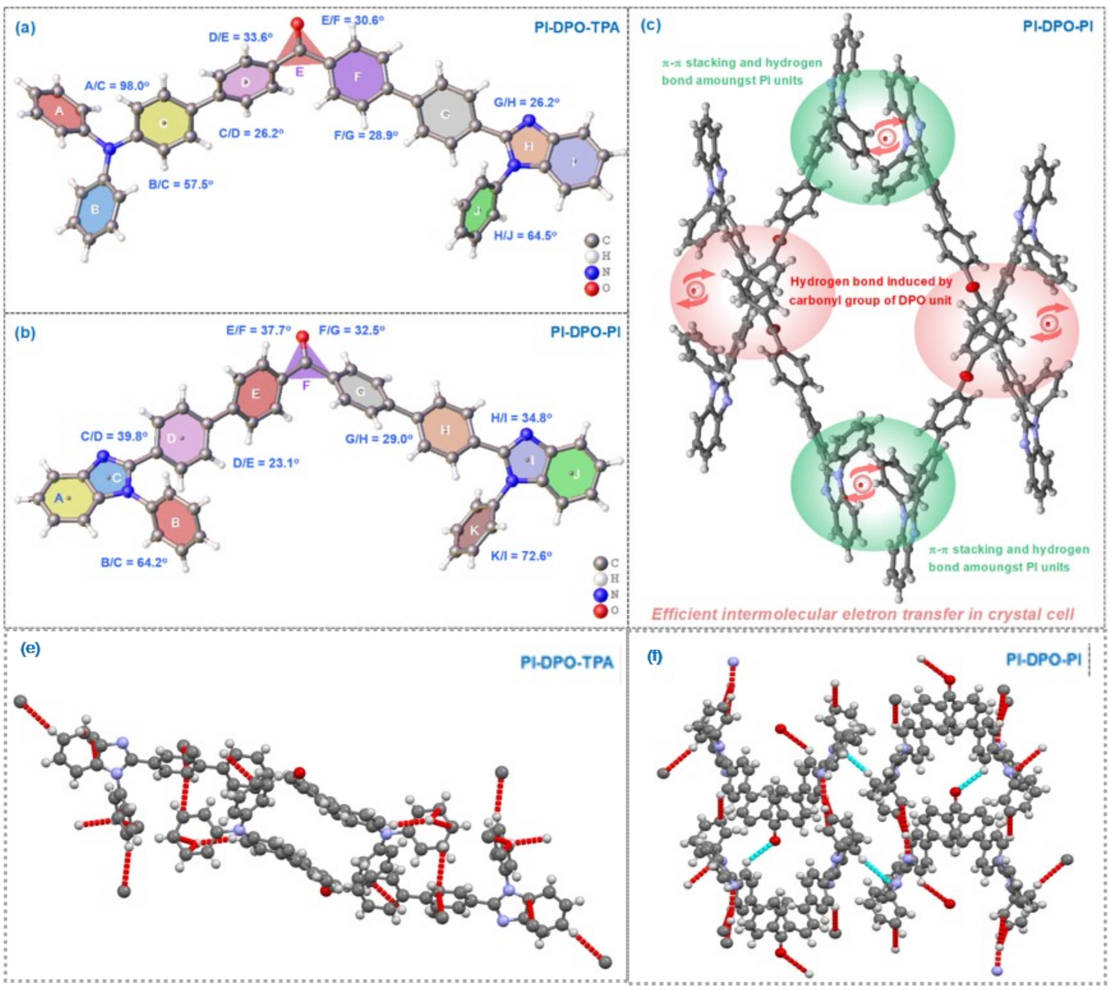

Figure S2 Torsion angle of (a) PI-DPO-TPA, (b) PI-DPO-PI in crystal cell, (c) the lattice conformation of PI-DPO-PI, (e) packing structure and multiple interactions of PI-DPO-TPA, and) packing structure and multiple interactions of PI-DPO-PI.

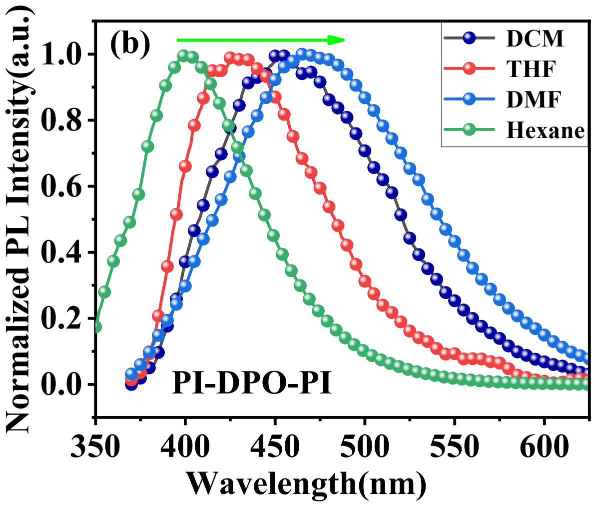

Figure S3 The emission of PI-DPO-PI in different solvents

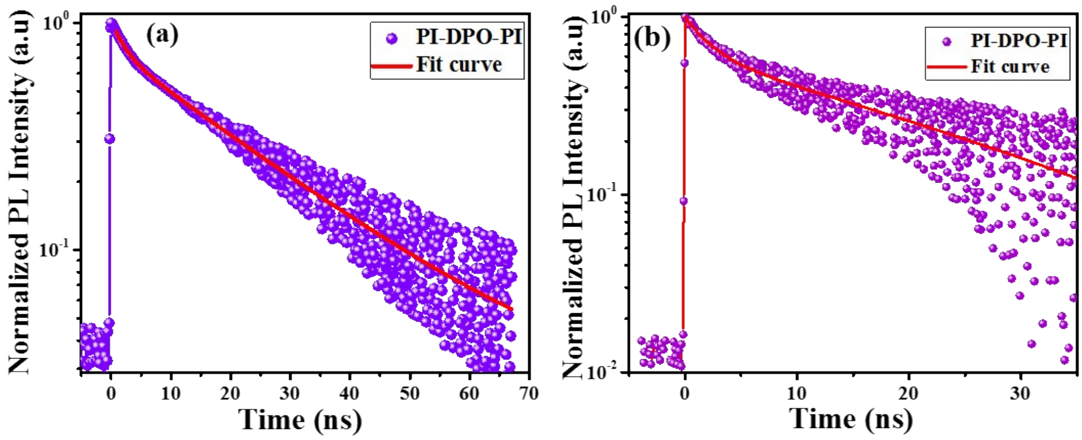

Figure S4 The fluorescent decay of PI-DPO-TPA and PI-DPO-PI in neat film

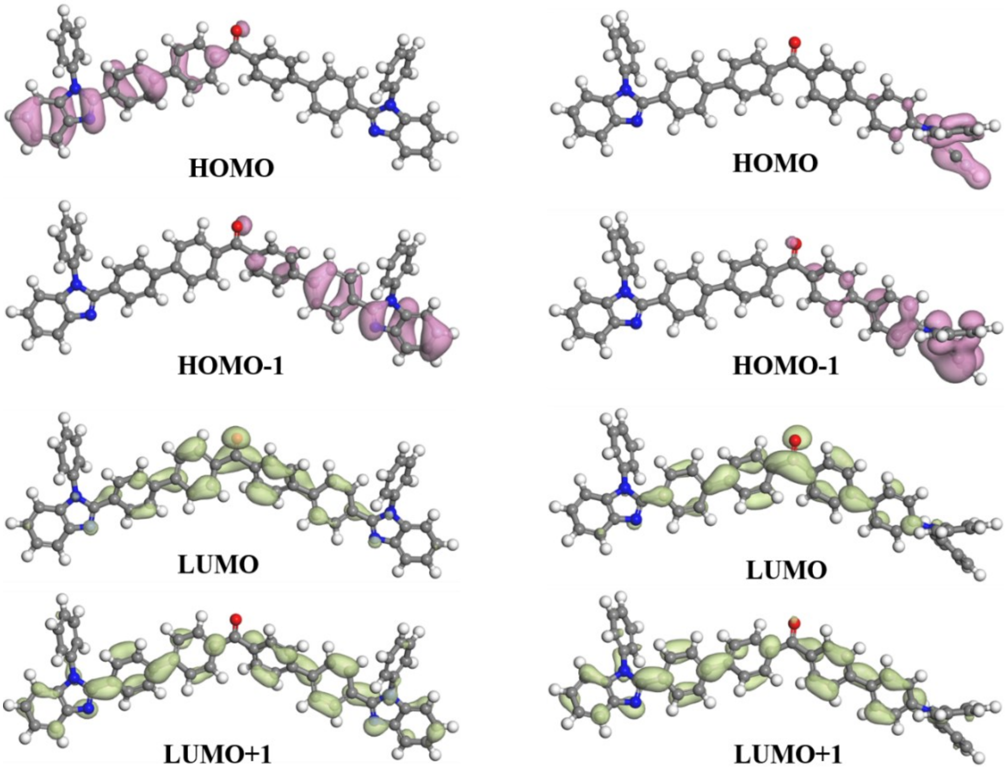

Figure S5 The densities of HOMOs and LUMOs of PI-DPO-TPA and PI-DPO-PI

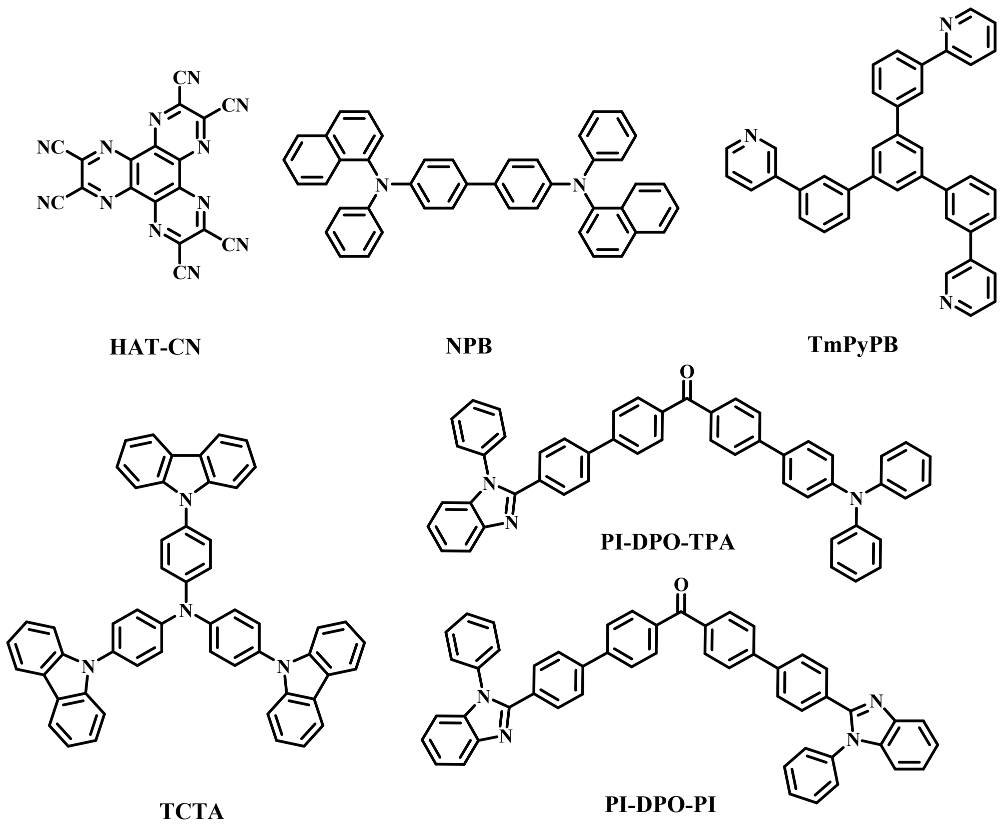

Figure S6 The chemical structures of the involved materials for the electroluminescent devices

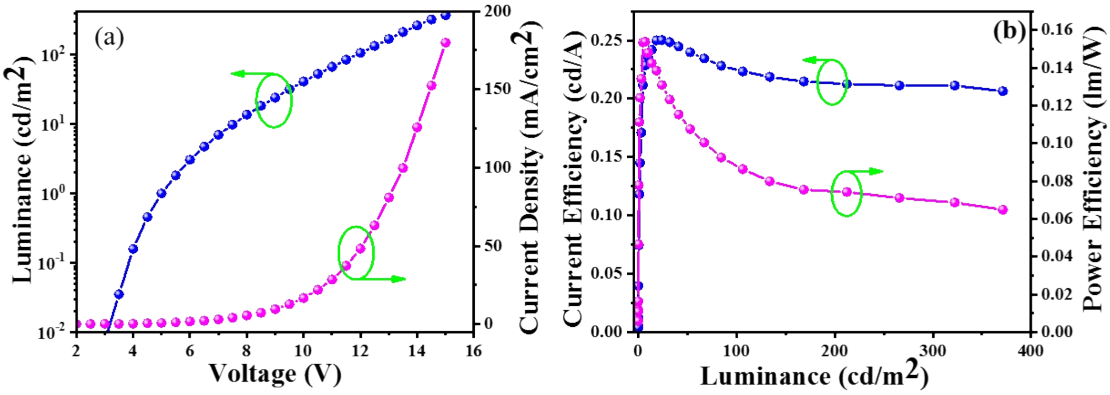

Figure S7 The device performance by using PI-DPO-PI as emitter and PI-DPO-TPA as EMT

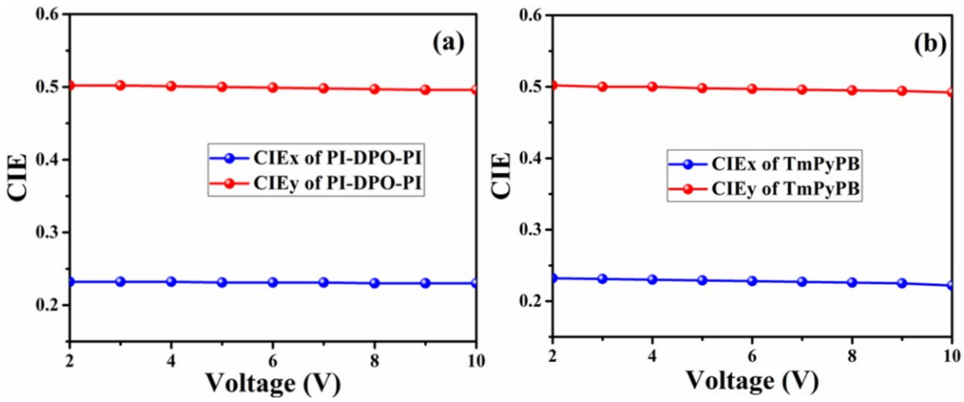

Figure S8 The CIE coordinates deviation of EL spectra in response to the voltage change of PI-DPO-PI and TmPyPB devices

Table S1. Crystal data and structure refinement for PI-DPO-TPA

Compound	**PI-DPO-TPA**
Empirical formula	$C_{50}H_{35}N_3O$
Formula weight	693.81
Temperature/K	296(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.8097(19)
b/Å	9.863(2)
c/Å	19.713(4)
α/°	88.450
β/°	78.609
γ/°	80.356
Volume/Å^3	1843.3(6)
Z	2
ρ_{calc}g/cm^3	1.250
μ/mm^{-1}	0.075
F(000)	728
Crystal size/mm^3	0.21 × 0.18 × 0.16
Radiation	Mo Kα (λ = 0.71073)
Index ranges	$-12 \le h \le 8$, $-12 \le k \le 12$, $-24 \le l \le 25$
Reflections collected	11630
Goodness-of-fit on F^2	0.965
Final R indexes [I>=2σ (I)]	R_1 = 0.0609, wR_2 = 0.1355
Final R indexes [all data]	R_1 = 0.1393, wR_2 = 0.1072
Largest diff. peak/hole / e Å^{-3}	0.001/0.0

Table S2. Crystal data and structure refinement for PI-DPO-PI

Compound	**PI-DPO-PI**
Empirical formula	$C_{54}H_{34}N_4O$
Formula weight	754.85
Temperature/K	296(2)
Crystal system	monoclinic
Space group	P21/n
a/Å	10.674(5)
b/Å	23.048(10)
c/Å	17.005(7)
α/°	90
β/°	91.185(5)
γ/°	90
Volume/Å^3	4182(3)
Z	4
ρ_{calc}g/cm^3	1.199
μ/mm^{-1}	0.072
F(000)	1576
Crystal size/mm^3	0.19 × 0.17 × 0.15
Radiation	Mo Kα (λ = 0.71073)
Index ranges	$-13 \leq h \leq 13$, $-29 \leq k \leq 18$, $-21 \leq l \leq 22$
Reflections collected	9528
Goodness-of-fit on F^2	0.957
Final R indexes [I>=2σ (I)]	R_1 = 0.0616, wR_2 = 0.1457
Final R indexes [all data]	R_1 = 0.1595, wR_2 = 0.1862
Largest diff. peak/hole / e Å^{-3}	0.0/-0.0

Table S3. Photophysical property of the neat PI-DPO-TPA and PI-DPO-PI films

compounds	ϕ_{PL} [%]	τ_{PF} [ns]	τ_{DF} [ns]	k_{PF} [10^8 s^{-1}]	k_{DF} [10^8 s^{-1}]	k_{ISC} [10^8 s^{-1}]	k_{hRISC} [10^8 s^{-1}]	k_r^s [10^8 s^{-1}]	k_{nr}^s [10^8 s^{-1}]	k_{IC}^{Tn} [10^8 s^{-1}]	ϕ_{ISC} [%]	ϕ_{hRISC} [%]	ϕ_{hRISC}/ϕ_{ISC}
PI-DPO-TPA	60.6	2.19	22.1	4.57	0.45	2.83	1.18	1.05	0.68	1.89	61	61	1.0
PI-DPO-PI	5.2	2.26	26.81	4.42	0.37	2.50	0.83	0.11	2.02	1.05	54	54	1.0

Table S4. Comparison on device performance of different emitters with hot-exciton characterization

Light color	Emitters	V_{on} (V)	EQE (%)	PE (lm/w)	CE (cd/A)	Literatures
Green	PI-DPO-TPA	2.0	8.45	16.91	18.87	This work
	CzP-BZP	4.0	6.95	16.38	23.99	[1]
	CADPPI	2.8	4.78	10.84	9.85	[2]
	DPIAPPB	2.8	4.15	6.16	6.56	
	Emitter 1	4.1	7.0	14.5	23.1	[3]
	Emitter 2	4.2	8.1	15.6	24.9	
	2EHO-TPA-CNPE	3.5	5.5	5.4	6.1	[4]
Blue	MPPIS-Cz	5.2	1.48	1.30	1.52	[5]
	MPPIS-TPA	6.1	1.34	1.28	1.46	
	PABP	4.1	6.31	4.65	5.85	[6]
	PAIDO	3.7	8.82	7.27	7.64	
Red	TPPI-BZPCN	2.8	3.33	4.28	7.60	[7]

Table S5. Comparison on device performance of ITO/HAT-CN/NPB/TCTA/emitters/ ETMs/LiF/Al with different ETMs

Emitter/ETMs	V_{on} (V)	EQE (%)	PE (lm/w)	CE (cd/A)	Literatures
PI-DPO-TPA/PI-DPO-PI	2.0	8.45	16.91	18.87	This work
PI-DPO-TPA/TmPyPB	4.5	4.20	4.02	12.32	This work
TPA-SO2/TPBi	2.7	3.91	5.46	5.26	[8]
DPAC-TAn-BI/TmPyPB	3.0	5.81	6.78	6.48	[9]
TPB-PAPC/TmPyPB	2.5	6.00	4.20	4.10	[10]
PAC/TPBi	4.4	10.03	6.94	12.37	[11]
CDE1/B3PYMPM	4.3	5.20	5.00	15.00	[12]
SBDBQ-PXZ/Bephen	2.4	5.60	10.50	12.00	[13]
o-ACSO2/TmPyPB	5.2	5.90	7.80	14.10	[14]
DCPDAPM/TmPyPB	6.1	1.34	1.28	1.46	[15]

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