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

Electronic Supplementary Information

Dibenzofuran/Dibenzothiophene as the secondary electron-donors for highly efficient blue thermally activated delayed fluorescence emitters

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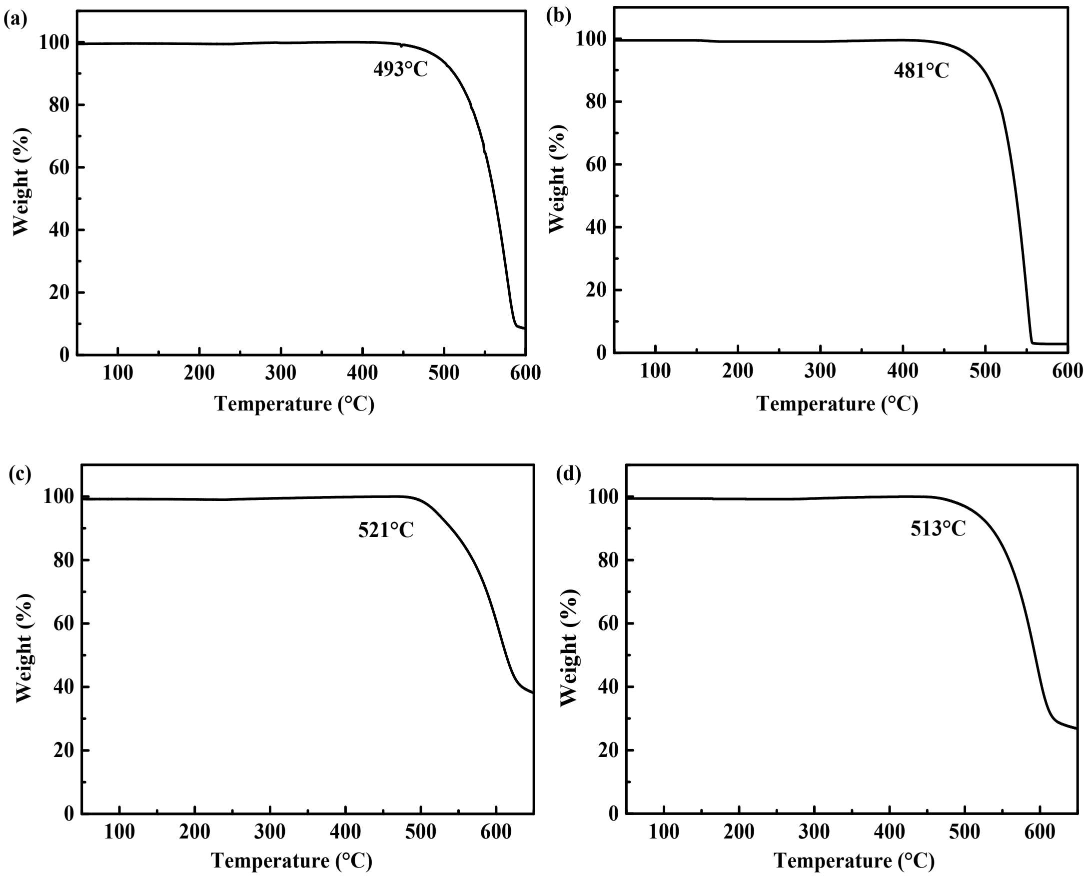
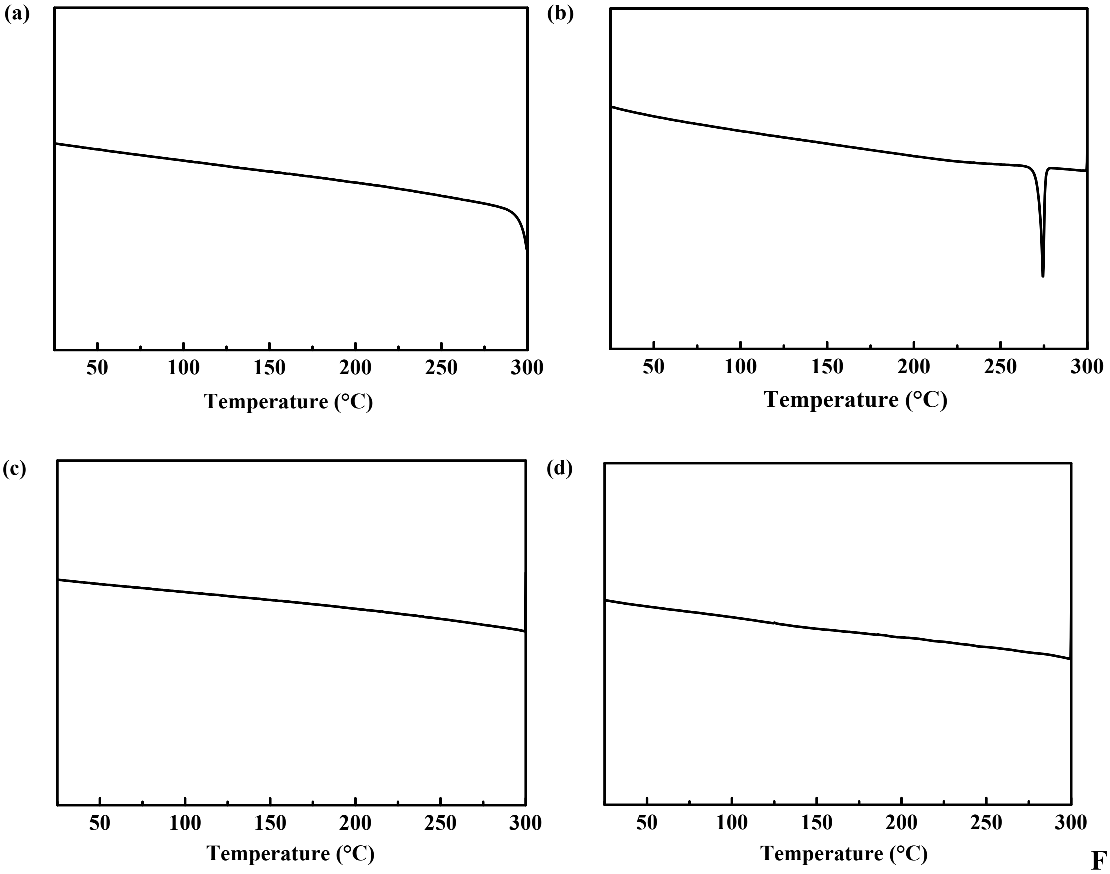


Fig. S1 Thermogravimetric analysis curves of DBTCz-Trz (a), DBFCz-Trz (b), BDBTCz-Trz (c) and BDBFCz-Trz (d) under nitrogen atmosphere.



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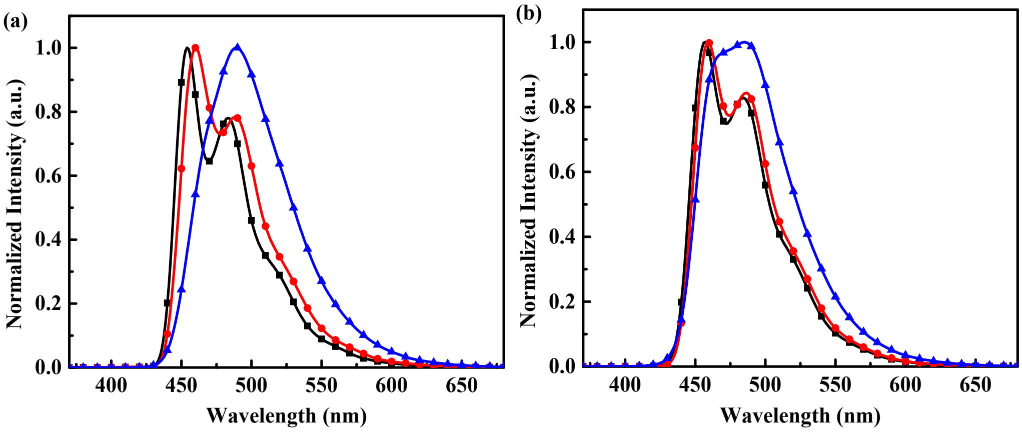
ig. S2 Differential Scanning Calorimeter analysis curves of DBTCz-Trz (a), DBFCz-Trz (b), BDBTCz-Trz (c) and BDBFCz-Trz (d) under nitrogen atmosphere.



(e)

Compounds	TOL	EA	DMF
DBTCz-Trz	2.74 eV	2.70 eV	2.54 eV
DBFCz-Trz	2.73 eV	2.71 eV	2.54 eV
BDBTCz-Trz	2.70 eV	2.67 eV	2.59 eV
BDBFCz-Trz	2.72 eV	2.68 eV	2.57 eV

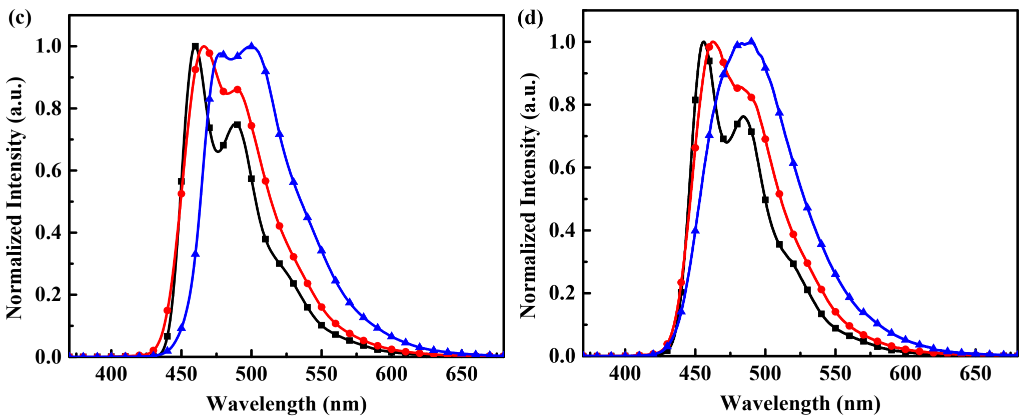


Fig. S3 Normalized phosphorescence spectra of (a) DBTCz-Trz, (b) DBFCz-Trz, (c) BDBTCz-Trz and (d) BDBFCz-Trz in TOL (black), EA (red)) and DMF (blue) at 77K and the corresponding estimated triplet energy level (T_1) from the first phosphorescence peaks.

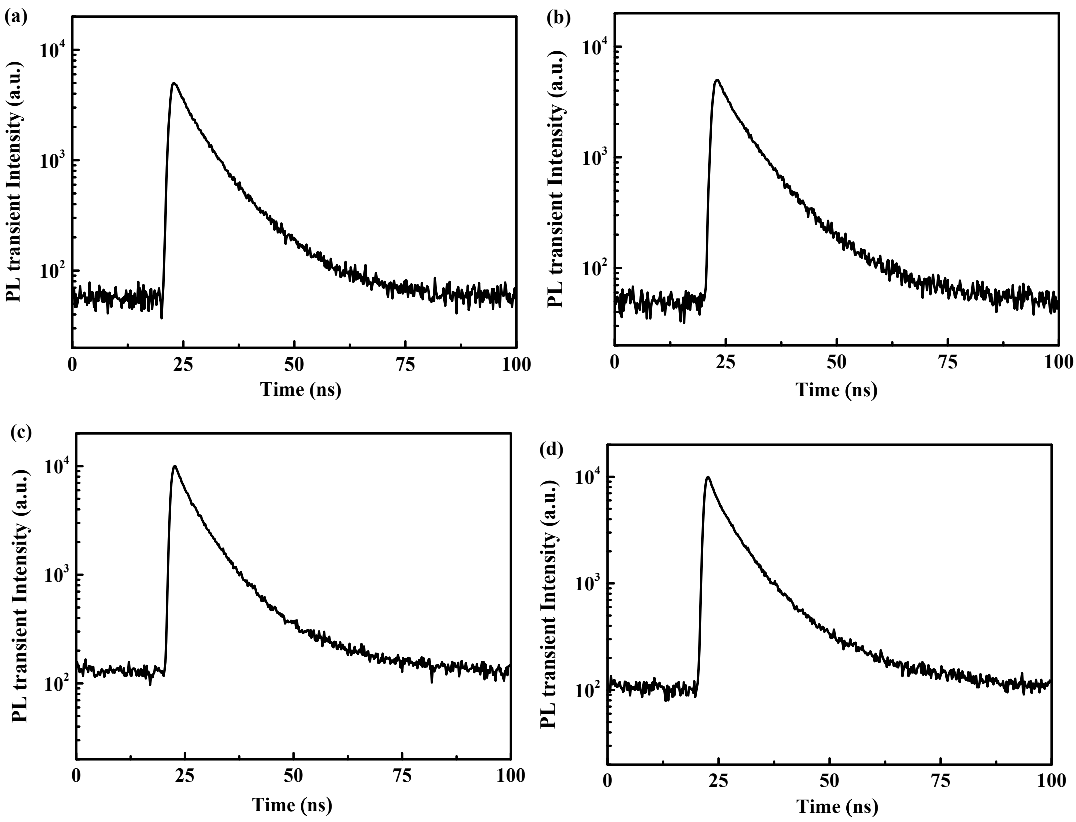
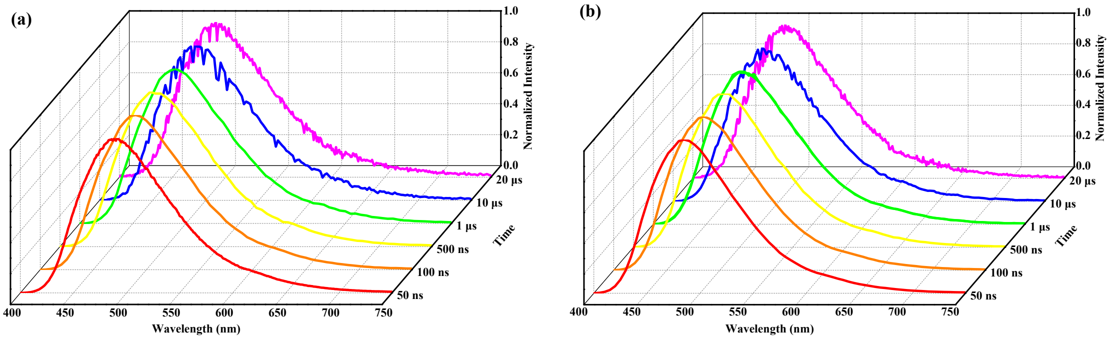


Fig. S4 Transient PL decay curves of prompt emission of DBTCz-Trz (a), DBFCz-Trz (b), BDBTCz-Trz (c) and BDBFCz-Trz (d) 15 wt% doped film at room temperature.



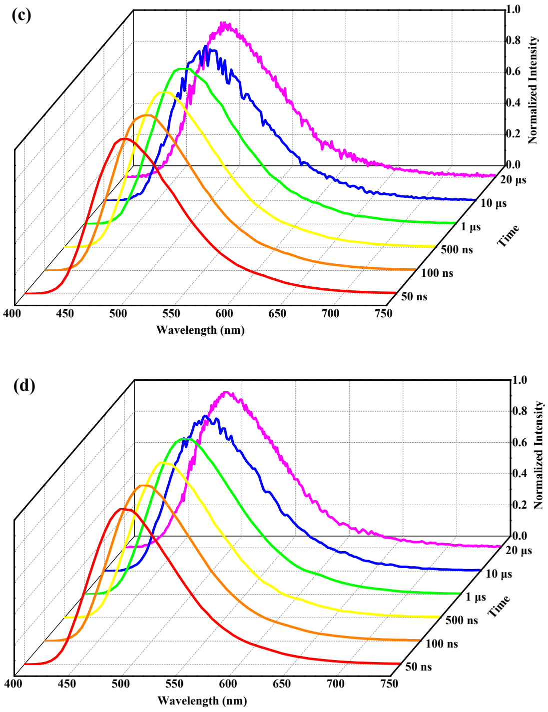


Fig. S5 Time resolved spectra of (a) DBTCz-Trz, (b) DBFCz-Trz, (c) BDBTCz-Trz and (d) BDBFCz-Trz 15 wt% doped film at room temperature with different time scales: 50 ns, 100 ns, 500 ns, 1μs, 10 μs and 20 μs.

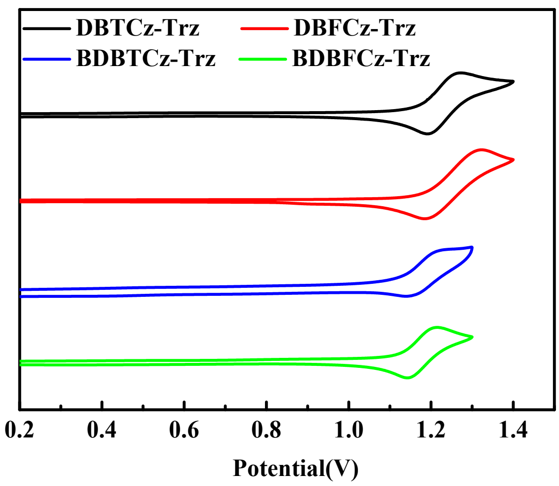


Fig. S6 Cyclic voltammograms of Oxidative curves in DCM.

Serious efficiency roll-off of the DBF and DBT substituted derivatives were analyzed by utilizing the singlet exciton-polaron annihilation (SPA) model [1] and the corresponding results were exhibited in Fig. S7. The simulated external quantum efficiency (EQE) fitted well with that of experimental results which could be ascribed to the low carrier mobility of the host DPEPO.

$$\eta_{ext}^{SP}(j) = \frac{\eta_0}{1 + \left(\frac{j}{j_0}\right)^{\frac{1}{1+l}}}$$

Where $\eta_{ext}^{SP}(j)$ and η_0 are the EQE in the presence absent of SPA and initial external quantum efficiency at very low current densities respectively. j_0 is the critical current density where $\eta = \eta_0/2$ and l is the fitting parameter. Corresponding key parameter of j_0 and l are listed in the following figures.

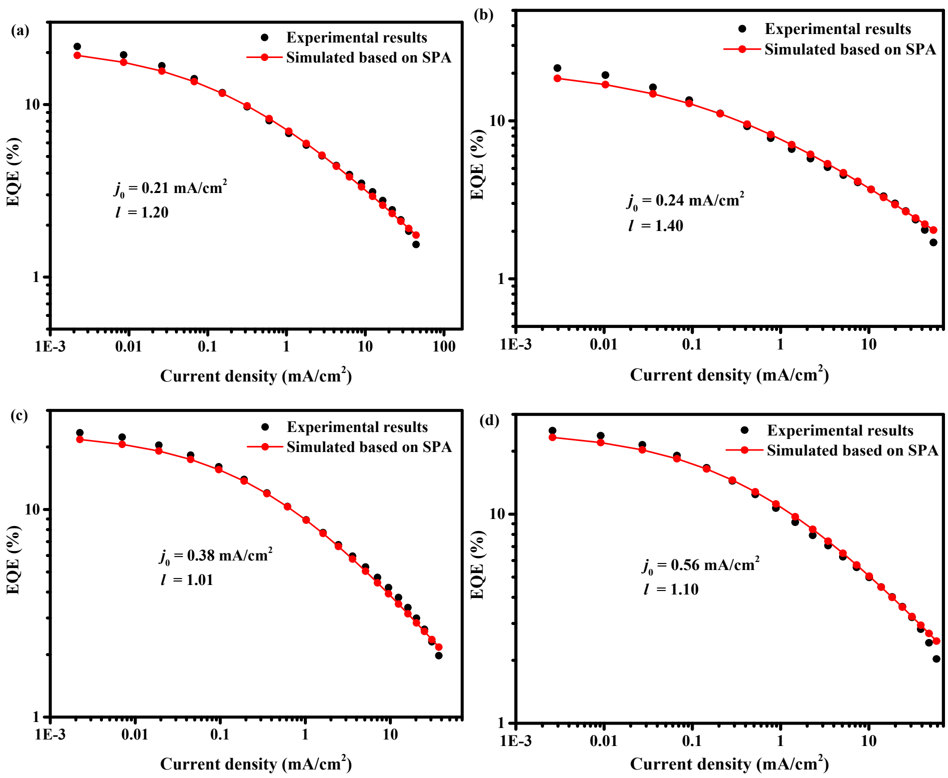


Fig. S7 External quantum efficiency-current density curve of the measured (black) and simulated (red) upon considering the SPA model for (a) DBTCz-Trz, (b) DBFCz-Trz, (c) BDBTCz-Trz and (d) BDBFCz-Trz respectively.

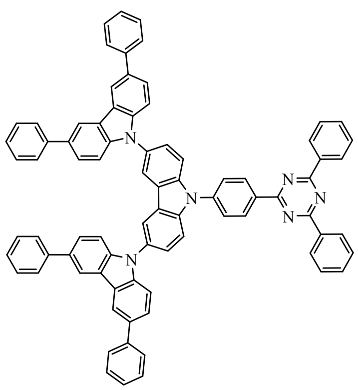
Table S1. Data extracted from the transient characterization in the range of 400 μs.

Compounds	Prompt Component		Delayed Component				r_p [b]	r_d [b]
	τ_1 [a] (μs)	A_1 [a]	τ_2 [a] (μs)	τ_3 [a] (μs)	A_2 [a]	A_3 [a]		
DBTCz-Trz	1.25	1.70	13.14	145.10	0.062	0.0040	0.61	0.39
DBFCz-Trz	1.25	2.15	12.78	137.10	0.10	0.0050	0.58	0.42
BDBTCz-Trz	1.25	2.49	11.31	99.27	0.28	0.036	0.32	0.68
BDBFCz-Trz	1.25	2.55	10.70	102.50	0.31	0.030	0.33	0.67

[a] Obtained from the multi-exponential fitting of the transient decay curves on a 400 μs scale; [b] The intensity ratio between prompt (r_p) and delayed (r_d) components were calculated by the equation of $r_p = \tau_1A_1/(\tau_1A_1+\tau_2A_2+\tau_3A_3)$ and $r_d = 1 - r_p$ according to the literature.[2]

Table S2. Summary of electroluminescence performances for TADF emitters with secondary D groups.

Emitter	EL (nm)	EQE_{max} (%)	CIE (x,y)	Ref
DBTCz-Trz	472	21.7	(0.17, 0.28)	This work
DBFCz-Trz	472	21.6	(0.17, 0.28)	This work
BDBTCz-Trz	492	23.4	(0.19, 0.37)	This work
BDBFCz-Trz	488	25.1	(0.18, 0.35)	This work
2a	487	20.6	(0.19,0.35)	3
2b	478	16.8	(0.17,0.27)	3
2c	477	14.8	(0.18,0.28)	3
BCz-TRZ	490	20.5	(0.18, 0.34)	4
3Cz-TRZ	-	12.2	(0.18, 0.32)	4
SFCC	456	10.59	(0.17,0.21)	5
DACT-II	520	29.6	-	6
G2TAZ	-	2.4	-	7
G3TAZ	-	3.4	-	7
G4TAZ	-	1.5	-	7



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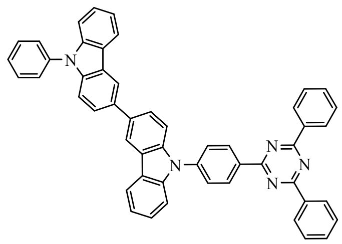
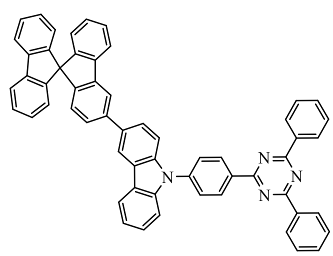


BCz-TRZ



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