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

Supporting Information

Highly efficient green organic light emitting diodes with phenanthroimidazole-based thermally activated delayed fluorescence emitters

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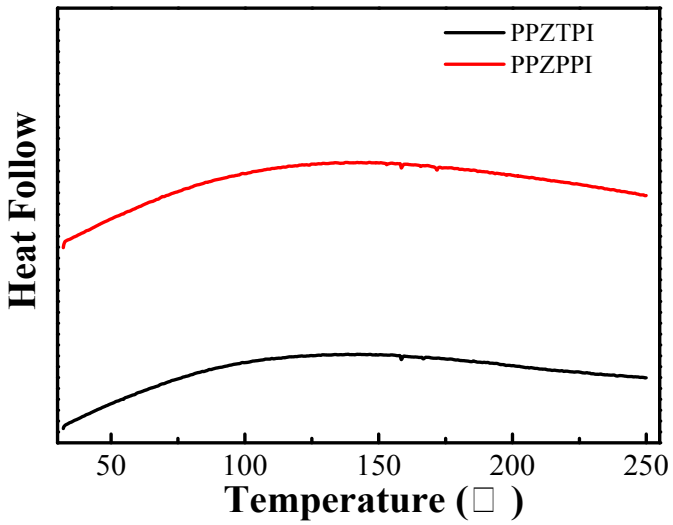

Fig. S1. DSC curves of **PPZTPI** and **PPZPPI**.

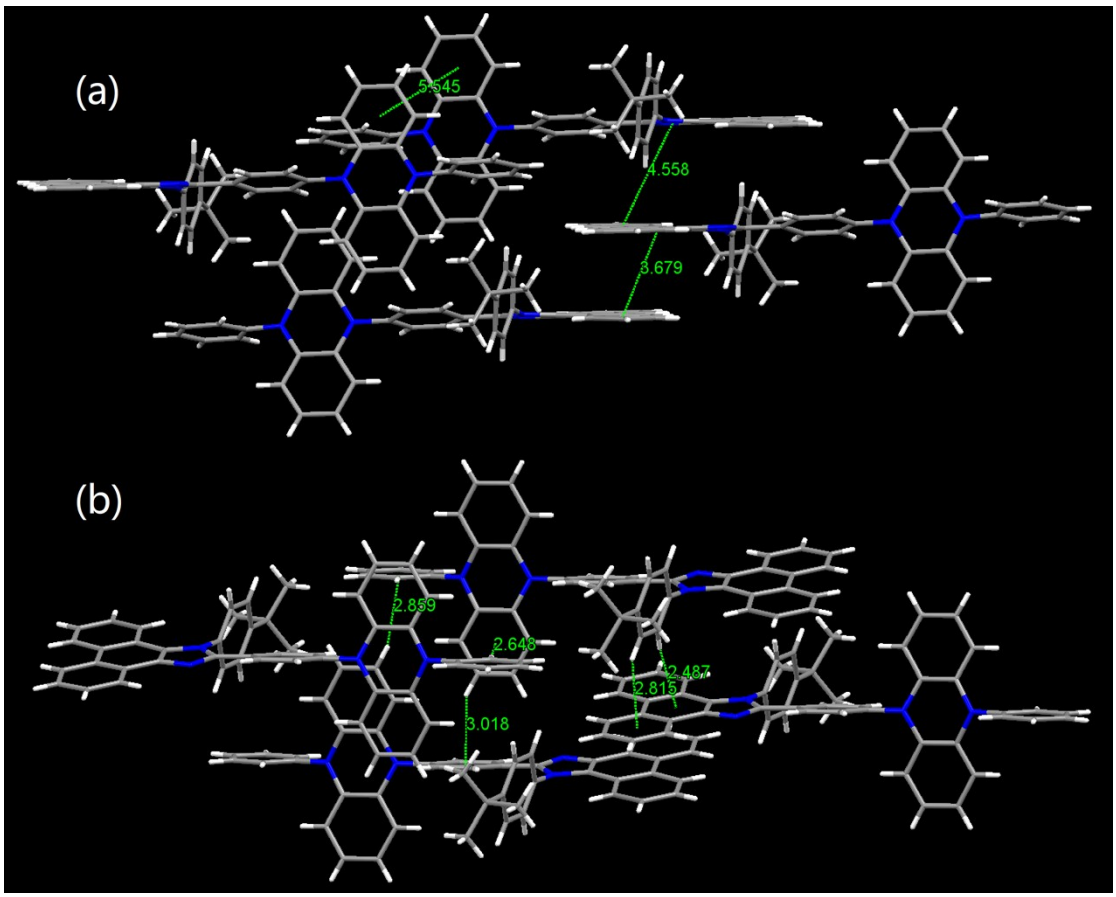

Fig. S2. Single-crystal structure of **PPZTPI**: (a) Distance of intermolecular π-π interaction; (b) Distance of intermolecular C−H···π interaction.

Table S1. Crystal data and structure refinement for **PPZTPI**

CCDC	1577557
Empirical formula	$C_{49}H_{38}N_4$
Formula weight	682.83
T, K	160(80)
Crystal system	triclinic
Space group	P-1
a/Å	9.2776(4)
b/Å	11.1340(7)
c/Å	18.0446(4)
α/°	95.121(3)
β/°	96.138(3)
γ/°	103.446(4)
Volume/Å^3	1789.87(15)
Z	2
ρ_{calc}g/cm^3	1.267
μ/mm^{-1}	0.572
F(000)	720.0
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	4.96 to 147.84
Index ranges	$-8 \leq h \leq 11$, $-13 \leq k \leq 10$, $-22 \leq l \leq 18$
Reflections collected	18583
Independent reflections	7007 [R_{int} = 0.0631, R_{sigma} = 0.0665]
Data/restraints/parameters	7007/0/481
Goodness-of-fit on F^2	1.100
Final R indexes [I>=2σ (I)]	R_1 = 0.0719, wR_2 = 0.2192
Final R indexes [all data]	R_1 = 0.0827, wR_2 = 0.2288
Largest diff. peak/hole / e Å^{-3}	0.84/-0.61

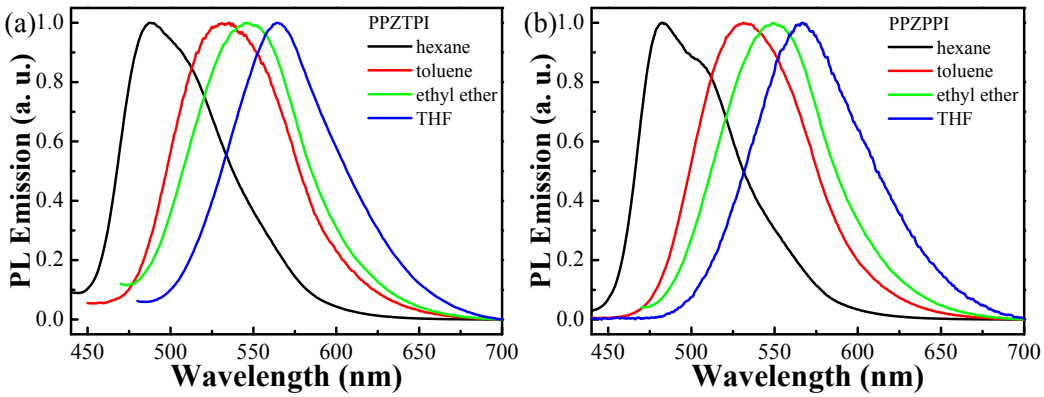

Fig. S3. Solvatochromic of **PPZTPI** and **PPZPPI** in different solvents.

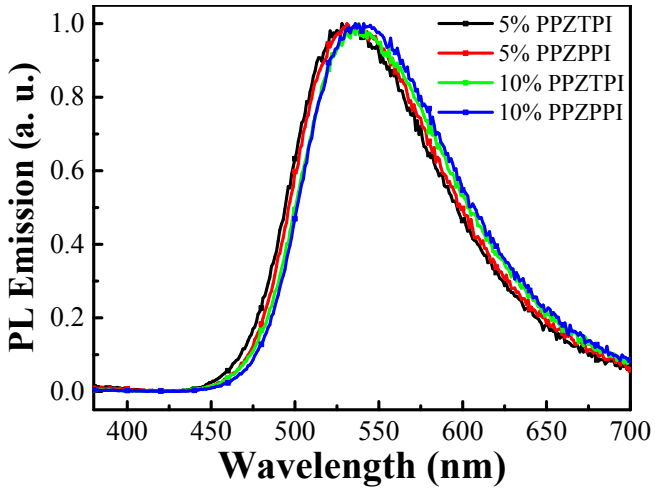

Fig. S4. PL spectra of **PPZTPI** and **PPZPPI** doped in CBP films.

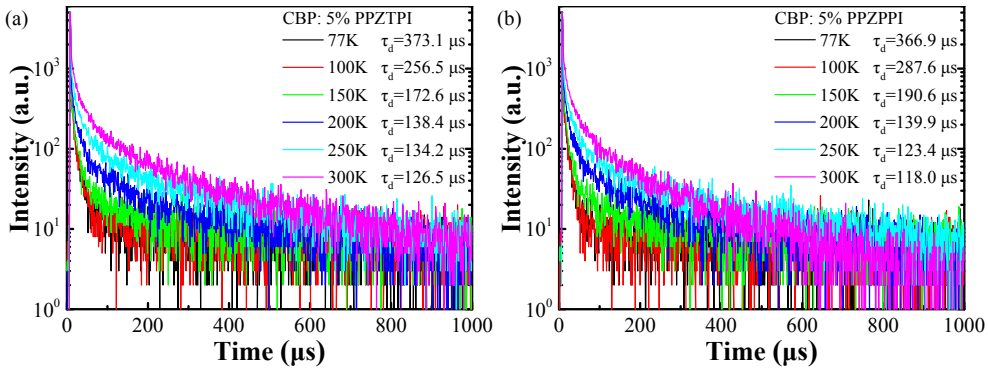

Fig. S5. Temperature-dependence of the transient PL characteristics for **PPZTPI** and **PPZPPI** doped in CBP films (5 wt%).

Table S2. The detail kinetic parameters

	PPZTPI	**PPZPPI**
Φ	0.731	0.990
Φ_p	0.364	0.577
Φ_d	0.367	0.413
τ_p(ns)	3.26	3.0
τ_d(μs)	126.5	118.0
$k_p(s^{-1})$	$1.12*10^8$	$1.92*10^8$
$k_d(s^{-1})$	$5.78*10^3$	$8.39*10^3$
$k_{ISC}(s^{-1})$	$1.54*10^8$	$1.39*10^8$
$k_{RISC}(s^{-1})$	$4.22*10^3$	$8.31*10^3$

To further compare the TADF characteristics of both compounds, the main kinetic parameters of both compounds were calculated according to the literature[1, 2]:

$$k_p = \Phi_p/\tau_p$$

$$\Phi = k_p/(k_p + k_{IC})$$

$$\Phi_p = k_p/(k_p + k_{IC} + k_{ISC})$$

$$\Phi_{IC} = k_{IC}/(k_p + k_{IC} + k_{ISC})$$

$$\Phi_{ISC} = 1 - \Phi_p - \Phi_{ISC} = k_{ISC}/(k_p + k_{IC} + k_{ISC})$$

$$k_d = \frac{\Phi_d}{\Phi_{ISC}\tau_d}$$

$$k_{RISC} = \frac{k_p k_d \Phi_d}{k_{ISC}\Phi_p}$$

where Φ is absolute photoluminescence quantum yield, Φ_p and Φ_d are the prompt and delayed fluorescence quantum yields, τ_p and τ_d are the prompt and delayed fluorescence decay lifetimes, k_p and k_d are the prompt and delayed fluorescence decay rate constants, Φ_{IC} and Φ_{ISC} are the internal conversion and intersystem crossing quantum yield, k_{IC} and k_{ISC} are the internal conversion and intersystem crossing decay rate constants, k_{RISC} is the rate constants for the reverse intersystem crossing from T_1 to S_1.

Table S3. The maximum EQE of **PPZTPI** and **PPZPPI** as dopants at different concentrations.

	3%	5%	10%	20%
PPZTPI	16.78%	20.52%	15.44%	-
PPZPPI	16.97%	21.06%	17.37%	12.09%

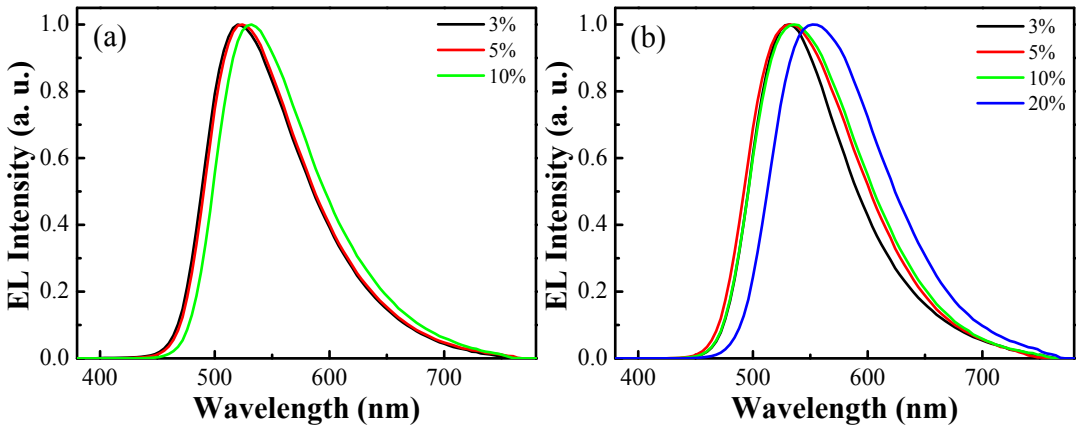

Fig. S6. EL spectra of **PPZTPI** (a) and **PPZPPI** (b) at different concentrations.

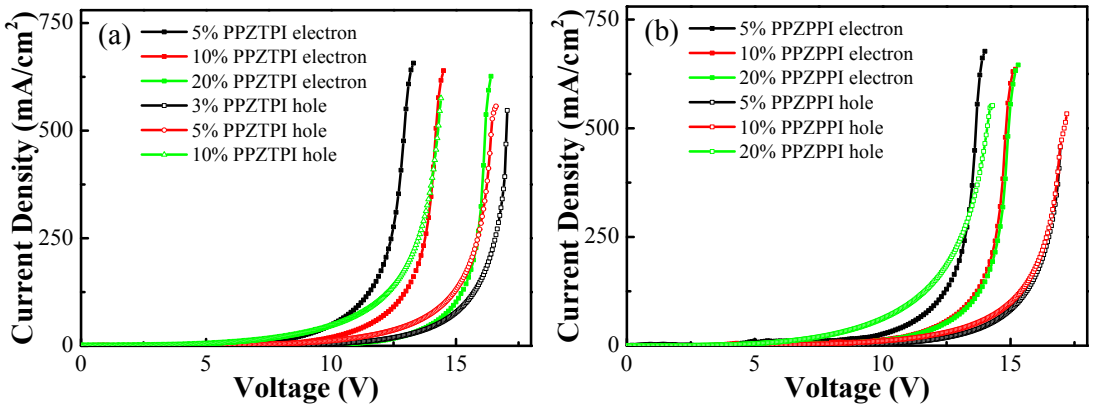

Fig. S7. Current density-voltage characteristics of hole-only and electron-only devices with different concentrations for **PPZTPI** (a) and **PPZPPI** (b).

Table S4. Recently reported OLEDs based on green TADF materials

emitter	EL_{max} (nm)	ΔE_{ST} (eV)	EQE	Ref.
PPZTPI	528	0.11	20.52 %	This work
PPZPPI	528	0.12	21.06 %	This work
4CzIPN	513	0.08	19.3 %	3
TXO-PhCz	520	0.09	21.5 %	4
ACRDSO2	534	0.058	19.2 %	5
PHzBCO	520	0.006	19.6 %	6
PXZ-DPS	507	0.08	17.5 %	7
Px2BP	539	0.03	10.7 %	8
DTCBPy	514	0.04	27.2 %	9
PXZPhPM	528	0.03	24.6 %	10
OSTFCN	530	0.09	20.4 %	11
4CzCNPy	524	0.07	10.4 %	12
DCZ-TTR	512	0.03	20.1 %	13
AI-Cz	510	0.06	23.2 %	14
AI-TBCz	540	0.03	21.1 %	14
mPTBC	516	0.006	18.1 %	15

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