

## Electronic Supplementary Information (ESI)

### **Triazatruxene-based thermally activated delayed fluorescence small molecules with aggregation-induced emission property for solution-processable nondoped OLEDs with low efficiency roll-off**

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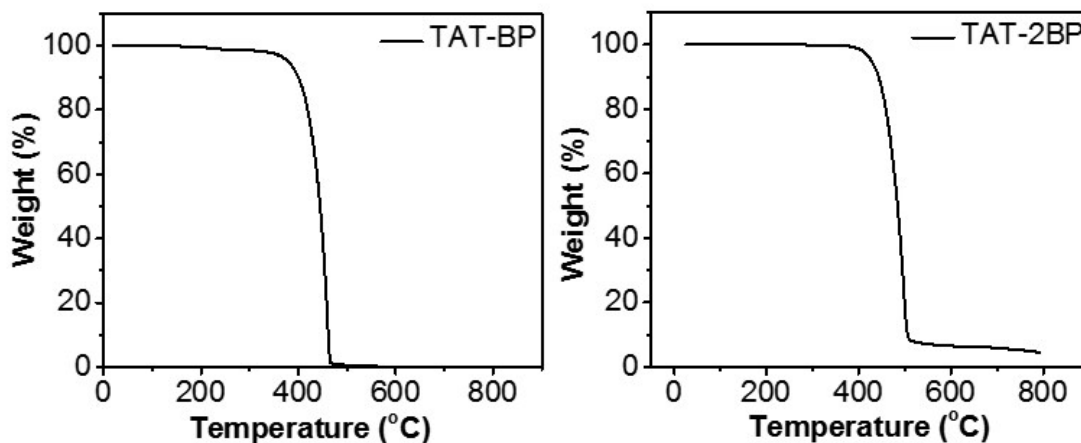


Fig. S1 TGA curves of TAT-BP and TAT-2BP.

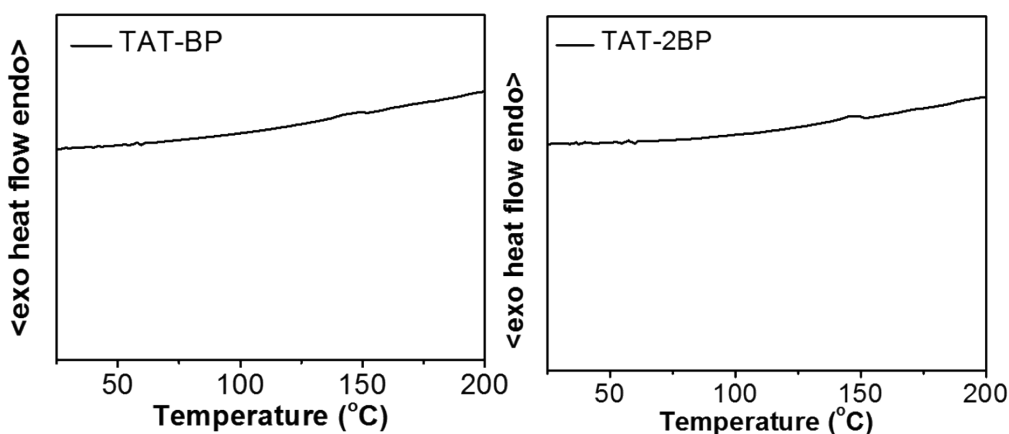


Fig. S2 DSC curves of TAT-BP and TAT-2BP.

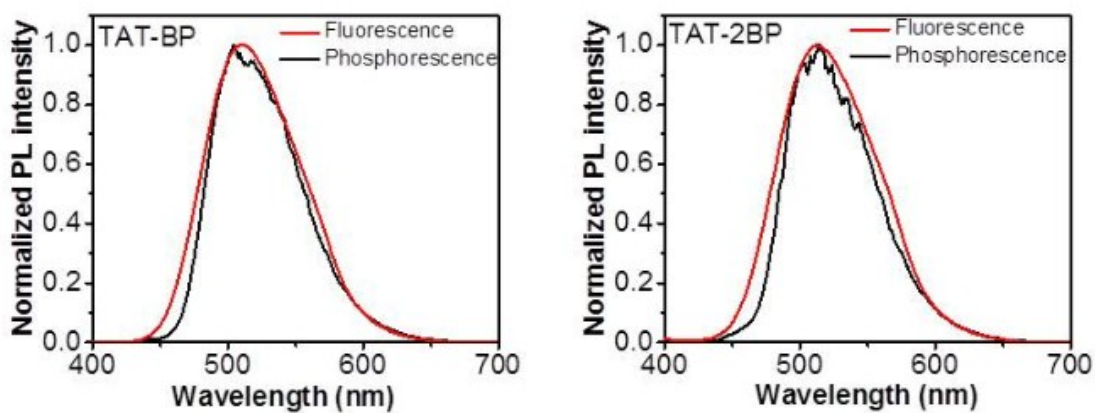
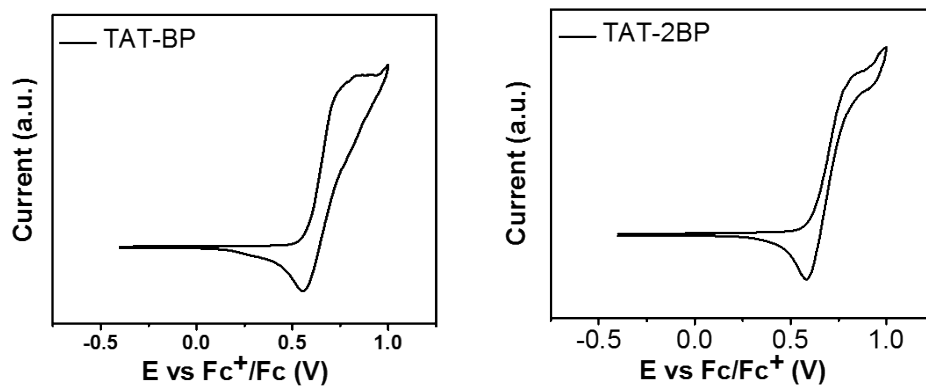


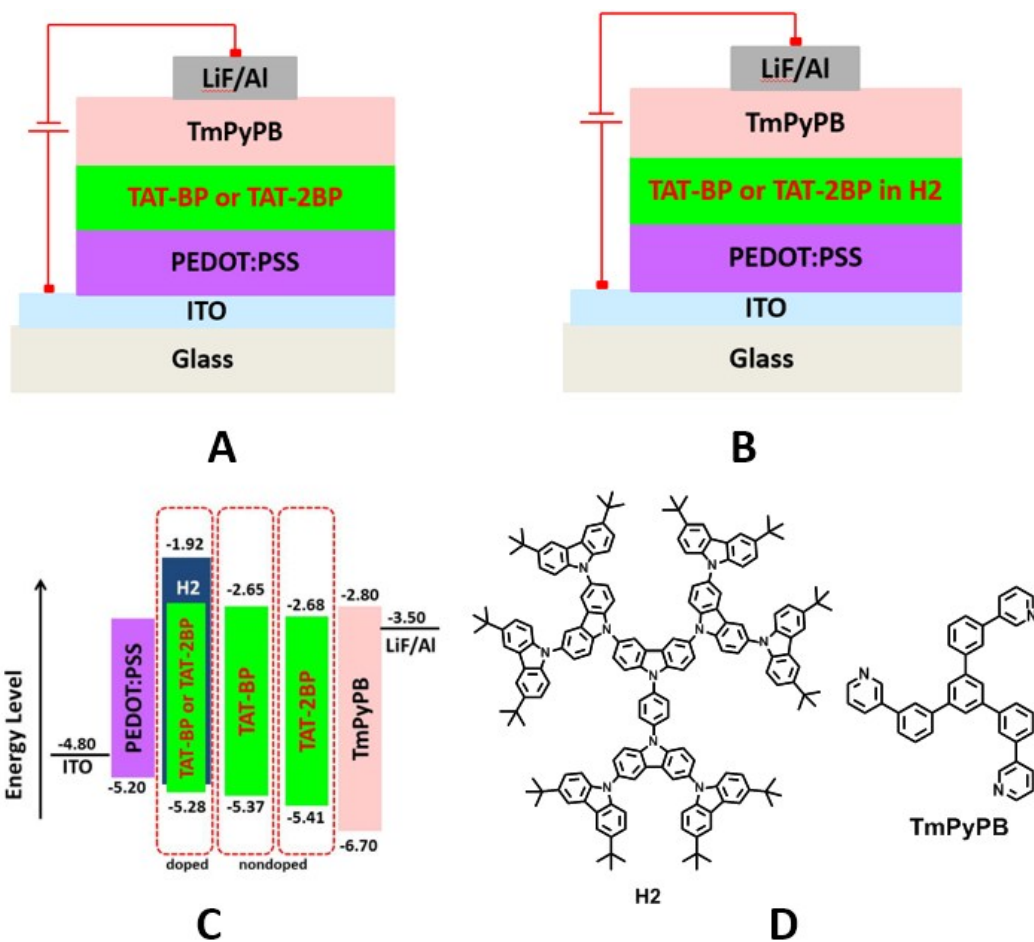
Fig. S3 Fluorescence spectra (red line) at room temperature and phosphorescence at (black line) spectra at 77K of TAT-BP and TAT-2BP in neat films.



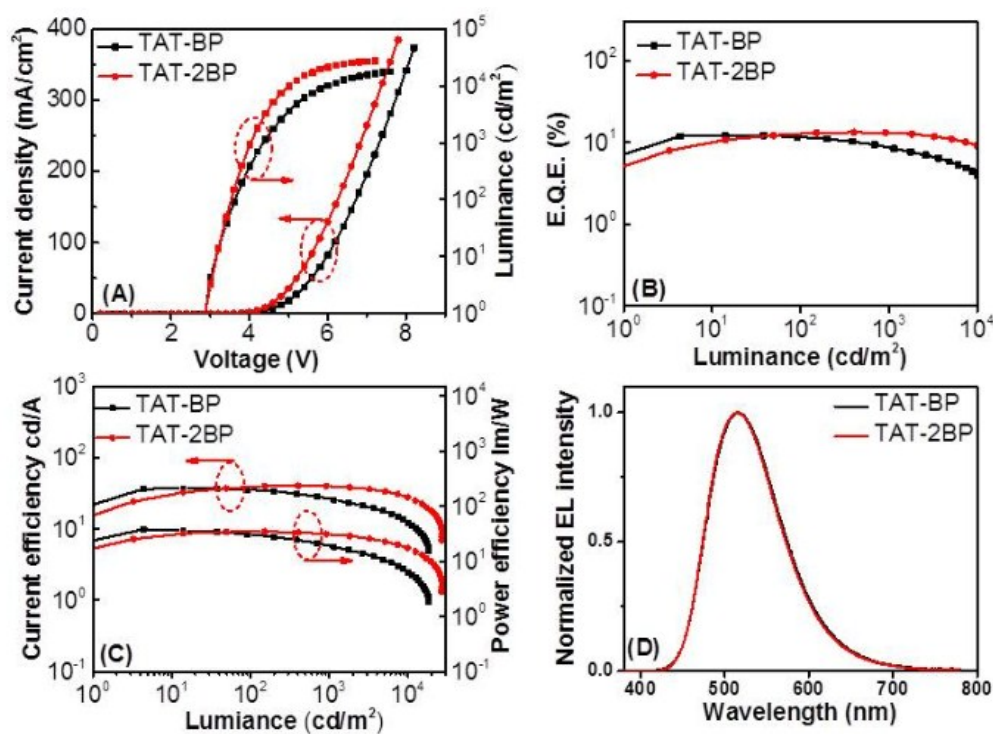
**Fig. S4** Cyclic voltammetry analysis of TAT-BP and TAT-2BP.

**Table S1** DFT calculation results of TAT-BP and TAT-2BP.

Emitters	HOMO (eV)	LUMO (eV)	$E_g$ (eV)	$S_1$ (eV)	$T_1$ (eV)	$\Delta E_{ST}$ (eV)	$f$
TAT-BP	-4.91	-1.82	3.09	2.68	2.59	0.09	0.0217
TAT-2BP	-5.03	-1.87	3.16	2.73	2.61	0.12	0.0346



**Fig. S5** (A) Nondoped device configuration. (B) Doped device configuration with 30 wt% emitters doped in H2 host. (C) Energy level diagrams the multilayer OLEDs. (D) Chemical structure of H2 and TmPyPB.

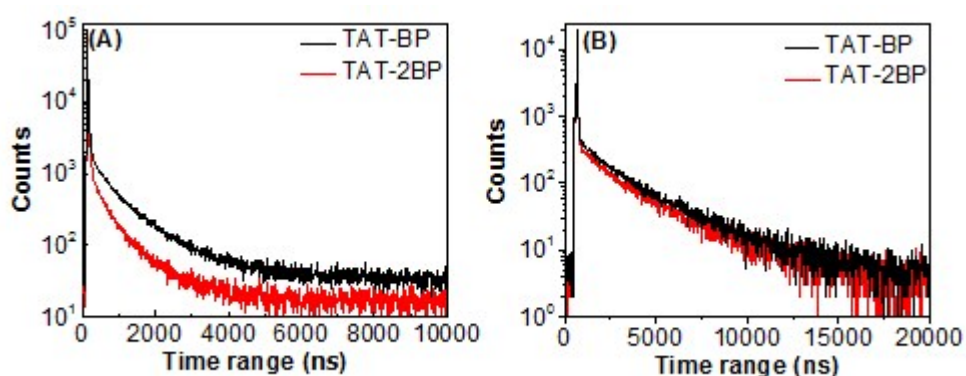


**Fig. S6** EL performance of the OLEDs based on TAT-BP and TAT-2BP doped in H2 host.

(A) The current density-voltage-luminance characteristics. (B) External quantum efficiency-luminance characteristics. (C) Current efficiency-luminance and power efficiency-luminance characteristics. (D) Electroluminescence spectra (EL) at 1000 cd m<sup>-2</sup>

**Table S2** EL performance of the doped OLEDs based on TAT-BP and TAT-2BP.

Device	Maximum values				Values at 1000 cd m <sup>-2</sup>			
	V <sub>on</sub> (V)	LE(cd/A)	PE(lm/W)	EQE(%)	LE(cd/A)	PE(lm/W)	EQE(%)	Roll-off ratio (%)
TAT-BP(30 wt %):H2	2.9	37.1	38.2	12.1	26.8	19.7	8.8	27.3
TAT-2BP(30 wt %):H2	2.9	40.4	34.8	13.2	40.0	30.6	12.9	2.3

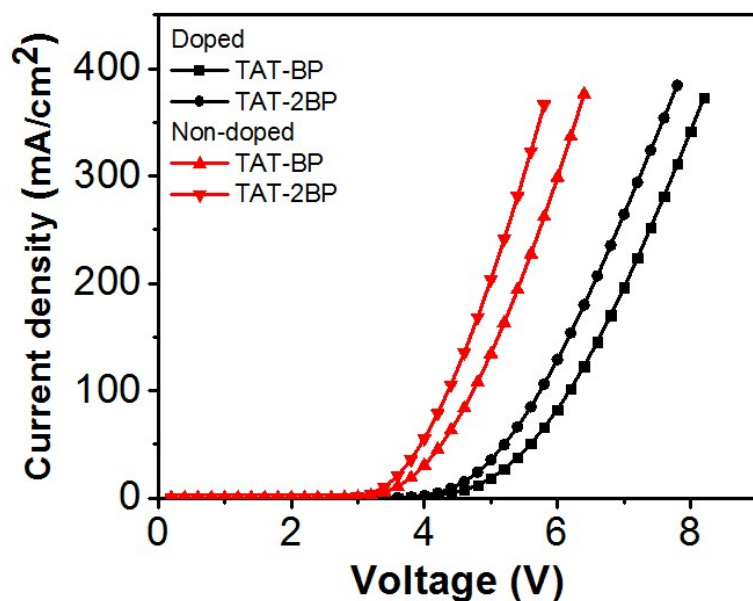


**Fig. S7** Transient photoluminescence decay curves of emitters in neat films (A) and emitters (30 wt %) doped in H2 films (B) measured at 300 K under argon atmosphere.

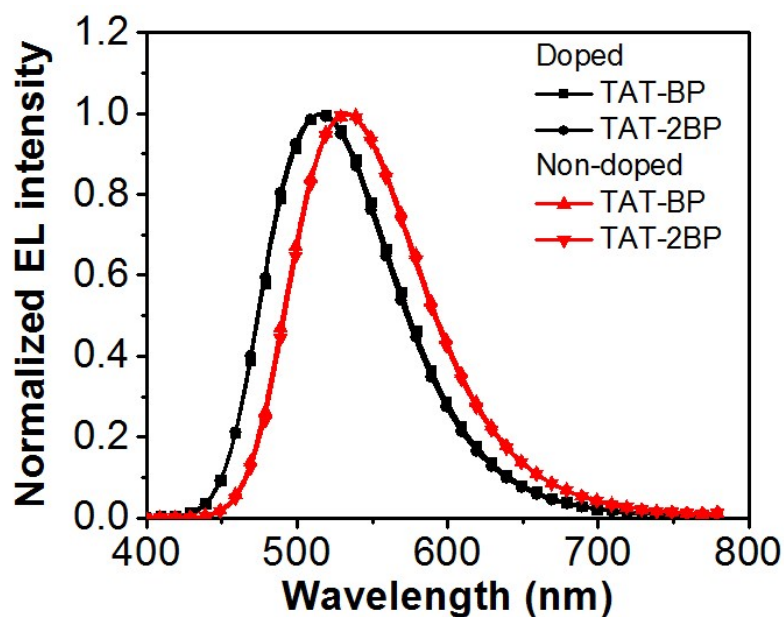
**Table S3** Fluorescence lifetimes and quantum yields (PLQYs) of the nondoped and doped films of TAT-BP and TAT-2BP.

	$\tau_p$ (ns)	$\tau_d$ ( $\mu$ s)	PLQY
TAT-BP neat film	46.7	0.79	51%
TAT-2BP neat film	37.3	0.54	44%
TAT-BP doped film	51.3	2.15	80%
TAT-2BP doped film	50.2	2.04	76%

The doped films have delay fluorescence lifetimes of 2.15  $\mu$ s for TAT-BP and 2.04  $\mu$ s for TAT-2BP, which are longer than non-doped ones (0.79  $\mu$ s for TAT-BP, 0.54  $\mu$ s for TAT-2BP). Meanwhile, doped films exhibit PLQY of 80% for TAT-BP and 76% for TAT-2BP, which are higher than the non-doped ones (51% for TAT-BP, 44% for TAT-2BP). The longer delayed fluorescence lifetimes and higher PLQYs in doped films should be attributed to the reduced exciton quenching.



**Fig. S8** The J-V curves of doped (black line) and non-doped (red line) devices based on TAT-BP and TAT-2BP.



**Fig. S9** The EL spectra of doped (black line) and non-doped (red line) devices based on TAT-BP and TAT-2BP.

TAT-BP and TAT-2BP exhibit similar EL spectra in both doped devices and non-doped devices. Their doped devices show the emission maximum at 516 nm, while their non-doped devices show the emission maximum at 533 nm. Compared to the nondoped devices, the blue-shifted emission in the doped devices should be attributed to the suppressed intermolecular dipole-dipole interaction and weakened intramolecular charge transfer in the less polar doped films.