

Supporting information

Effect of Substituents in a Series of Carbazole-based Host Materials toward High-Efficiency Carbene-based Blue OLEDs

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1. DFT calculations

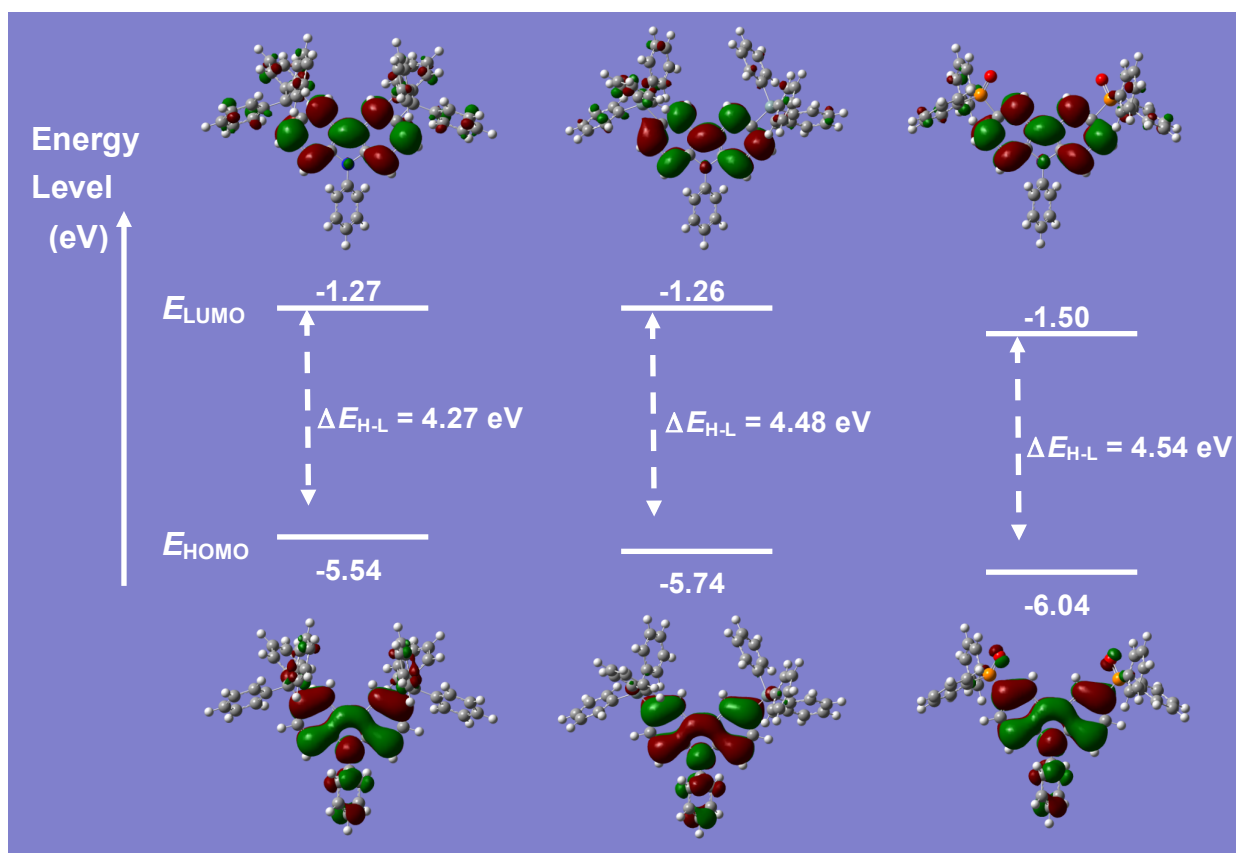
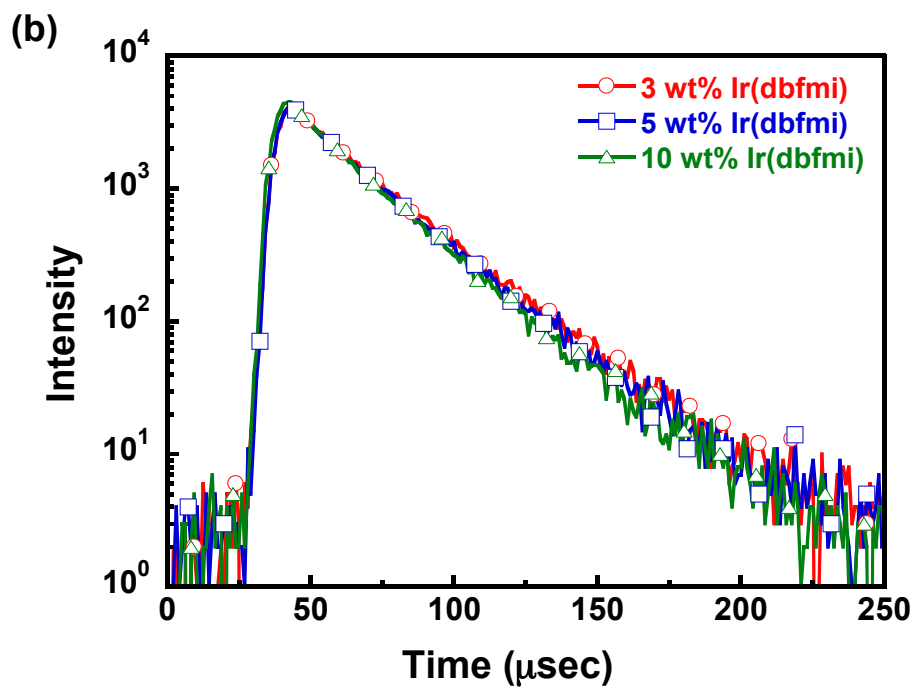
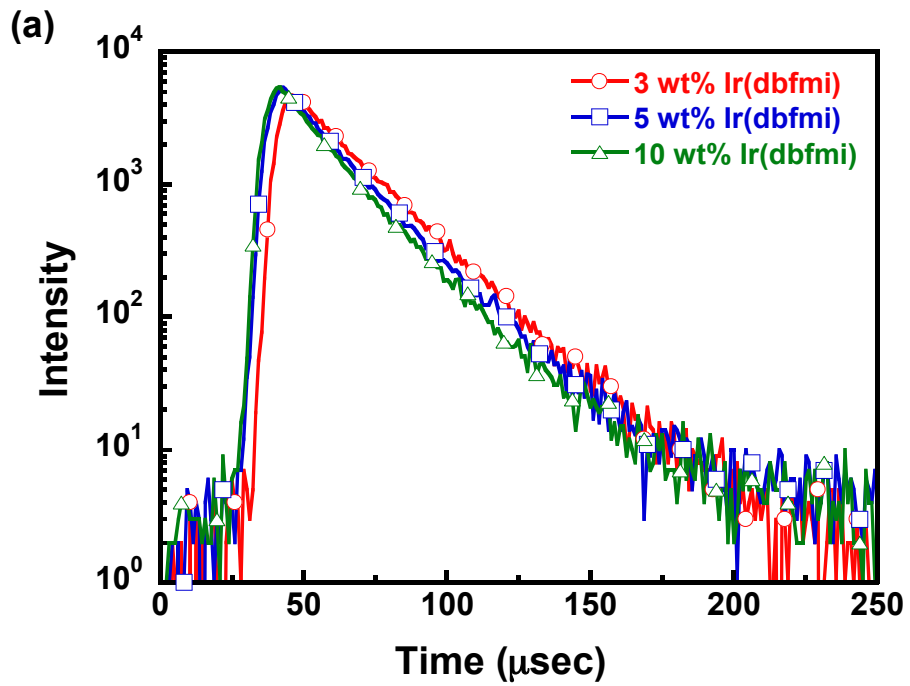


Figure S1. The optimized structures and the spatial distributions of the HOMOs and

LUMOs for the carbazole based hosts, as calculated at the

RB3LYP/6-311+G(d,p)//RB3LYP/6-31G(d,p) level.



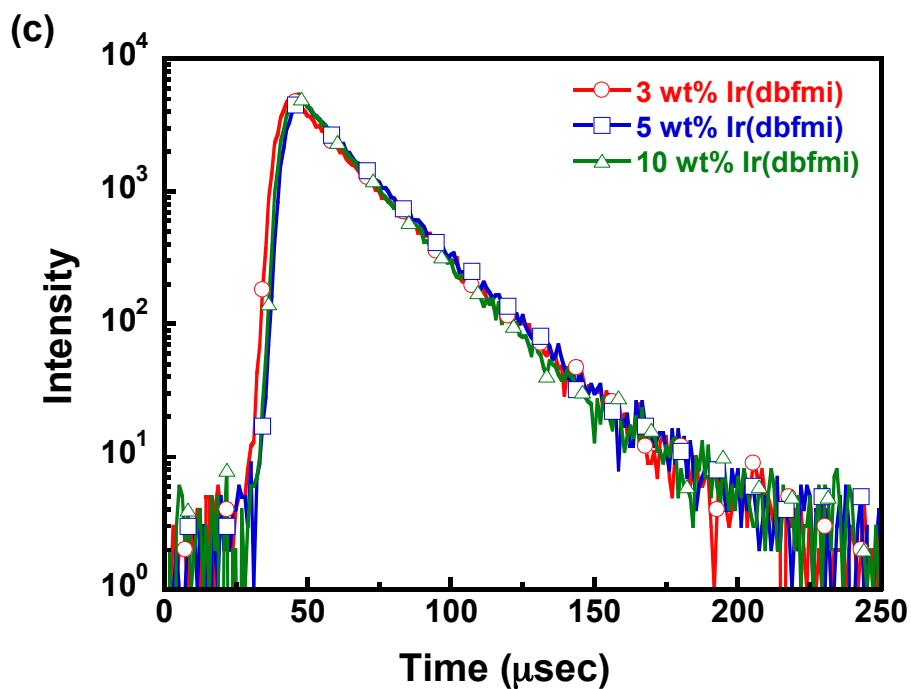


Fig. S2 Phosphorescent decay curves of co-deposited film depending on doping concentration. (a)CCz, (b)SiCz, (c)PO9.

Table S1 Phosphorescent lifetime of co-deposited film depending on doping concentration.

Host	3 wt%				5 wt%				10 wt%			
	η_{PL}	τ_p	$k_r \times 10^5$	$k_{nr} \times 10^5$	η_{PL}	τ_p	$k_r \times 10^5$	$k_{nr} \times 10^5$	η_{PL}	τ_p	$k_r \times 10^5$	$k_{nr} \times 10^5$
	[%]	[μ s]	[s^{-1}]	[s^{-1}]	[%]	[μ s]	[s^{-1}]	[s^{-1}]	[%]	[μ s]	[s^{-1}]	[s^{-1}]
CCz	61	21.4	0.28	0.18	54	19.6	0.27	0.23	49	18.1	0.27	0.28
SiCz	75	25.6	0.29	0.098	75	24.9	0.30	0.10	63	23.9	0.26	0.15
PO9	72	21.2	0.34	0.13	71	21	0.34	0.14	59	19.6	0.30	0.20

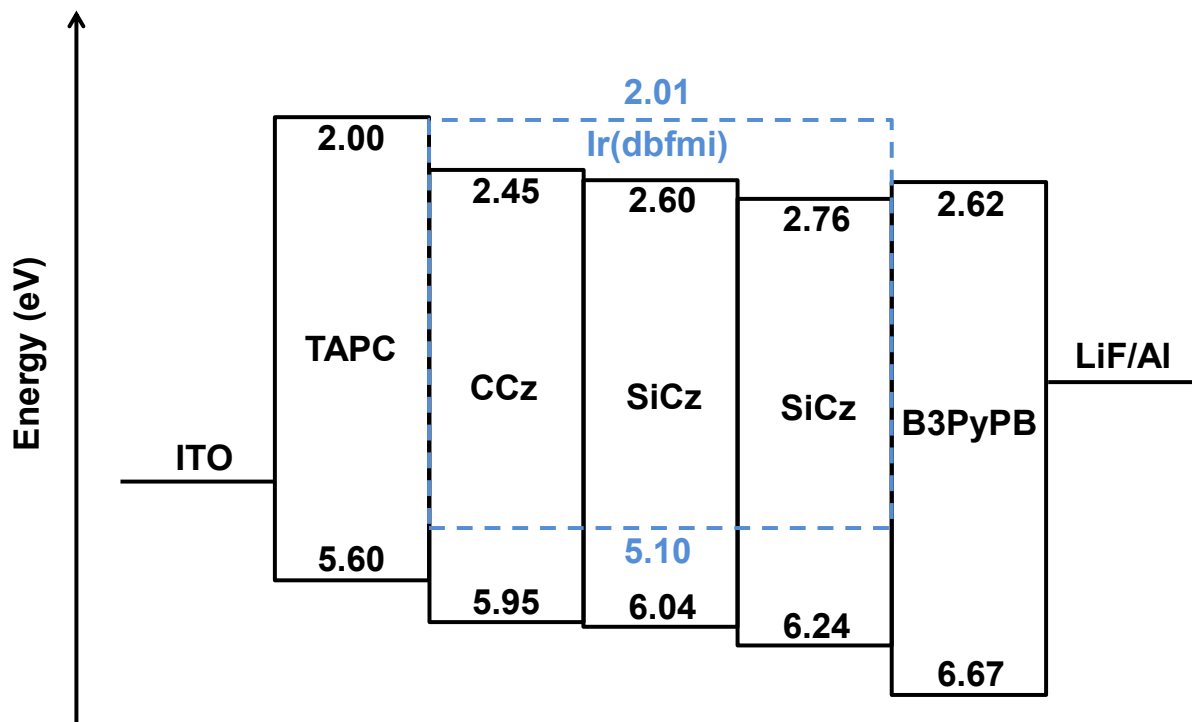
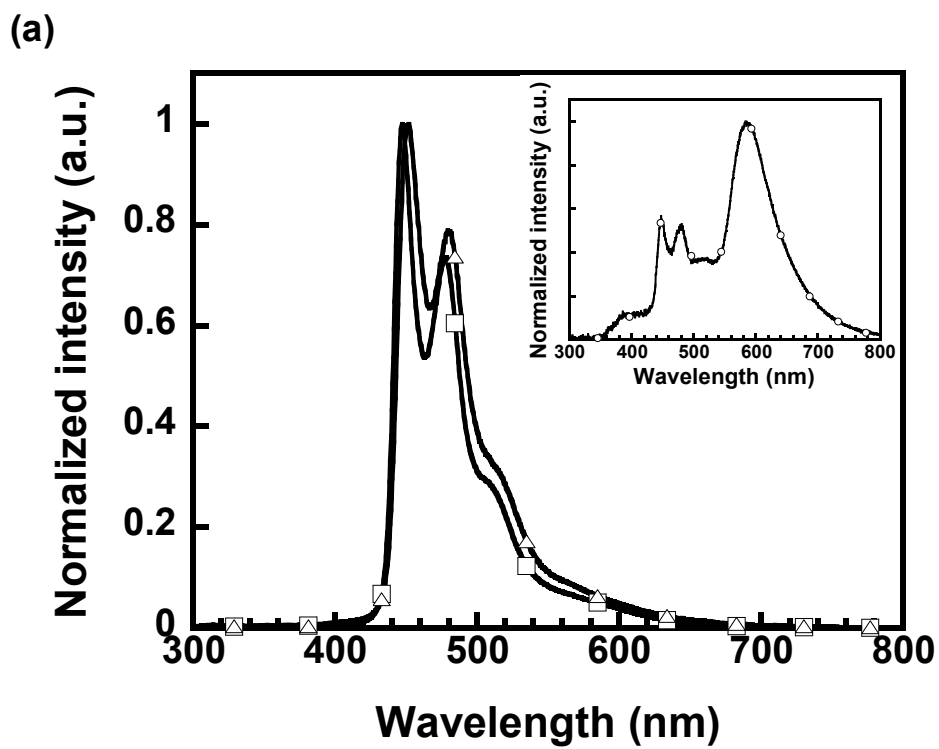


Figure S3. Energy diagram of deep blue phosphorescent organic LED.



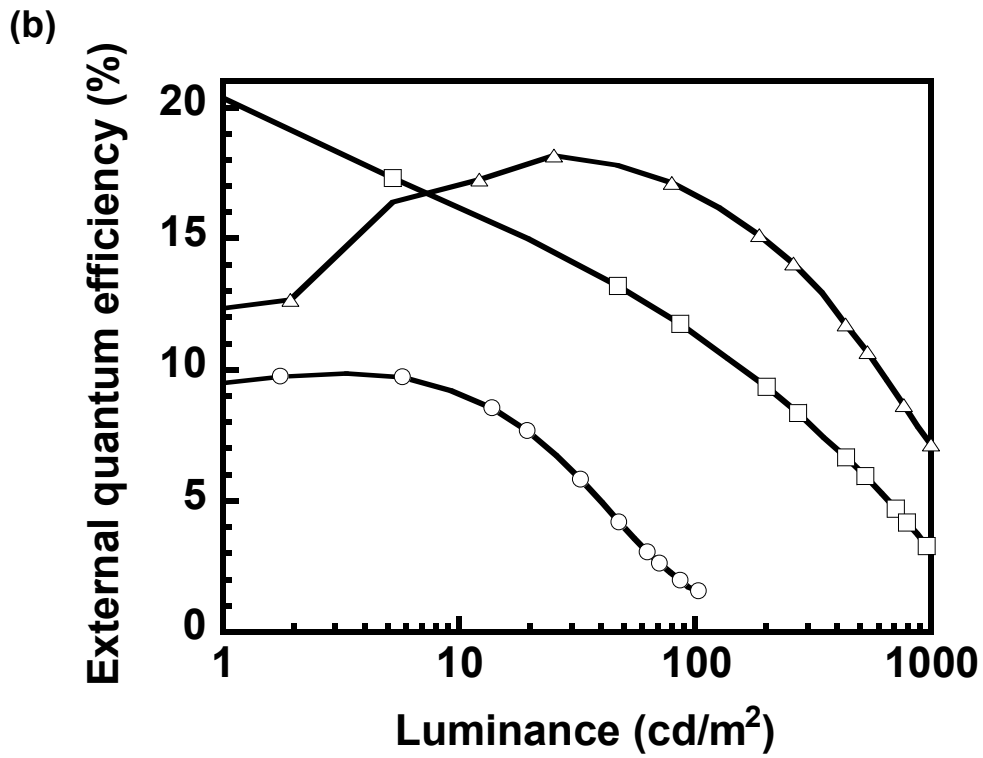


Fig. S3 (a) EL spectra at 1mA. Inset: EL spectrum of CCz based OLED. (b) $\eta_{\text{ext}}-L$ characteristics of deep blue OLEDs using CCz (circle), SiCz (square) and PO9 (triangle), respectively.