

Highly Efficient Orange Phosphorescent Organic Light-Emitting Diodes Based on Iridium (III) Complex with Diethyldithiocarbamate (S[^]S) as the Ancillary Ligand

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1. GC-MS, High Resolution MS Spectra, ¹H-NMR, ¹³C NMR Spectra and EI-MS spectra

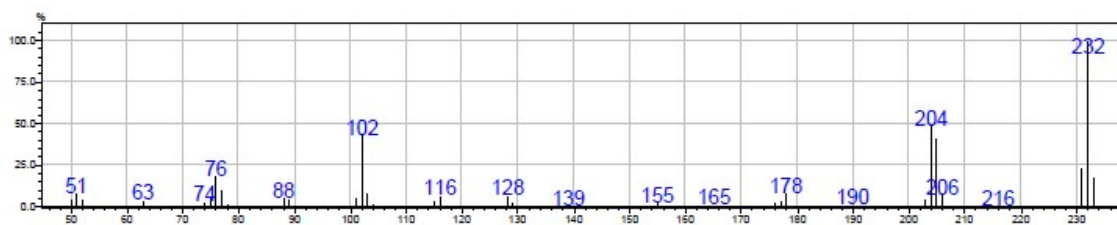


Figure S1. GC-MS of 4,6-Diphenyl pyrimidine in THF

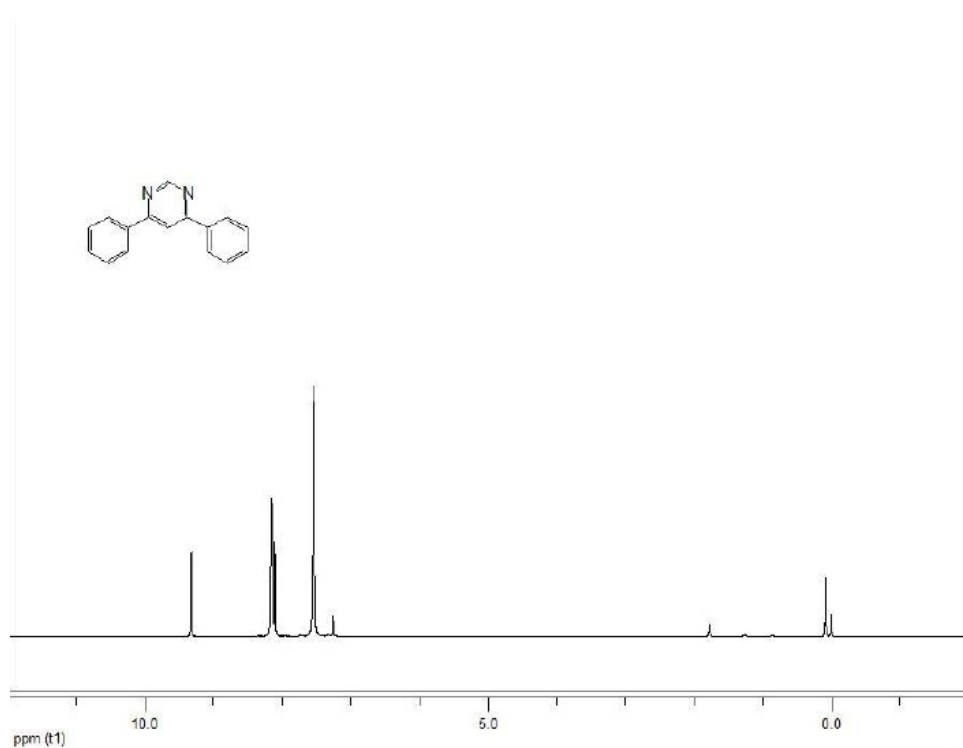


Figure S2. ¹H NMR of 4,6-Diphenyl pyrimidine in CDCl₃

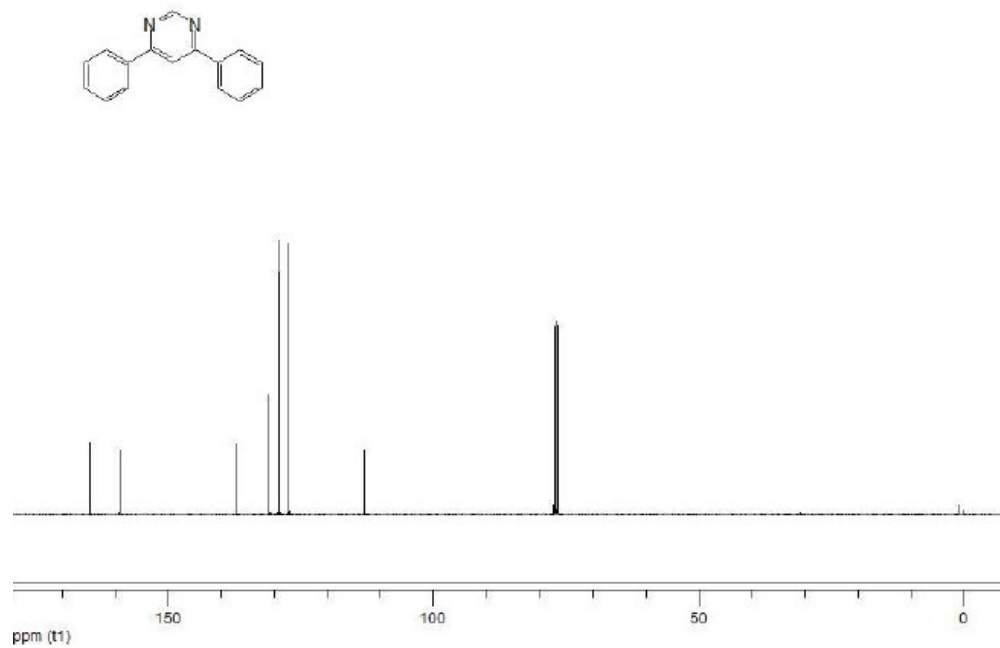


Figure S3. ^{13}C NMR of 4,6-Diphenyl pyrimidine in CDCl_3

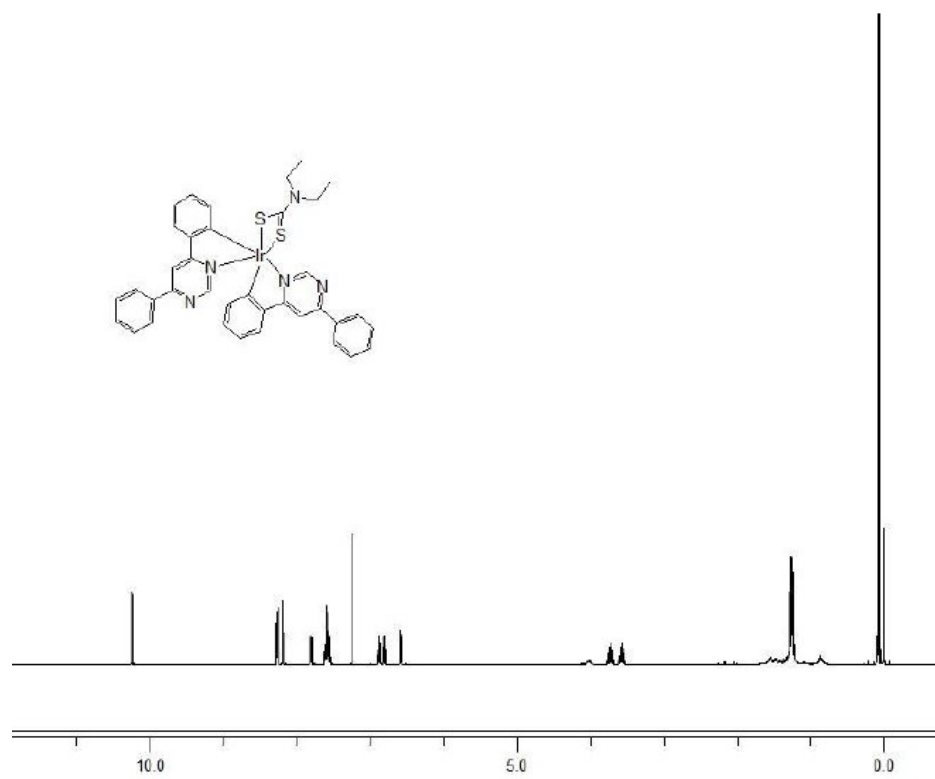


Figure S4. ^1H NMR of $\text{Ir}(\text{dpp})_2\text{dta}$ in CDCl_3

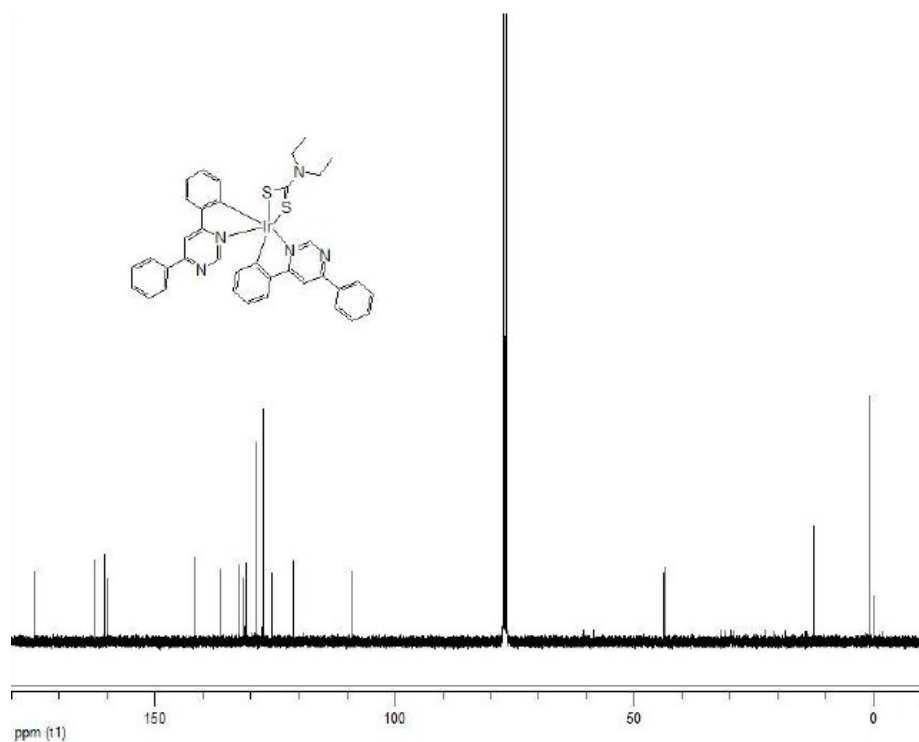


Figure S5. ^{13}C NMR of $\text{Ir}(\text{dpp})_2\text{dta}$ in CDCl_3

$\text{Ir}(\text{dpp})_2(\text{dta})$

Spectrum from 1030pos11.wiff (sample 1) - Sample011, Experiment 1, +TOF MS (100 - 2000) from 0.213 to 0.456 min

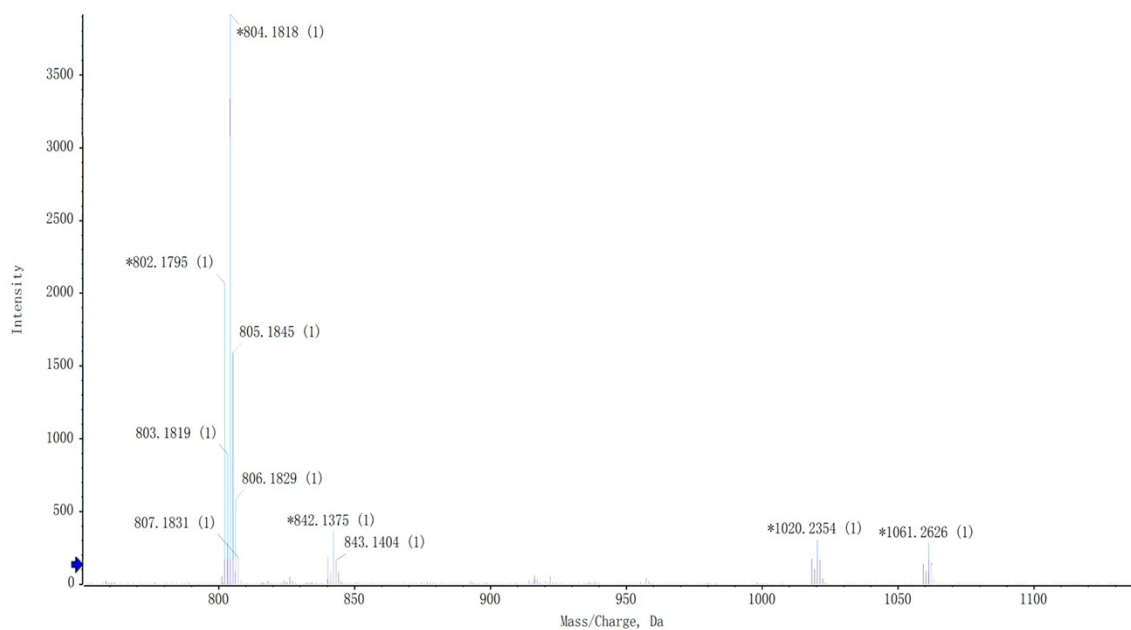


Figure S6. High resolution MS spectra of $\text{Ir}(\text{dpp})_2(\text{dta})$.

2.The X-ray crystallography of Ir(dpp)₂(dta)

(CCDC 1402238 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via <https://www.ccdc.cam.ac.uk/deposit>)

Table S1. Crystal data and structure refinement for Ir(dpp)₂(dta).

Identification code	Ir(dpp)₂(dta)
Empirical formula	C ₃₇ H ₃₂ Ir N ₅ S ₂
Formula weight	804.00
Temperature	293 K
Wavelength	0.71073 Å
space group	P-1
Unit cell dimensions	a = 10.4442(7) Å alpha = 72.086(1) deg. b = 13.1344(10) Å beta = 88.803(2) deg. c = 15.5974(12) Å gamma = 81.704(1) deg.
Volume	2014.0(3) Å ³
Z, Calculated density	2, 1.464 Mg/m ³
Absorption coefficient	3.583 mm ⁻¹
F(000)	880.0
F(000)	878.47
Theta range for data collection	2.35 to 27.45 deg.
Reflections collected / unique	10037 / 9736
Data completeness	97.0 %
Max. and min. transmission	0.616 and 0.506
Final R indices [I>2sigma(I)]	R1 = 0.0354, wR2 = 0.0963

Table S2. Bond lengths [Å] and angles [deg] for Ir(dpp)₂(dta).

Ir(2)-C(38)	2.009(4)
Ir(2)-C(54)	2.019(4)
Ir(2)-N(7)	2.051(3)
Ir(2)-N(9)	2.048(3)
Ir(2)-S(1)	2.4644(9)
Ir(2)-S(2)	2.44785(9)
C(38)-Ir(2)-C(54)	89.96(15)
C(38)-Ir(2)-N(9)	96.11(14)

C(54)-Ir(2)-N(9)	80.00(14)
C(38)-Ir(2)-N(7)	80.02(14)
C(54)-Ir(2)-N(7)	93.21(14)
N(9)-Ir(2)-N(7)	172.23(11)
C(38)-Ir(2)-S(1)	98.97(10)
C(54)-Ir(2)-S(1)	170.71(11)
N(9)-Ir(2)-S(1)	96.42(9)
N(7)-Ir(2)-S(1)	90.85(9)
C(38)-Ir(2)-S(2)	170.01(10)
C(54)-Ir(2)-S(2)	99.75(11)
N(9)-Ir(2)-S(2)	87.94(9)
N(7)-Ir(2)-S(2)	96.98(9)
S(1)-Ir(2)-S(2)	71.44(3)

3. Life time of Ir(dpp)₂(dta)

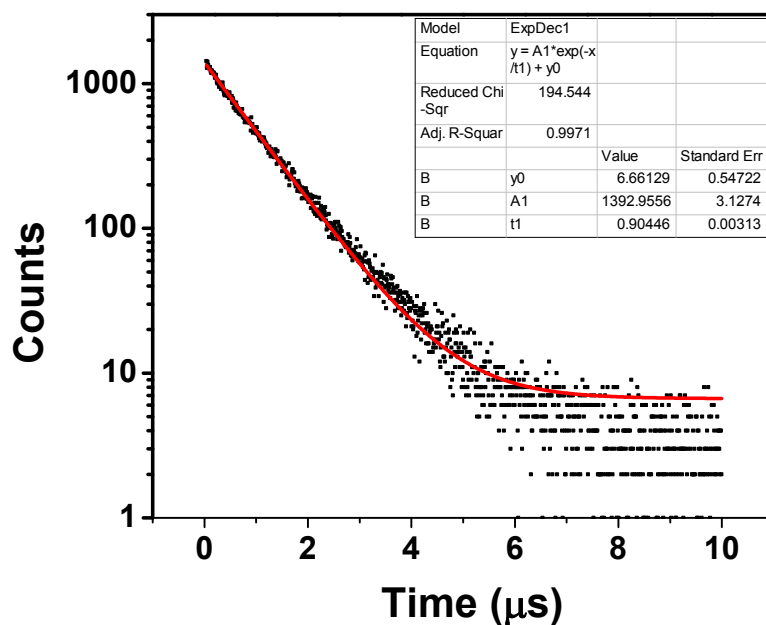


Fig.S7 Life time of Ir(dpp)₂(dta) in 1% PMMA film.

4. Electrochemical properties of ferrocene/ferricenium (Fc/Fc⁺) and Ir(dpp)₂(dta).

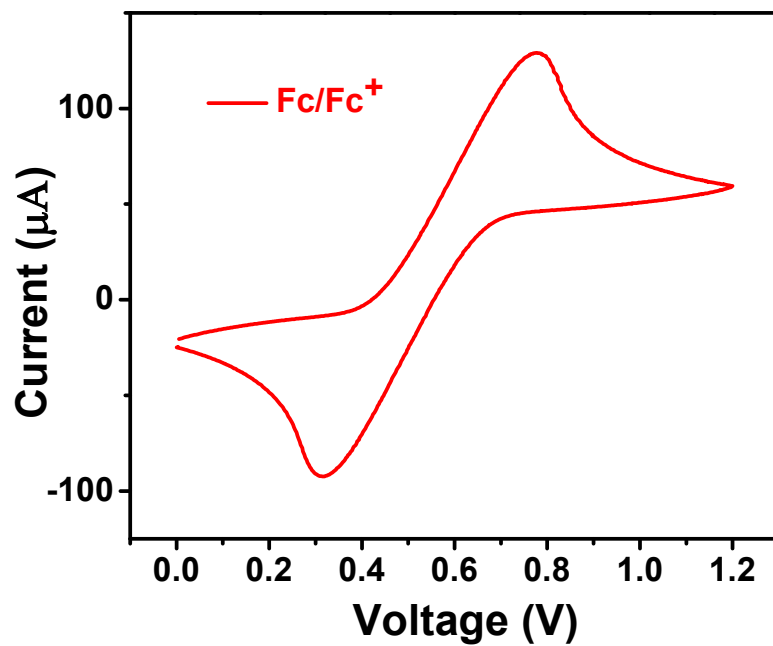


Fig.S8 Cyclic voltammogram of ferrocene/ferricenium (Fc/Fc⁺)

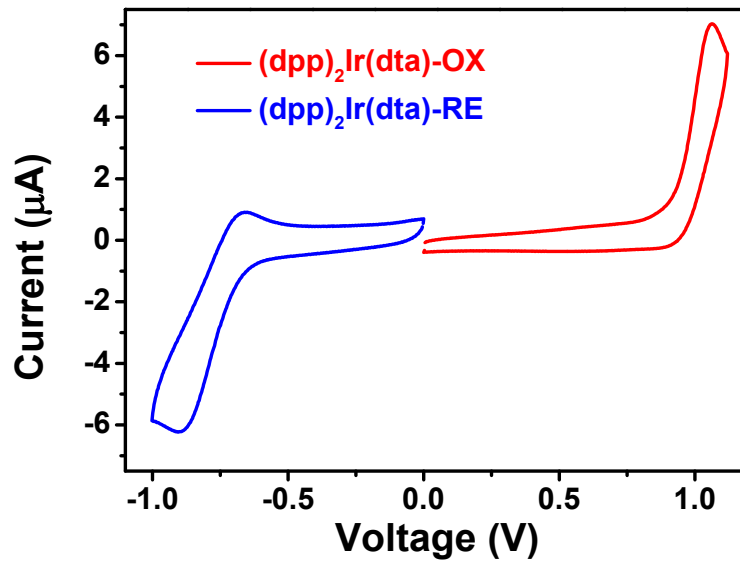


Fig.S9 Cyclic voltammogram of Ir(dpp)₂(dta)

5. Data of Photophysical properties

Table S3. Data of Photophysical properties of Ir(dpp)₂(dta).

	DCM solution	1% PMMA film		Powder	
	$\lambda_{\text{max, abs}}$ (nm)	λ_{PL} (nm)	τ (us)	Φ_{film}	Φ_{power}
(dpp) ₂ Ir(dta)	304, 398, 503	575	0.90	86%	14%

6. PL spectra for different doping concentrations

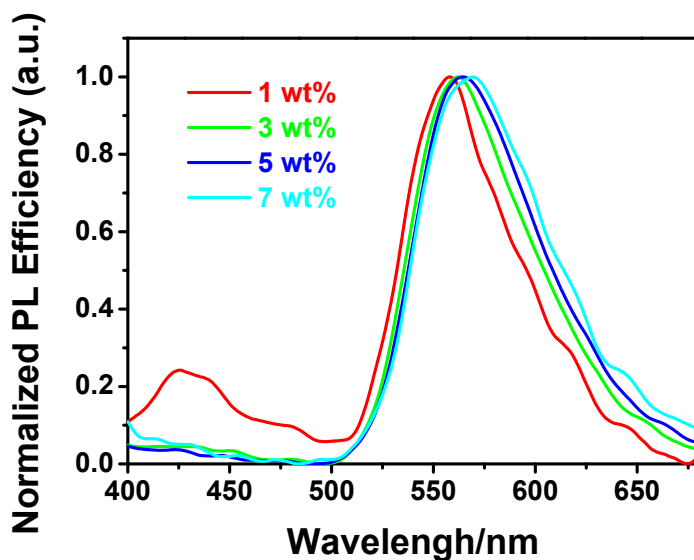
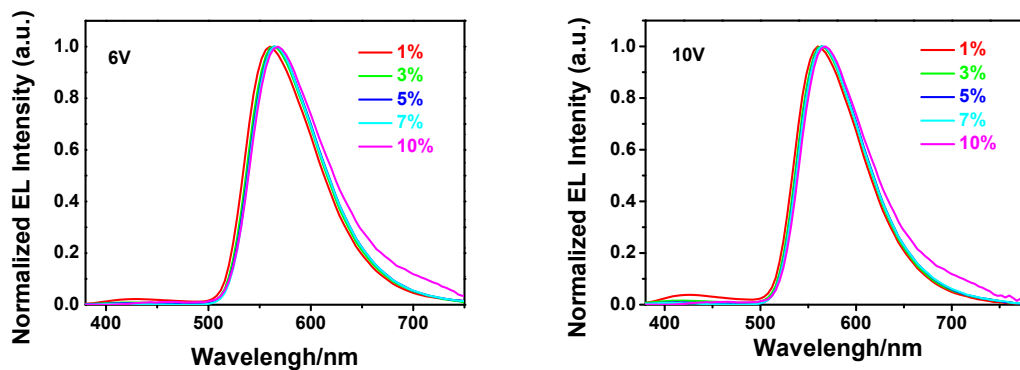


Fig.S10 PL spectra for different doping concentrations

7. The data of Ir(dpp)₂dta doping density from 1% to 10%



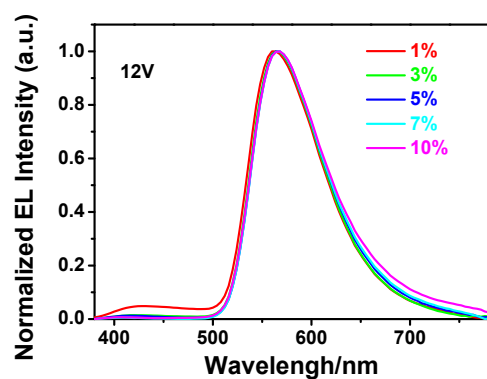


Fig.S11 Electroluminescence spectra of the devices at different density

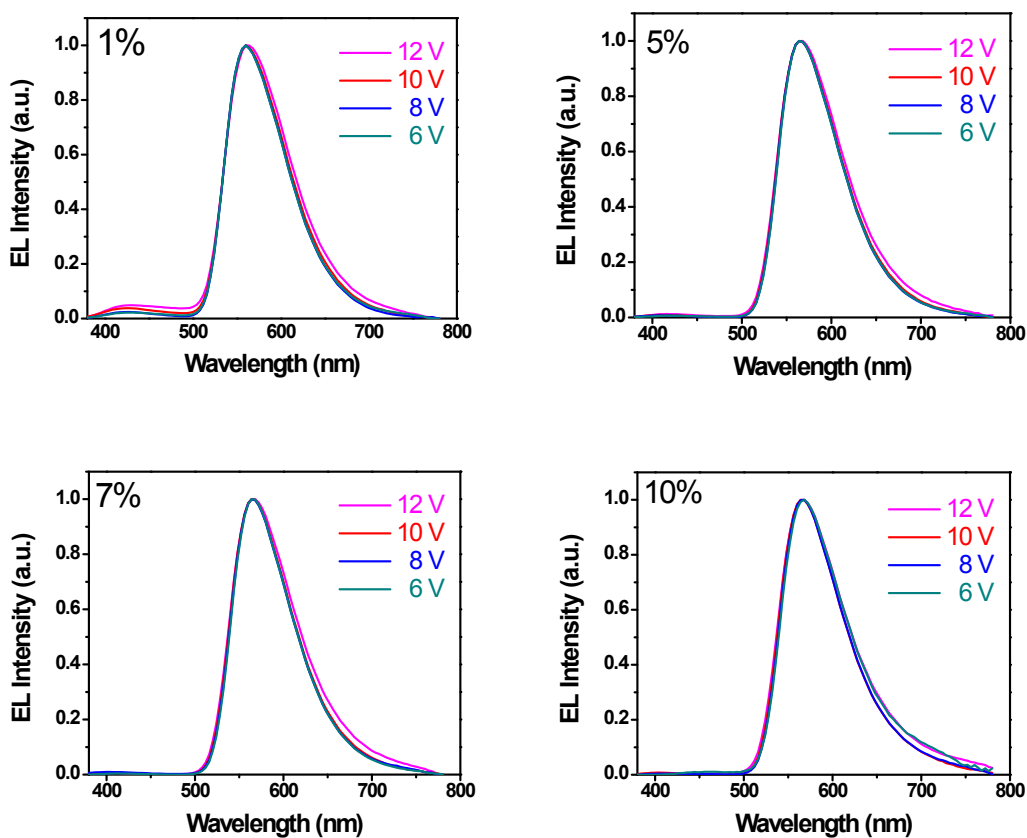


Fig.S12 Electroluminescence spectra of the devices at different voltage

8. CIE plot of $\text{Ir}(\text{dpp})_2(\text{dta})$

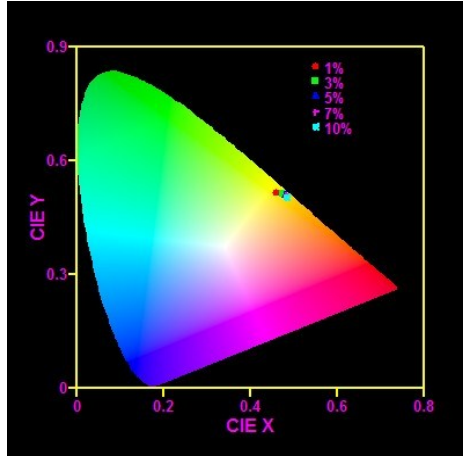


Fig.S13 CIE plot of Ir(dpp)₂(dta)

9. External quantum efficiency–Luminance of the devices

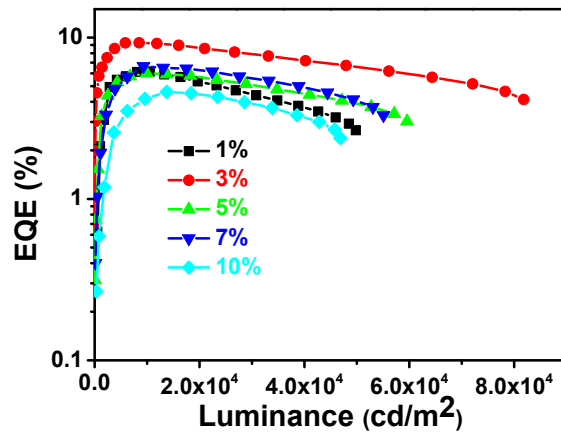


Fig.S14 External quantum efficiency–Luminance of the devices