Electronic Supplementary Information (ESI)

Iridium(III) complexes adopting 1,2-diphenyl-1*H*-benzoimidazole ligands for highly efficient organic light-emitting diodes with low efficiency roll-off and non-doped feature

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Table S1 Crystal data and structure refinements for complex **1**.

Complex **1**			
Formula	$C_{49}H_{45}IrN_8O_3$	V/Å^3	4355(2)
Formula weight	985.79	Z	4
Crystal system	Monoclinic	$D_{calcd.}$[g cm^{-3}]	1.504
Space group	P2(1)/c	μ/mm^{-1}	3.118
a /Å	13.303(5)	F(000)	1983
b /Å	22.847(5)	Observed reflection/unique	22928/7896
c /Å	19.514(5)	R_{int}	0.0557
α/°	90.00	Goodness-of-fit on F^2	0.778
β/°	132.756(15)	R_1[a], wR_2[b][I>2σ(I)]	0.0387, 0.1010
γ/°	90.00	R_1, wR_2 (all data)	0.0708, 0.1240

[a]$R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b]$wR_2 = |\Sigma w(|F_o|^2-|F_c|^2)|/\Sigma|w(F_o^2)^2|^{1/2}$.

Table S2 Comparison between theory and experiment for selected bond lengths [Å] and bond angles [°] in complex **1**.

Complex **1**	Experiment values	Theory values
Ir(1)-C(27)	2.026(7)	2.01777
Ir(1)-C(28)	2.013(6)	2.00576
Ir(1)-N(1)	2.173(5)	2.19861
Ir(1)-N(2)	2.112(5)	2.12396
Ir(1)-N(5)	2.031(5)	2.04201
Ir(1)-N(7)	2.040(5)	2.05165
C(27)-Ir(1)-N(5)	79.4(2)	79.37765
C(28)-Ir(1)-N(7)	80.3(2)	79.55712
C(28)-Ir(1)-N(2)	97.2(2)	97.80971
N(5)-Ir(1)-N(2)	99.7(2)	97.63101
N(7)-Ir(1)-N(2)	88.2(2)	87.00887
C(28)-Ir(1)-N(1)	173.0(2)	173.56553
N(7)-Ir(1)-N(1)	98.4(2)	98.55110
N(2)-Ir(1)-N(1)	75.8(2)	75.90024

Table S3 Calculated triplet states for complexes **1** and **2** by a TD-DFT approach.

Complex	States	E (eV)	f	Assignment[a]	Nature[b]
1	T_1	2.20	0	H→L (82%)	^{3}MLCT/^{3}LLCT/^{3}LC
2	T_1	2.45	0	H→L+1 (45%)	^{3}MLCT/^{3}LC
				H→L (43%)	^{3}MLCT/^{3}LLCT

[a]H and L denote HOMO and LUMO, respectively. [b]MLCT, LLCT and LC denote metal-to-ligand charge transfer, ligand-to-ligand and ligand centered charge transfer, respectively.

Table S4 Photophysical data for **1** and **2** doped in PMMA films (**a**–**d** for **1** and **e**–**i** for **2**).

PMMA films	**a**	**b**	**c**	**d**	**e**	**f**	**g**	**h**	**i**
PL (nm)	520	505	501	498	540	530	522	508	504

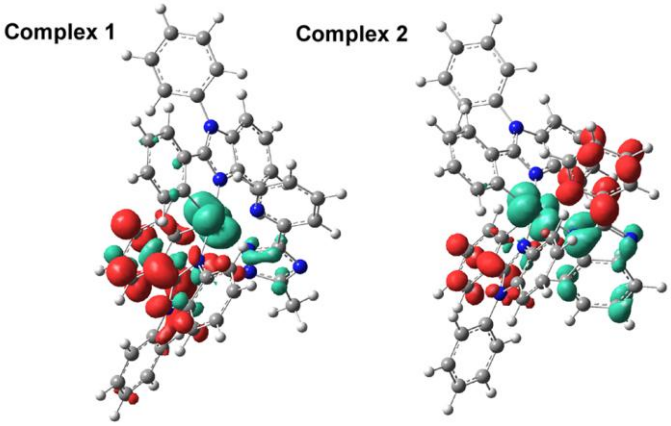

Fig. S1 Difference electron density computed by subtracting the electron densities of the T_1 and S_0 states for complex **1** and **2**. The charge goes from the green to the red areas.

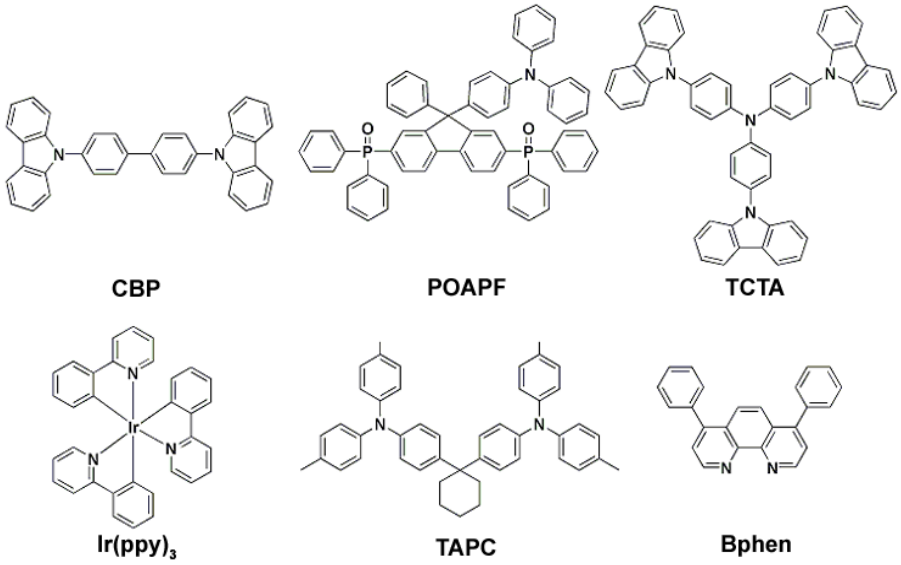

Fig. S2 Chemical structures of the materials used in OLEDs.

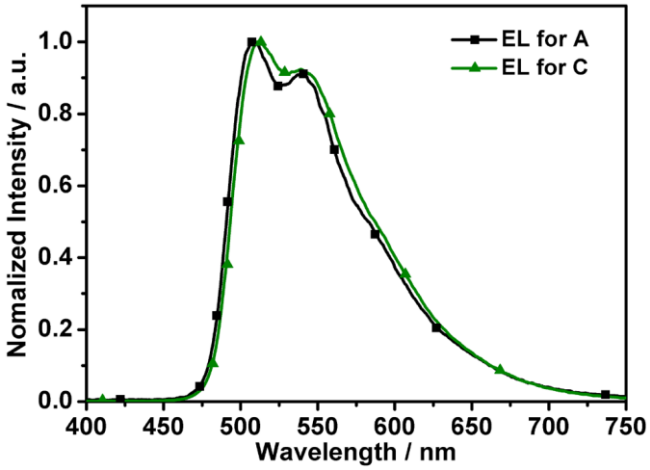

Fig. S3 The EL spectra for devices **A** and **C** at 4.5 V.

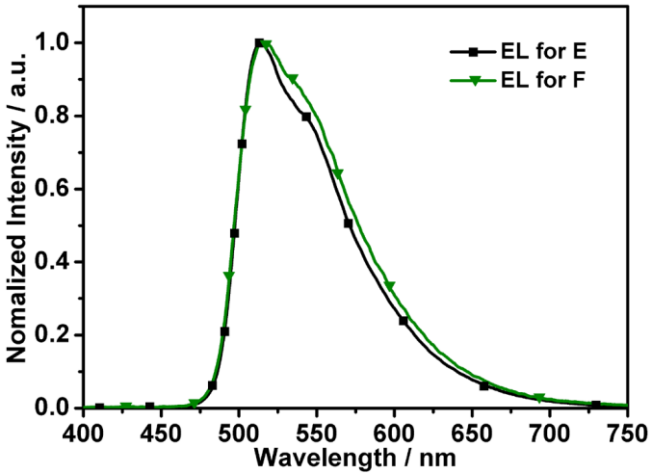

Fig. S4 The EL spectra for devices **E** (at 6 V) and **F** (at 7 V).

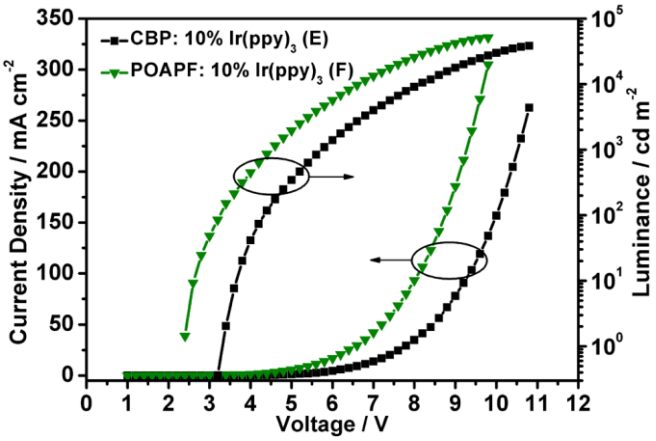

Fig. S5 The current density–voltage–luminance characteristics for devices **E** and **F**.

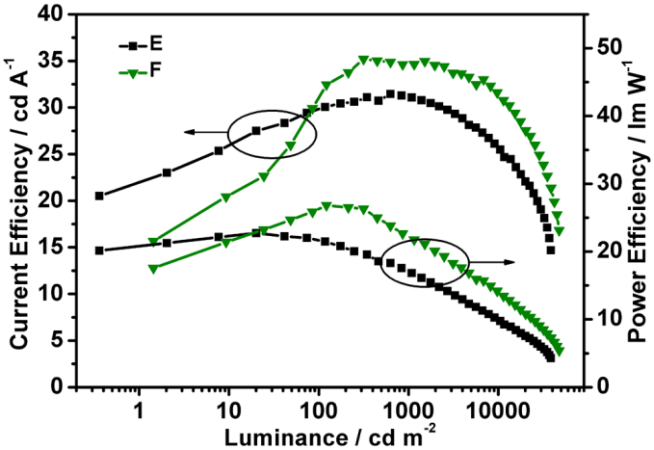

Fig. S6 The current efficiency–luminance–power efficiency characteristics for devices **E** and **F**.

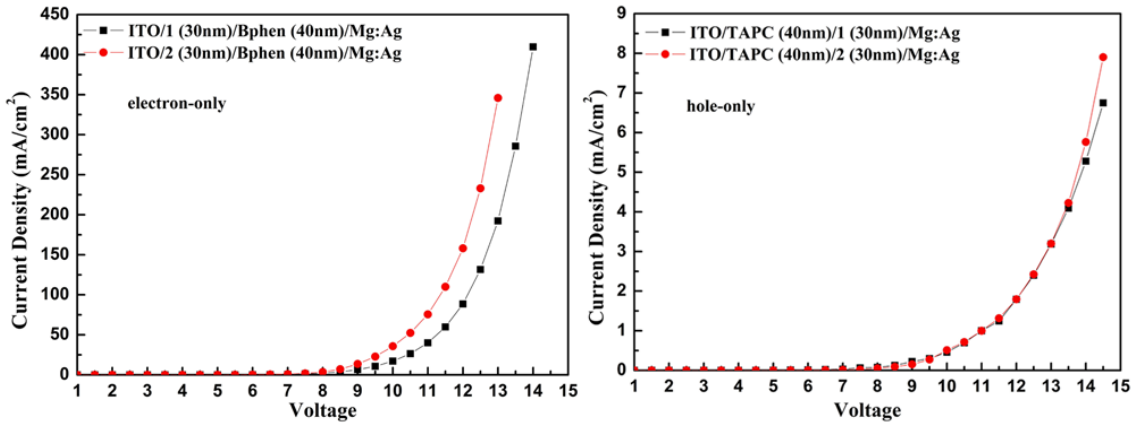

Fig. S7 Current density–voltage curves of single-carrier devices based on **1** and **2**.

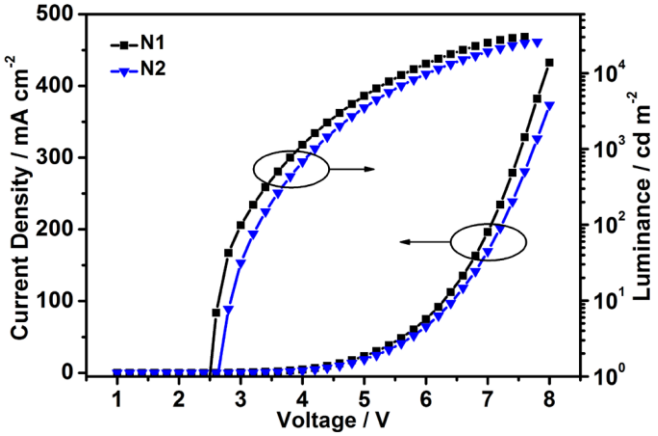

Fig. S8 The current density–voltage–luminance characteristics for devices **N1** and **N2**.