## Supporting Information

Highly efficient chlorine functionalized blue iridium(III) phosphors for blue and white phosphorescent organic light-Emitting diodes with external quantum efficiency exceeding 20%

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## **1.** General Experimental Information

All operations were performed under an inert nitrogen atmosphere using standard Schlenk unless otherwise stated. All solvents were used after distillation and stored over activated molecular sieves (5 Å). All reagents and chemicals were purchased from commercial sources and used without further purification. The NMR spectra were recorded in CDCl<sub>3</sub> or CD<sub>2</sub>Cl<sub>2</sub> with a Bruker spectrometer at ambient temperature. Mass spectra were obtained on SHIMADZU matrix-assisted laser desorption/ionization time-of-flight mass pectrometer (MALDI-TOF-MASS). Elemental analyses were carried out with a VarioEL III O-Element Analyzer system. The UV-vis absorption spectra were recorded on a Shimadzu UV-2550 spectrometer. Steady-state emission experiments at room temperature or 77 K were measured on an Edinburgh LFS-920 spectrometer. Excited-state lifetime studies were performed with an Edinburgh LFS-920 spectrometer with a hydrogen-filled excitation source. The data were analyzed by a software package provided by Edinburgh Instruments. The absolute quantum yields of the complexes were determined through an absolute method by employing an integrating sphere. The solution was degassed by three freeze-pump-thaw cycles. Cyclic voltammetry measurements were carried out in  $CH_2Cl_2$  (5×10<sup>-4</sup> M) with a three-electrode cell configuration consisting of platinum working and counter electrodes and a Ag/AgNO<sub>3</sub> (0.01 M in CH<sub>3</sub>CN) reference electrode at room temperature. Tetra-n-butylammonium hexafluorophosphate (0.1 M in CH<sub>2</sub>Cl<sub>2</sub>) was used as the supporting electrolyte. The redox potentials were recorded at a scan rate of 100 mV/s and are reported with reference to the ferrocene/ferrocenium (Fc/Fc<sup>+</sup>) redox couple.

## 2. Device Fabrication

The devices were fabricated on pre-patterned ITO glass substrates with a sheet resistance of  $15\Omega$ /square. The ITO glass substrates were sequentially cleaned by the detergent, acetone, isopropyl alcohol and deionized water before use. Prior to the thin film deposition, the substrates were treated with the UV ozone to improve the work function and also to remove the possible chemical residuals left on the ITO surface during the wet cleaning processes. Afterwards, the ITO glass substrates were loaded in a vacuum chamber for deposition of organic layers using thermal evaporation under a base pressure of  $5 \times 10^{-4}$  Pa. The film thicknesses and the corresponding deposition rates were controlled by the calibrated crystal quartz sensors. Deposition rates of functional organic layers, the cathode interlayer LiF and the top Al contact were about 1 Å/s, 0.1 Å/s and 3-6 Å/s, respectively. The active emissive area of the devices is 3 mm × 3 mm, defined by the overlap between ITO anode and Al cathode.

The EL spectra, CIE coordinates, CRI, and CCT of OLEDs were measured using a computer controlled PR-655 spectra scan spectrometer. The *J-V-L* were measured by a computer-controlled Keithley 2400 source meter integrated with a BM-70A luminance meter. The *CE* and *PE* were calculated from the plot of *J-V-L*. The *EQE* was calculated from the *J-V-L* curve and spectra data. All samples were characterized immediately after thin films deposition without encapsulation.

The above detailed OLEDs preparation and characterization processes are consistent with the previously reported work by Miao et al.<sup>[S1-S2]</sup>

complex	$\delta$ (ppm)		
	H <sup>a)</sup>		
Ir1	6.48, 6.24		
Ir2	6.54, 6.31		
Ir3	6.49, 6.36		
Ir4	6.55, 6.45		

Table S1 Selected chemical shifts of Ir1-Ir4.

<sup>a)</sup> Protons adjacent to the C-Ir bonds of the phosphors.

Complex	Absorption <sup>a)</sup>	Emission <sup>b)</sup>	Rigidochromic shift <sup>c)</sup>	
	$\lambda_{abs}$ [nm]	$\lambda_{\rm em}$ [nm]	$\lambda_{\Delta}[nm]$	
Ir1	265, 280, 355, 378	465, 501 (sh)	3	
Ir2	263, 284, 328, 387, 422	472, 508 (sh)	4	
Ir3	269, 289, 355, 413	468, 503 (sh)	7	
Ir4	260, 277, 339, 377	465, 500 (sh)	3	

Table S2 Absorption, luminescence data for Ir1-Ir4.

<sup>a)</sup>At a concentration of  $1.0 \times 10^{-5}$  mol/L in CH<sub>2</sub>Cl<sub>2</sub>; <sup>b)</sup> At a concentration of  $1.0 \times 10^{-5}$  mol/L in 2-MeTHF glass matrix at 77 K,  $\lambda_{ex} = 365$  nm; <sup>c)</sup> The difference between the PL peaks measured at room temperature and at 77 K.

Table S3	Photophysical	properties	for some	reported	blue	iridium(III)	phosphors	in solution
state <sup>[S3-S4]</sup> .								

C 1		Emission			
Complex	$\lambda_{ m em}$	FWHM	τ	$\phi_{ m PL}$	
	[nm]	[nm]	[µs]	12	
FIrpic	468, 495 (sh)	-	1.72	0.62	
1	464, 493 (sh)	67	0.79	0.76	
2	480, 506 (sh)	60	1.27	0.81	
3	458, 489 (sh)	52	2.51	0.98	
4	465, 497 (sh)	57	2.02	0.88	
5	457, 488 (sh)	54	3.08	0.71	
6	457, 488 (sh)	52	1.02	0.64	



Fig. S1 The chemical structures of some reported blue iridium(III) phosphors<sup>[S4]</sup>.



Fig. S2 Thermogravimetric curves under  $N_2$  atmosphere of Ir1–Ir4.

**Probe devices:** 

**Device D1**: ITO/ MoO<sub>3</sub>(3 nm)/ TAPC(40 nm)/ DCJTB(0.5 nm)/ TCTA (20 nm)/ TmPyPb(50 nm)/ LiF(1 nm)/ Al(100 nm)

Device D2: ITO/ MoO<sub>3</sub>(3 nm)/ TAPC(40 nm)/ TCTA(5 nm)/ DCJTB(0.5 nm)/ TCTA (15 nm)/ TmPyPb(50 nm)/ LiF(1 nm)/ Al(100 nm)

Device D3: ITO/ MoO<sub>3</sub>(3 nm)/ TAPC(40 nm)/ TCTA(15 nm)/ DCJTB(0.5 nm)/ TCTA (5 nm)/ TmPyPb(50 nm)/ LiF(1 nm)/ Al(100 nm)

**Device D4**: ITO/ MoO<sub>3</sub>(3 nm)/ TAPC(40 nm)/ TCTA(20 nm)/ DCJTB(0.5 nm)/ TmPyPb(50 nm)/ LiF(1 nm)/ Al(100 nm)



**Fig. S3** The normalized EL spectra of the probe devices D1 to D4 at different voltages of 4V, 5V, 6V, and 7V.



Fig. S4 Schematic diagram of the device structure and energy levels of the white OLEDs.































## Notes and references

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