Electronic Supporting Information (ESI)

Hybrid nanospheres of silica covalently containing a yellow-emitting cationic iridium(III) complex: preparation and application in white light-emitting diodes†

Haoju Li,a,b,‡ Jing Qin,a,‡ Shanglan Xian,a Huaijun Tang,*,a Yuxiang Jiao,a Meifang Zhang,c Long Wang,a Qiang Zhou,a and Zhengliang Wang,a

† The first two authors contributed equally to this work.

a Key Laboratory of Green-Chemistry Materials in University of Yunnan Province, National and Local Joint Engineering Research Center for Green Preparation Technology of Biobased Materials, School of Chemistry & Environment, Yunnan Minzu University, Kunming 650500, P. R. China.

E-mail: tanghuaijun@sohu.com

b School of Materials and Energy, Guangdong University of Technology, No. 100 Waihuan Xi Road, Guangzhou Higher Education Mega Center, Guangzhou 510006, China.

c Institute of Carbon Neutral New Energy Research, Yuzhang Normal University, Nanchang 330031, China.

E-mail: mfzhang@whu.edu.cn
## Table of Contents

*Synthesis of [(dfppy)$_2$Ir(NCCH$_3$)$_2$]PF$_6$* ............................................................... 1  

**Fig. S1** $^1$H NMR spectrum of [(dfppy)$_2$Ir(NCCH$_3$)$_2$]PF$_6$ ........................................ 1  

**Fig. S2** $^1$H NMR spectrum of [(dfppy)$_2$Ir(TBD)]PF$_6$ .................................................. 2  

**Fig. S3** MS spectrum of [(dfppy)$_2$Ir(TBD)]PF$_6$ .............................................................. 2  

**Fig. S4** EL emission spectrum of 455 nm GaN-based blue-emitting chip .......................... 3  

**Fig. S5** The PL decay curves and corresponding tri-exponential fitting lines of pure solid [(dfppy)$_2$Ir(TBD)]PF$_6$ and hybrid nanospheres ......................... 3
Synthesis of \([(dfppy)_2Ir(NCCH_3)_2]PF_6\)

The dimer \((dfppy)_2Ir(\mu-Cl)_2Ir(dfppy)_2\) (1.00 g, 0.82 mmol) was added in 60.0 mL CH_3CN and heated to 60~70 °C, after the dimer was dissolved, AgPF_6 (0.42 g, 1.66 mmol) was added into the solution and stirred in the dark at 60~70 °C for 12 h (overnight), the reaction mixture was filtered over a Celite pad to separate a yellow solution from the gray precipitate (Ag and AgCl). The solution was concentrated to about 1.0 mL in vacuo, and diethyl ether (10.0 mL) was added to give a yellow precipitate. The precipitate was collected by filtration and redissolved in about 1.0 mL CH_3CN, the precipitate was regenerated after diethyl ether (10.0 mL) was added. The product was collected by filtration again and dried under vacuum, yellow solid, yield 82.1% (1.08 g). ^1H NMR (400 MHz, CDCl_3, ppm, Fig. S1 in Electronic Supporting Information), δ: 8.97 (d, 2H, J = 2.6 Hz, ArH), δ: 8.24 (d, 2H, J = 4.2 Hz, ArH), δ: 7.92 (t, 2H, J = 8.0 Hz, ArH), δ: 9.37−9.41 (m, 2H, ArH), δ: 6.33−6.39 (m, 2H, ArH), 5.42 (d, 2H, J = 8.4 Hz, ArH), δ: 2.33 (s, 6H, −CH_3).

Fig. S1 ^1H NMR spectrum of \([(dfppy)_2Ir(NCCH_3)_2]PF_6\), 400 MHz, CDCl_3.
Fig. S2 $^1$H NMR spectrum of [(dfppy)$_2$Ir(TBD)]PF$_6$, 400 MHz, CDCl$_3$.

Fig. S3 MS spectrum of [(dfppy)$_2$Ir(TBD)]PF$_6$. 
**Fig. S4** EL emission spectrum of 455 nm GaN-based blue-emitting chip. Inset: The photographs of the chip under natural light and its working state.

**Fig. S5** The PL decay curves (black) and corresponding tri-exponential fitting lines (red) of (a) pure solid [(dfppy)$_2$Ir(TBD)]PF$_6$ and (b) hybrid nanospheres. Inset: Fitting data.