Supplementary Information

Design, synthesis and characterization of a new blue phosphorescent Ir complex

Chuang Yao,[‡] Jingxian Li,[‡] Jinshan Wang, Xinjun Xu,* Ronghua Liu and Lidong Li*

School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, P. R. China. E-Mail: xuxj@mater.ustb.edu.cn; lidong@mater.ustb.edu.cn



Fig. S1 The phosphorescent spectra of compound 2 in CH_2Cl_2 at 77 K.



Fig. S2 The transient photoluminescence decay curves of FIrpic and **Cz-C8-FIrpic** in both neat and doped (in PVK:OXD-7) thin films measured at 477 nm (at room temperature). The doping concentrations of FIrpic and **Cz-C8-FIrpic** are 5 wt% and 7.5 wt%, respectively, to ensure a same molar ratio.

Photoluminescence Quantum Yields

In order to improve the precision of quantum yield measurement, the concentration of FIrpic and **Cz-C8-FIrpic** in degassed acetonitrile solutions was controlled very low with the absorption optical density below 0.1 at 335 nm. The quantum yield of **Cz-C8-FIrpic** was calculated using the equation:

$$Q = Q_R \frac{I}{I_R} \frac{dD_R}{dD} \frac{d^2}{n_R^2}$$

In this equation Q is the quantum yield, I is the integrated intensity, n is the refractive index, OD is the optical density, and the subscript R refers to the reference dye with a known quantum yield. Here we use FIrpic as the reference whose absolute quantum yield is known as 61% in degassed acetonitrile solution.^{S1} So the quantum yield of **Cz-C8-FIrpic** was measured to be 58%.



Fig. S3. Curves of a),c),e) the current efficiency *versus* current density and b),d),f) external quantum efficiency (EQE) *versus* luminance for device 1,2 (80 °C); 3,4 (120 °C); and 5,6 (150 °C). All the devices have a structure of ITO/PEDOT:PSS /PVK:OXD-7: FIrpic or Cz-C8-FIrpic/Ca/Al



Fig. S4 The normalized EL spectra (a) and zoom-in spectra around 540–700 nm (b) for devices doped with FIrpic at different concentrations (1 wt%, 5 wt% and 10 wt%).

Table S1. Frontier molecular orbital (MO) energies (E, eV) and MO compositions (%) of **Cz-C8-FIrpic** in the lowest-lying triplet excited state in CH₂Cl₂.

| MO ^a | Energy eV | MO composition (%) ^b | | | Assignment | |
|-----------------|--------------|---------------------------------|--------|-------|-----------------|--|
| | | Ir | ligand | Cz-C8 | rssignment | |
| L | -1.91 | 5 | 95 | 0 | $\pi^*(ligand)$ | |
| Н | -5.37 | 0 | 0 | 100 | π(Cz-C8) | |
| H-1 | -5.43 | 38 | 62 | 0 | d(Ir)+π(ligand) | |
| Н-3 | -6.02 | 44 | 56 | 0 | d(Ir)+π(ligand) | |
| H-4 | -6.13 | 26 | 74 | 0 | d(Ir)+π(ligand) | |

^a H = HOMO, H-1 = HOMO-1, H-3 = HOMO-3, H-4 = HOMO-4, L = LUMO; ^b ligand = ligand in FIrpic unit, Cz-C8 = 9-phenyl-9*H*-carbazole linked with alkyl chain.

Table S2. Calculated orbital transition analyses based on the optimized geometry of the lowest-lying triplet state by TD-DFT/B3LYP method.

| State | Configuration ^a | Composition (%) | Assignment | MLCT ^b | |
|--------------------------------|-----------------------------------|--------------------|---|-------------------|--|
| S ₀ -T ₁ | $\text{H-1} \rightarrow \text{L}$ | 70 | $d(Ir)+\pi(Iigand) \rightarrow \pi^*(Iigand)$ | | |
| | $H-3 \rightarrow L$ | 6 | $d(Ir)+\pi(Iigand) \rightarrow \pi^*(Iigand)$ | 29% | |
| | $H-4 \rightarrow L$ | 16 | $d(Ir)+\pi(Iigand) \rightarrow \pi^*(Iigand)$ | | |

^a H-1 = HOMO-1, H-3 = HOMO-3, H-4 = HOMO-4, L = LUMO; ^b MLCT denotes metal-to-ligand charge transfer.

To investigate the spatial distribution of Ir element in these films, the dark-field scanning transmission

electron microscopy (STEM) and energy-dispersive X-ray spectroscopy (EDS) mapping of the same region were shown in Fig. S5. The EDS mapping of Ir implied that the distribution of FIrpic unit in both films is uniform, but it is hard to get a quantitative analysis of the distribution of FIrpic unit in these films.



Cz-C8-FIrpic doped PVK:OXD-7 film

Fig. S5 The STEM images recorded from the FIrpic and **Cz-C8-FIrpic** doped films (left). Elemental mapping of the same region, indicating spatial distribution of Ir (right).

Reference

S1 J. Frey, B. F. Curchod, R. Scopelliti, I. Tavernelli, U. Rothlisberger, M. K. Nazeeruddin and E. Baranoff, *Dalton. Trans.*, 2014, **43**, 5667.