

**The crystal structures and chiral luminescence of three Iridium(III) complexes  
with the maximum EQE of 10.7% at 5000 cd/m<sup>2</sup>**

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**Abstract**

In this paper, three Iridium(III) complexes, Ir(dnfppy)<sub>2</sub>(Cl/Pyrrole), Ir(dfppy)<sub>2</sub>(dpp) and Ir(tfmqz)<sub>2</sub>(sdpp), have been designed and synthesized. They emitted deep-blue, blue or red photoluminescence with high quantum yields, for ((Ir(dnfppy)<sub>2</sub>(Cl/Pyrrole):  $\lambda_{\max}$  = 447 nm, F = 62.4%; Ir(dfppy)<sub>2</sub>(dpp):  $\lambda_{\max}$  = 467 nm, F = 25%; Ir(tfmqz)<sub>2</sub>(sdpp):  $\lambda_{\max}$  = 609 nm, F = 73.7%), respectively. Two pairs of enantiomers of Ir(dfppy)<sub>2</sub>(dpp) and Ir(tfmqz)<sub>2</sub>(sdpp) have been separated by column chromatography. The maximum external quantum efficiency (EQE<sub>max</sub>) of OLEDs based on Ir(tfmqz)<sub>2</sub>(sdpp) was 13.8%, showing a relatively low efficiency roll-off with the EQE of 10.7% at 5000 cd/m<sup>2</sup>.

**Keywords:** Circularly polarized luminescence, Double chiral centers, Iridium(III) complexes

## 1. Introduction

Circularly polarized luminescence (CPL) has attracted considerable attention because of its wide applications in optical data storage, backlights in 3D displays and liquid-crystal display, spin sources in optical spintronics and information carriers in quantum computation.<sup>[1]</sup> Although chiral luminophores with circularly polarized photoluminescence (CPPL) have made considerable progress so far<sup>[2]</sup>, the development of circularly polarized electro-luminescence (CPEL) emitters, which would be more practical for future display and photonic technologies, still lag behind.<sup>[3]</sup> For CPEL, the luminescence dissymmetry factor (*g* factor) is an important parameter to evaluate the degree of polarization, which is defined as  $g_{EL} = \Delta I / I = 2(I_L - I_R) / (I_L + I_R)$ , where  $I_L$  and  $I_R$  represent the left and right-handed luminescence polarized intensity values, respectively.<sup>[4]</sup> At present, the  $|g_{EL}|$  values were mostly in the order of  $10^{-3}$  for the emitting devices based on CPL-active organic molecules. Therefore, it is necessary to study the relationship of the structure and photo-physical properties of chiral luminescence materials to further improve the  $|g_{EL}|$  factors.

Phosphorescent materials based on complexes of heavy metals such as Pt( II )<sup>5</sup>, Os( II )<sup>6</sup> and Ru( II )<sup>7</sup> are able to achieve theoretically 100% internal quantum efficiency through harvesting singlet and triplet excitons, because they can be synchronously utilized by spin-orbit coupling interactions due to the metal effect. Among the heavy-metal complexes used in phosphorescent OLEDs, Ir( III ) complexes, which are used as emitters in organic light-emitting diodes (OLEDs) due to the high phosphorescent quantum efficiency and broad emission colors range.<sup>[8]</sup> To the best of our knowledge, there are few reports about the utilization of chiral phosphorescent Iridium(III) complexes to construct the emitting device.<sup>[9]</sup> For example, Zheng et al. reported a series of Iridium(III) complex isomers by introducing chiral phosphine atoms in the ancillary ligand. The two pairs of enantiomers for Ir(dfppy)<sub>2</sub>(L), (where dfppy is 2-(2,4-difluorophenyl) pyridine, and L is sulfur-dipyridinylphosphinate oxide), based on  $\Lambda$  or  $\Delta$  isomer together with chiral phosphine center (*R* or *S*), have been designed and studied.<sup>[10]</sup> Meanwhile, the OLEDs based on enantiomeric isomers of Iridium(III) complexes as emitters showed the obvious CPEL signals with the maximum external quantum efficiency (EQE) of 14.6%. As well as we know,  $\Lambda$  ( $\lambda$ ) and  $\Delta$  ( $\delta$ ) isomers of Iridium(III) complexes can be obtained by chiral column separation. However, the process to separate or purify  $\Lambda$  and  $\Delta$  isomers was complicated.<sup>[11]</sup> In addition, most of Iridium(III) complexes also exhibited a low  $|g_{PL}|$  factor.<sup>[12]</sup> We are interested that what will happen to the chirality of the luminescence for the Iridium(III) complex, when the chiral phosphorus atoms are linked to different atoms in comparison with Ir(dfppy)<sub>2</sub>(L), or when the main ligands change.

Herein, we have designed and synthesized three Iridium(III) complexes to investigate the effect of chiral phosphorus auxiliary ligands on the photo-electric properties. They were only one or double chiral centers for Ir(dnfppy)<sub>2</sub>(Cl/Pyrrrole), Ir(dfppy)<sub>2</sub>(dpp) and Ir(tfmqz)<sub>2</sub>(sdpp), respectively. The research results can provide a new, adaptable method for designing chiral emitters.

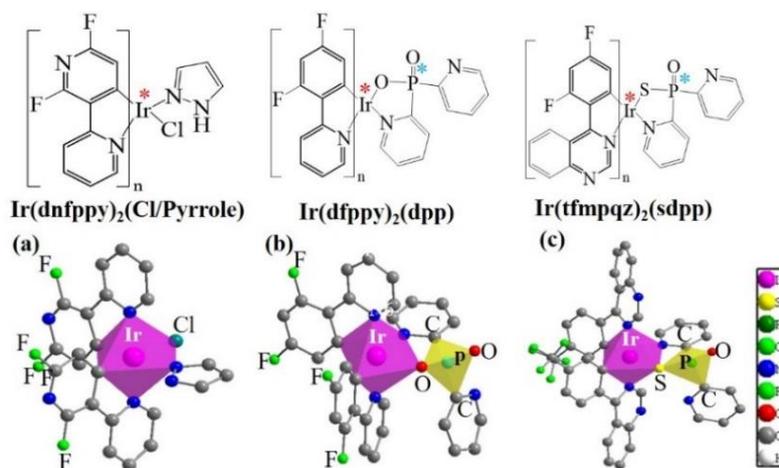
## 2. Experiment section

The cyclometallated chloro-bridged dimers (0.20 mmol) and 2.2 equivalent sodium di(pyridin-2-yl)phosphinothioate (0.44 mmol) were dissolved in 10 mL of dichloromethane. After degassed, the reaction was maintained at room temperature for about 10 min under argon. The solvent was removed and the crude compound purified by column chromatography with  $\text{CH}_2\text{Cl}_2$ : MeOH = 20:1 as eluent. Further purification was taken by gradient sublimation. And then four chiral Iridium(III) isomers were obtained by column chromatography.

$\text{Ir}(\text{dnfppy})_2(\text{Cl}/\text{Pyrrole})$ . EI-TOF-MS (M/Z): Calculated for  $\text{C}_{23}\text{H}_{14}\text{F}_4\text{IrN}_6$ ,  $[\text{M}+\text{H}]^+$  678.053, found 679.780.

$\text{Ir}(\text{dfppy})_2(\text{dpp})$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.79-8.68 (m, 2H), 8.53-8.38 (m, 2H), 8.37-8.27 (m, 2H), 8.24-8.10 (m, 2H), 8.00-7.85 (m, 4H), 7.81-7.71 (m, 4H), 7.69-7.61 (m, 1H), 7.35-7.24 (m, 1H), 7.16-7.04 (m, 3H), 7.03-6.96 (m, 1H), 6.59 (d,  $J=1.8$  Hz, 1H), 6.38 (dd,  $J=14.9, 1.8$  Hz, 1H).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -106.59 (1F), -108.49 (1F), -109.02 (1F), -110.64 (1F).  $^{31}\text{P}$  NMR (162 MHz,  $\text{CDCl}_3$ )  $\delta$  33.64. EI-TOF-MS (M/Z): Calcd for  $\text{C}_{40}\text{H}_{24}\text{F}_6\text{IrN}_6\text{OPS}$ ,  $[\text{M}+\text{H}]^+$  997.089, found 997.089.

$\text{Ir}(\text{tfmpqz})_2(\text{sdpp})$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.79-8.68 (m, 2H), 8.53-8.38 (m, 2H), 8.37-8.27 (m, 2H), 8.24-8.10 (m, 2H), 8.00-7.85 (m, 4H), 7.81-7.71 (m, 4H), 7.69-7.61 (m, 1H), 7.35-7.24 (m, 1H), 7.16-7.04 (m, 3H), 7.03-6.96 (m, 1H), 6.59 (d,  $J=1.8$  Hz, 1H), 6.38 (dd,  $J=14.9, 1.8$  Hz, 1H).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -106.59 (1F), -108.49 (1F), -109.02 (1F), -110.64 (1F).  $^{31}\text{P}$  NMR (162 MHz,  $\text{CDCl}_3$ )  $\delta$  33.64. EI-TOF-MS (M/Z): Calcd for  $\text{C}_{40}\text{H}_{24}\text{F}_6\text{IrN}_6\text{OPS}$   $[\text{M}+\text{H}]^+$  997.089, found 997.089.



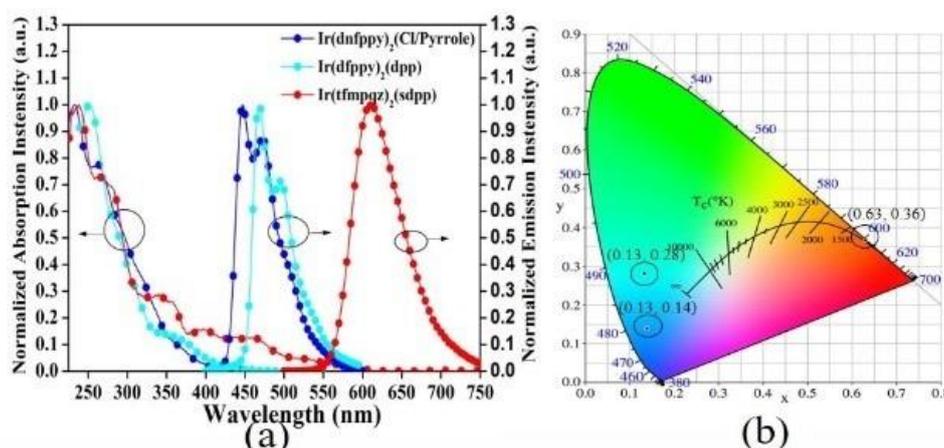
**Fig. 1.** The chemical and single crystal diffraction structures of  $\text{Ir}(\text{dnfppy})_2(\text{Cl}/\text{Pyrrole})$  (CCDC no. 1956569), (b)  $\text{Ir}(\text{dfppy})_2(\text{dpp})$  (CCDC no. 2025773), (c)  $\text{Ir}(\text{tfmqz})_2(\text{sdpp})$  (CCDC no. 2053656).

## 3. Results and discussion

### 3.1 Synthesis and characterization of Iridium(III) complexes

The designing strategy and synthetic routes of Ir(dnfppy)<sub>2</sub>(Cl/Pyrrrole), Ir(dfppy)<sub>2</sub>(dpp) and Ir(tfmqz)<sub>2</sub>(sdpp) were shown in Fig. 1. Single crystals of three Iridium(III) complexes were obtained by solvent evaporation method. As shown in Fig.1, Ir(dnfppy)<sub>2</sub>(Cl/Pyrrrole) adopted distorted octahedral coordination geometry with the distance of 2.45 Å between Ir and Cl atom. For Ir(dfppy)<sub>2</sub>(dpp), the angle of C-P-C is 106.4°, indicating different positions of two pyridine groups in space. Meanwhile, due to the coordination between iridium and nitrogen atoms in the pyridine group, P-O-Ir-N-C forms stable five-membered ring. Ir(tfmpqz)<sub>2</sub>(sdpp) also adopted distorted octahedral coordination geometry, and P-O-C-C-S in the ancillary ligand exhibited triangular conformation. The distance between chiral P atom and plane centroid of S-C-C in the ancillary ligand for λ-Ir(tfmpqz)<sub>2</sub>(S-sdpp) was 0.70 Å. Ir-N-C-P-S constituted a stable five-membered ring with the Ir.....P distance of 3.43 Å. Ir(tfmpqz)<sub>2</sub>(sdpp) exhibited excellent thermal stability with a high decomposition temperature (T<sub>d</sub>) of 323 °C (5% weight loss). The excellent thermal stabilities are necessary for improving the performance of OLEDs.

### 3.2 Photophysical properties

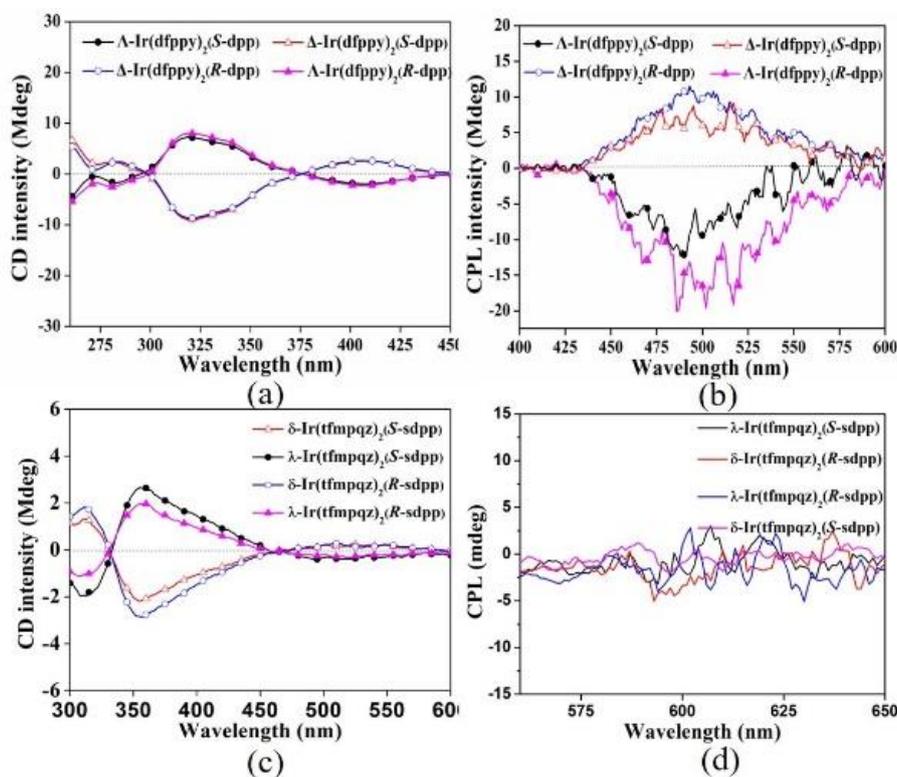


**Fig. 2.** (a) UV-vis absorption and emission spectra and (b) the Commission Internationale de L'Eclairage (CIE (x, y)) of Ir(dnfppy)<sub>2</sub>(Cl/Pyrrrole), Ir(dfppy)<sub>2</sub>(dpp) and Ir(tfmqz)<sub>2</sub>(sdpp).

The photophysical properties of three Iridium(III) complexes were investigated in CH<sub>2</sub>Cl<sub>2</sub> solution. As shown in Fig. 2, the maximum absorption peaks were 232, 238 and 254 nm for Ir(dnfppy)<sub>2</sub>(Cl/Pyrrrole), Ir(dfppy)<sub>2</sub>(dpp) and Ir(tfmqz)<sub>2</sub>(sdpp), respectively. Broad and intense high-energy absorption bands were assigned to the  $\pi$ - $\pi^*$  transition, which corresponded to the absorption bands of the main ligands. The weaker and broad low-energy transitions in the range of 450–600 nm were attributed to the mixed <sup>1</sup>MLCT/<sup>3</sup>MLCT transitions.<sup>[13]</sup> Meanwhile, three Iridium(III) complexes emitted deep-blue, blue or red photoluminescence with high quantum yields, for ((Ir(dnfppy)<sub>2</sub>(Cl/Pyrrrole):  $\lambda_{\text{max}} = 447$  nm, F = 62.4%; Ir(dfppy)<sub>2</sub>(dpp):  $\lambda_{\text{max}} = 467$  nm, F = 25%; Ir(tfmqz)<sub>2</sub>(sdpp):  $\lambda_{\text{max}} = 609$  nm, F = 73.7%), respectively. The Commission Internationale de L'Eclairage (CIE (x, y)) color coordinate was (0.13, 0.14), (0.13, 0.28), (0.63, 0.36), respectively. The triplet lifetime of Ir(tfmpqz)<sub>2</sub>(sddp) was 0.8  $\mu$ s, suggesting the efficient

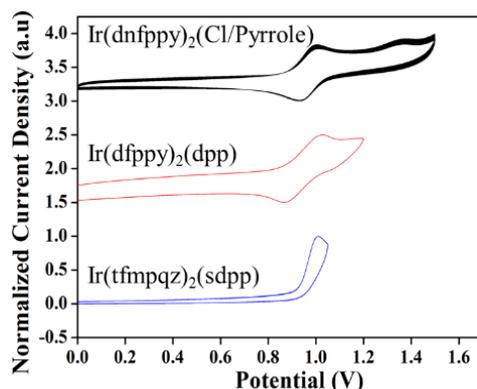
intersystem crossing from the singlet to triplet state. Two pairs of enantiomers of  $\text{Ir}(\text{dfppy})_2(\text{dpp})$  and  $\text{Ir}(\text{tfmqz})_2(\text{sdpp})$  have been separated by column chromatography, respectively. The isomers of  $\Lambda\text{-Ir}(\text{dfppy})_2(\text{S-dpp})$  and  $\Delta\text{-Ir}(\text{dfppy})_2(\text{R-dpp})$ ,  $\Lambda\text{-Ir}(\text{dfppy})_2(\text{R-dpp})$  and  $\Delta\text{-Ir}(\text{dfppy})_2(\text{S-dpp})$  have similar emission spectra with the maximum peaks at 467 and 494 nm. Meanwhile, the isomers of  $\Lambda\text{-Ir}(\text{tfmqz})_2(\text{S-L})$  and  $\Delta\text{-Ir}(\text{tfmqz})_2(\text{R-L})$ ,  $\Lambda\text{-Ir}(\text{tfmqz})_2(\text{R-L})$  and  $\Delta\text{-Ir}(\text{tfmqz})_2(\text{S-L})$  have also similar emission spectra with the maximum peak at 609 nm.

To investigate the chiral optical properties, CD and CPL spectra of the enantiomers were used for  $\text{Ir}(\text{dfppy})_2(\text{dpp})$  and  $\text{Ir}(\text{dfppy})_2(\text{sdpp})$ . From Fig. 3,  $\lambda\text{-Ir}(\text{dfppy})_2(\text{R-ddp})$  and  $\delta\text{-Ir}(\text{dfppy})_2(\text{S-ddp})$  exhibited mirror-image CD spectra with alternating negative and positive Cotton effects. By comparison,  $\delta\text{-Ir}(\text{dfppy})_2(\text{S-ddp})$  and  $\lambda\text{-Ir}(\text{dfppy})_2(\text{R-ddp})$  showed symmetrical and opposite absorption trend. The intense Cotton effects in short wavelength regions were assigned to the absorption caused by the intramolecular  $\pi$ -system transition. Meanwhile, the weak cotton effect at the longest-wavelength absorption band was caused by the MLCT<sup>[14]</sup>. Furthermore,  $g_{\text{lum}}$  values of  $\lambda\text{-Ir}(\text{dfppy})_2(\text{R-ddp})$ ,  $\delta\text{-Ir}(\text{dfppy})_2(\text{S-ddp})$ ,  $\delta\text{-Ir}(\text{dfppy})_2(\text{S-ddp})$  and  $\lambda\text{-Ir}(\text{dfppy})_2(\text{R-ddp})$  were  $4.8 \times 10^{-3}$ ,  $4.8 \times 10^{-3}$ ,  $4.8 \times 10^{-3}$ , and  $4.8 \times 10^{-3}$ , respectively, displaying mirror-image CPL characters. From Fig. 4c, compared with  $\text{Ir}(\text{dfppy})_2(\text{dpp})$ , CD spectra of  $\lambda\text{-Ir}(\text{tfmpqz})_2(\text{S-sdpp})$  and  $\delta\text{-Ir}(\text{dfppy})_2(\text{R-sdpp})$  also displayed perfect mirror symmetry with opposite polarization between 300 and 600 nm. However, the CPL spectra of two pairs of the enantiomers for  $\text{Ir}(\text{tfmpqz})_2(\text{sdpp})$  displayed little symmetry in 500-650 nm (Fig. 4d).

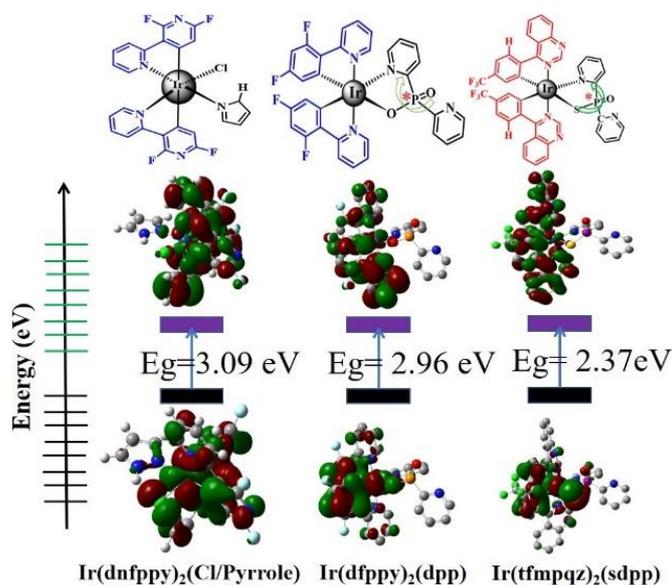


**Fig. 3.** (a) CD and (b) CPL spectra of  $\text{Ir}(\text{dfppy})_2(\text{dpp})$  and  $\text{Ir}(\text{tfmqz})_2(\text{sdpp})$  in  $\text{CH}_2\text{Cl}_2$  solution.

### 3.3 Electrochemical properties and DFT calculation



**Fig. 4.** Cyclic voltammograms of Ir(dnfppy)<sub>2</sub>(Cl/Pyrrrole), Ir(dfppy)<sub>2</sub>(dpp) and Ir(tfmpqz)<sub>2</sub>(sdpp) on platinum electrode in 0.1 mol/L Bu<sub>4</sub>NClO<sub>4</sub>, acetonitrile solution.

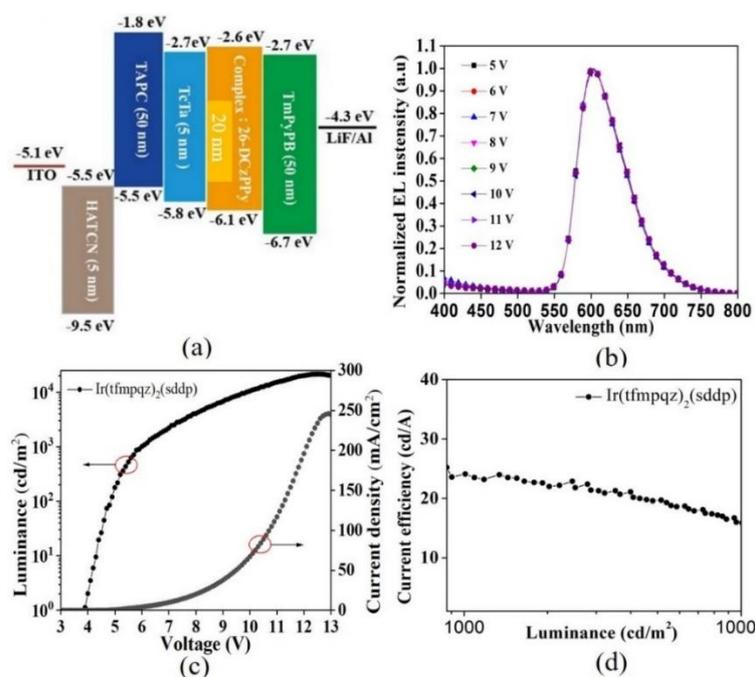


**Fig 5.** HOMO and LUMO electron distributions and energy levels of Ir(dnfppy)<sub>2</sub>(Cl/Pyrrrole), Ir(dfppy)<sub>2</sub>(dpp) and Ir(tfmpqz)<sub>2</sub>(sdpp).

The redox properties have been measured by cyclic voltammetry (CV) experiments. The oxidation processes were observed for Ir(dnfppy)<sub>2</sub>(Cl/Pyrrrole), Ir(dfppy)<sub>2</sub>(dpp) and Ir(tfmpqz)<sub>2</sub>(sdpp) with oxidation potential of 0.93, 1.01 and 1.0 V, respectively. Based on the first anodic peak potentials and the onset of the UV-vis absorption spectra<sup>[20]</sup>, HOMO energy levels were calculated to be -5.40/-5.48/-5.47 eV, respectively. LUMO energy levels were calculated to be -2.31 eV for Ir(dnfppy)<sub>2</sub>(Cl/Pyrrrole). Due to the increase of conjugation degree of main ligands, LUMO energy levels was decreased to -2.52/-3.1 eV for Ir(dfppy)<sub>2</sub>(dpp) and Ir(tfmpqz)<sub>2</sub>(sdpp) respectively. Time-dependent density functional theory calculations, based on the B3LYP function, 6-31G for C, H, O, S, P, and lanl2dz basis set for Ir atoms, were performed to investigate the electronic distribution of the four configuration isomers. The theoretical results indicated that the enantiomers featured double chiral emission characteristics.

### 3.4 Electroluminescent properties

Since the CPL properties of two pairs of enantiomers for  $\text{Ir}(\text{tfmpqz})_2(\text{sddp})$  were not obvious, their circular polarization luminescence properties of OLEDs were not investigated. We only fabricated the devices to study the light-emitting properties of  $\text{Ir}(\text{tfmpqz})_2(\text{sddp})$ .  $\text{Ir}(\text{tfmpqz})_2(\text{sddp})$  was used as emissive dopant to the architecture: ITO/HATCN (5 nm)/TAPC (50 nm)/10 wt%  $\text{Ir}(\text{tfmpqz})_2(\text{sddp})$ :26DCzPPY (20 nm)/TmPyPB (50 nm)/LiF (1 nm)/Al (100 nm) (Fig. 6a). The EL spectra of the device displayed a prominent red EL centered at 602 nm (Fig. 6b). The light emitting device achieved a maximum luminance of 36020  $\text{cd/m}^2$  at 12V. Notably, the device featured a turn-on voltage ( $V_T$ ) of 3.6 V, a maximum current efficiency, a maximum power efficiency and the maximum external quantum efficiency ( $\text{EQE}_{\text{max}}$ ) of 25.2  $\text{cd/A}$ , 17.9  $\text{lm/W}$  and 13.8%, respectively. Moreover, the device also showed a relatively low efficiency roll-off, and the EQE was 10.7% at a luminance of 5000  $\text{cd/m}^2$ .



**Fig. 5.** (a) The structure and energy diagram of OLEDs, (b) EL spectra, (c) luminance-voltage-current density curves, and (d) current efficiency luminance curve of  $\text{Ir}(\text{tfmpqz})_2(\text{sddp})$ .

### 4. Conclusions

In summary, three Iridium(III) complexes,  $\text{Ir}(\text{dnfppy})_2(\text{Cl}/\text{Pyrrole})$ ,  $\text{Ir}(\text{dfppy})_2(\text{dpp})$  and  $\text{Ir}(\text{tfmqz})_2(\text{sdpp})$ , have been designed and synthesized. The complexes emitted deep-blue, blue or red photoluminescence with high quantum yields. The CD spectra of two pairs of enantiomers of  $\text{Ir}(\text{tfmpqz})_2(\text{sddp})$  displayed symmetry with opposite polarization between 300 and 600 nm, but the CPL signals were not obvious in 500-650 nm. The light emitting device based on  $\text{Ir}(\text{tfmpqz})_2(\text{sddp})$  achieved a maximum luminance of 36020  $\text{cd/m}^2$  at 12 V, a maximum current efficiency of 25.2  $\text{cd/A}$  and  $\text{EQE}_{\text{max}}$  of 13.8%, respectively. These research results indicate that the iridium(III) complex containing the ancillary ligand with chiral

phosphine center (*R* or *S*) can provide a new pathway to design CP luminescent materials for OLEDs.

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## Conflict of Interest

The authors declare no conflict of interest.

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