

# **Electronic Supplementary Information**

**for**

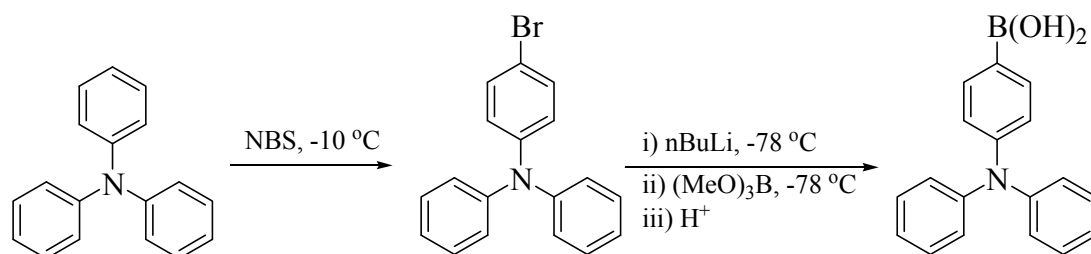
**Thiazole-based metallophosphors of iridium with balanced carrier injection/transporting features and their two-colour WOLEDs fabricated by both vacuum deposition and solution processing-vacuum deposition hybrid strategy**

X. Yang, Y. Zhao, X. Zhang, R. Li, J. Dang, Y. Li, G. Zhou,\* Z. Wu,\* D. Ma,\* W-Y. Wong,\*

X. Zhao, A. Ren, L. Wang and X. Hou

## Synthesis Details

The compounds (4-bromophenyl)diphenylamine and 4-triphenylaminoboronic acid were synthesized following the synthetic routes as shown in Scheme S1.



**Scheme S1.** The synthesis of the intermediate compounds derived from triphenylamine.

**Synthesis of (4-Bromophenyl)diphenylamine:** Under a N<sub>2</sub> atmosphere, triphenylamine (5.00 g, 20.38 mmol) in chloroform (150 mL) was cooled to ca. 0 °C by an ice bath. Then, NBS (3.66 g, 20.56 mmol) was added to the reaction mixture in small portions at the same temperature. After addition, the reaction mixture was allowed to warm to room temperature (rt) and was stirred overnight. The mixture was subsequently extracted with water (3 × 100 mL). The organic phase was separated and dried over MgSO<sub>4</sub>. The solvent was removed under reduced pressure and the residue was recrystallized from MeOH. The product was obtained as a white crystalline solid (6.01 g, 91%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.30 (d, *J* = 8.80 Hz, 2 H, Ar), 7.28–7.20 (m, 4 H, Ar), 7.06 (t, *J* = 8.00 Hz, 4 H, Ar), 7.01 (d, *J* = 7.20 Hz, 2 H, Ar), 6.94 (d, *J* = 8.80 Hz, 2 H, Ar); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 147.30, 132.10, 129.32, 125.08, 124.36, 124.11, 123.17, 114.70 (Ar).

**Synthesis of 4-Diphenylaminophenylboronic acid:** Under a N<sub>2</sub> atmosphere, (4-bromophenyl)diphenylamine (5.00 g, 15.42 mmol) in dry THF (50 mL) was cooled to -78 °C. *n*-Butyllithium (2.5 M in hexane, 6.79 mL, 16.96 mmol) was added slowly at -78 °C. After the

addition, the reaction mixture was kept at  $-78\text{ }^{\circ}\text{C}$  for 40 min. Then,  $(\text{MeO})_3\text{B}$  (1.76 g, 16.96 mmol) was added to the reaction mixture slowly at the same temperature. The reaction mixture was allowed to warm to rt slowly and stirred overnight. The HCl solution (0.2 M, 50 mL) was charged into the reaction mixture which was stirred for 30 min. The mixture was then extracted with  $\text{CH}_2\text{Cl}_2$  ( $3 \times 60\text{ mL}$ ). The organic phase was separated and dried over  $\text{MgSO}_4$ . After removal of most of the solvent, hexane was added to precipitate the title product as a greenish-white solid (2.53 g, 55%).  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ ):  $\delta$  (ppm) 7.90 (s, 2 H, BOH), 7.67 (d,  $J = 8.00\text{ Hz}$ , 2 H, Ar), 7.30 (t,  $J = 8.00\text{ Hz}$ , 4 H, Ar), 7.09–7.02 (m, 6 H, Ar), 6.90 (d,  $J = 8.40\text{ Hz}$ , 2 H, Ar);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ ):  $\delta$  (ppm) 148.75, 146.81, 135.27, 129.40, 124.24, 123.19, 121.13, 66.98 (Ar).

**Table S1** X-ray crystal data for **IrTZ1**.

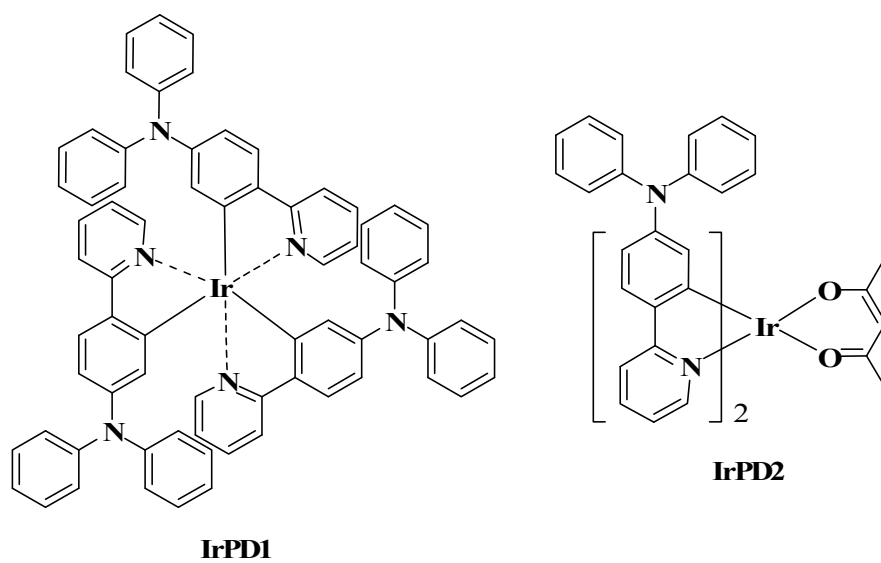
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CCDC no.	844253
formula	C <sub>63</sub> H <sub>45</sub> IrN <sub>6</sub> S <sub>3</sub> ·CHCl <sub>3</sub>
formula weight	1293.80
crystal system	Triclinic
space group	<i>P</i> $\bar{1}$
<i>a</i> (Å)	12.609(1)
<i>b</i> (Å)	13.176(1)
<i>c</i> (Å)	17.001(2)
$\alpha$ (deg)	84.885(2)
$\beta$ (deg)	85.729(2)
$\gamma$ (deg)	82.363(2)
<i>V</i> (Å <sup>3</sup> )	2782.6(5)
<i>Z</i>	2
<i>D</i> <sub>calcd</sub> (g cm <sup>-3</sup> )	1.544
$\mu$ (mm <sup>-1</sup> )	2.703
<i>F</i> (000)	1296
$\theta$ range (deg)	2.54–28.27
reflections collected	16990
unique reflections	12428
<i>R</i> <sub>int</sub>	0.0316
observed reflections	9688
no. of parameters	694
<i>R</i> 1, <i>wR</i> 2 [ <i>I</i> > 2.0 $\sigma$ ( <i>I</i> )] <sup>a</sup>	0.0474, 0.1129
<i>R</i> 1, <i>wR</i> 2 (all data)	0.0726, 0.1259
GoF on <i>F</i> <sup>2</sup> <sup>b</sup>	1.008

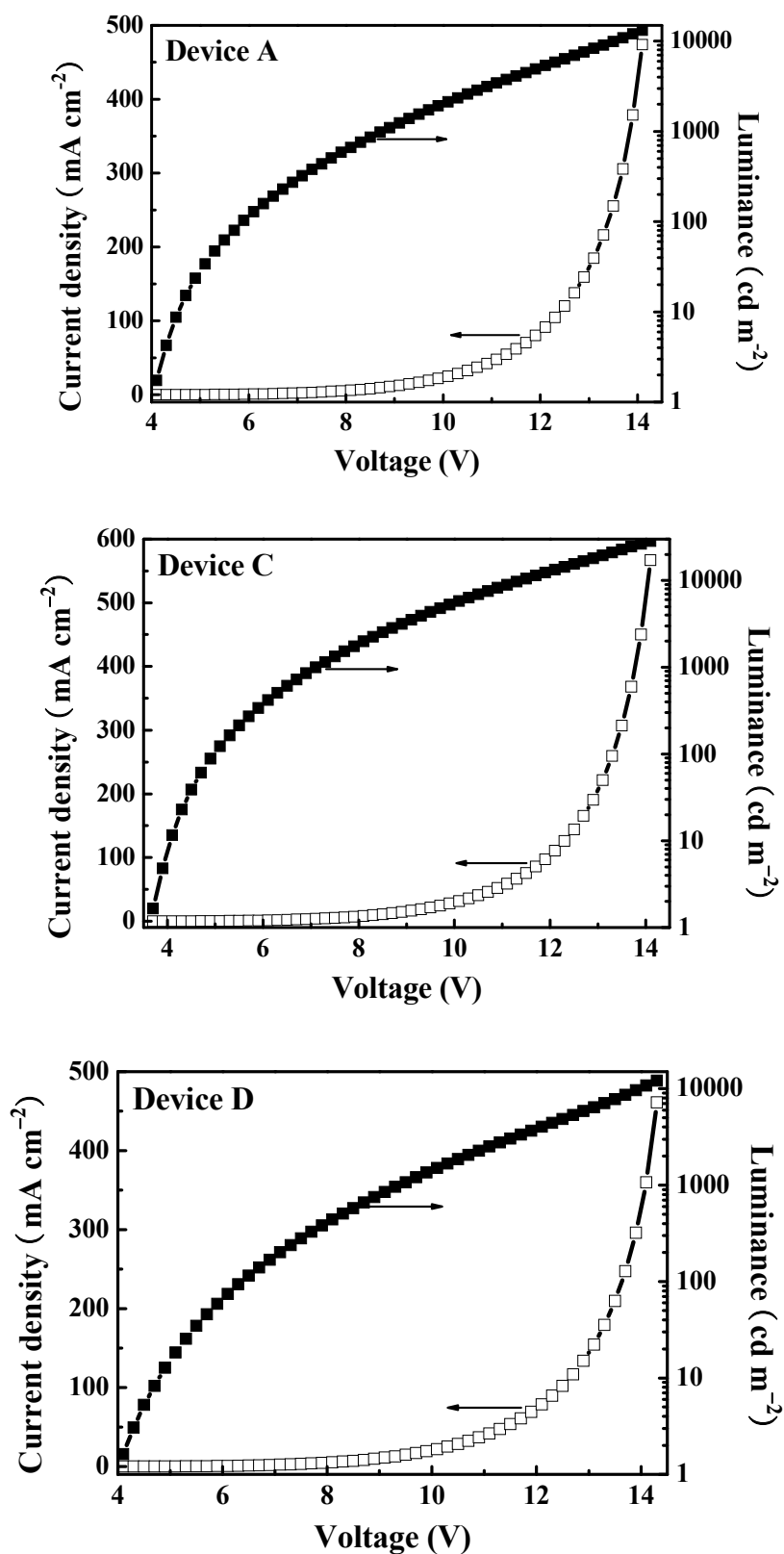
<sup>a</sup>  $R1 = \sum ||F_o| - |F_c|| / \sum |F_o|$ .  $wR2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$ .

<sup>b</sup>  $GoF = [(\sum w|F_o| - |F_c|)^2 / (N_{obs} - N_{param})]^{1/2}$ .

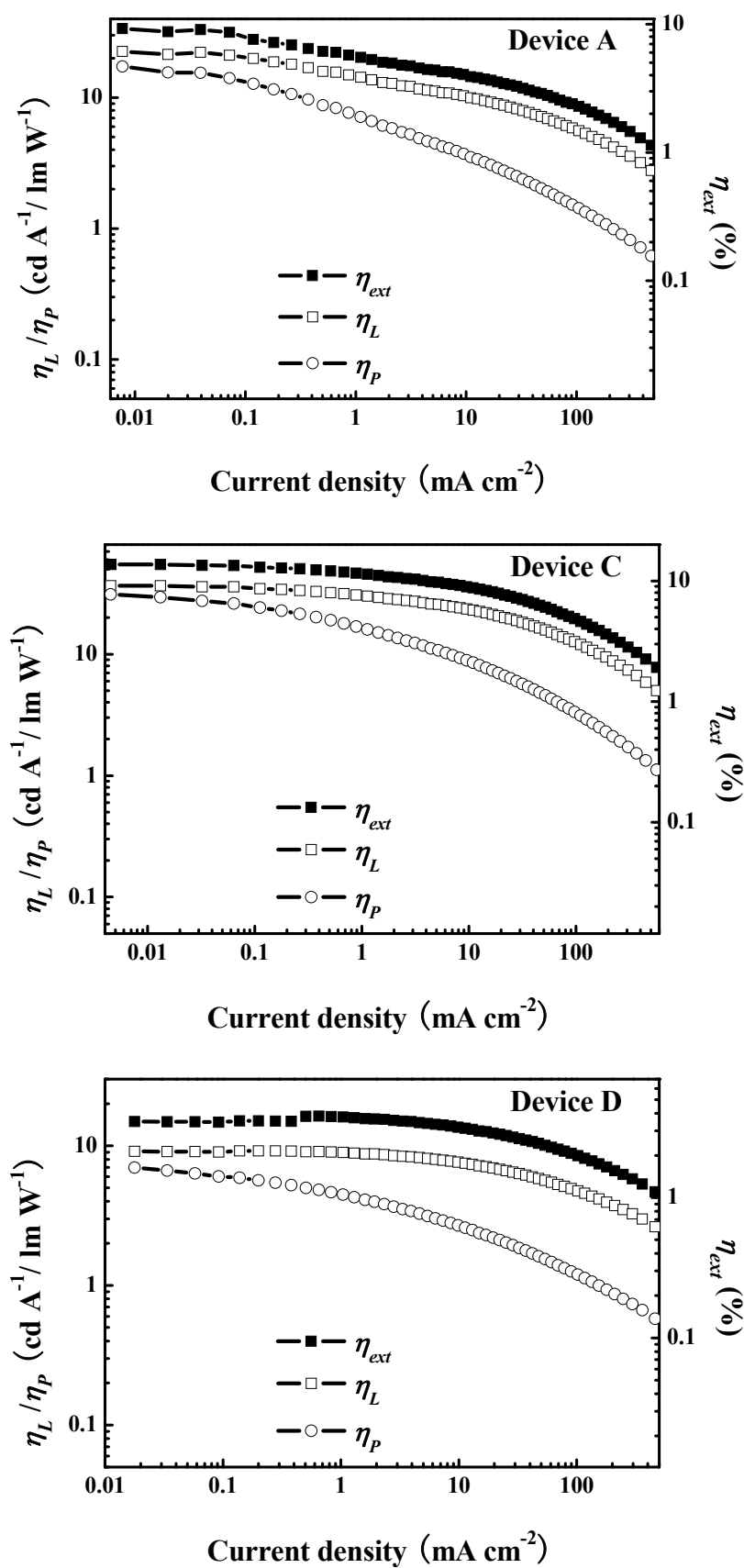
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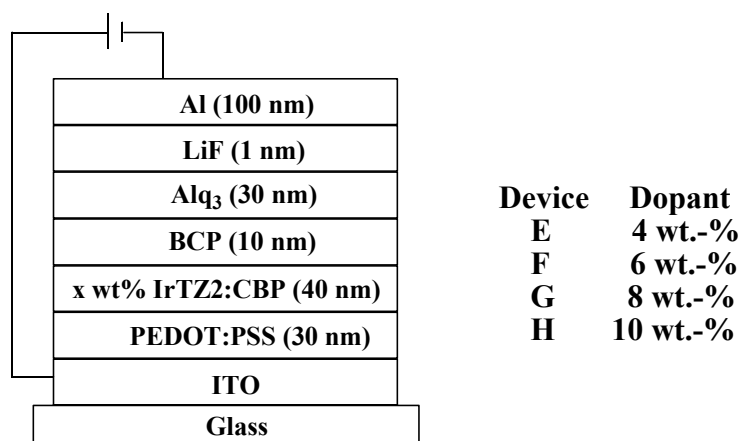
**Figure S1.** Chemical structures for the control complexes **IrPD1** and **IrPD2**.



**Figure S2.** The  $J$ - $V$ - $L$  curves for the monochromatic electrophosphorescent OLEDs A, C and D made from IrTZ1.

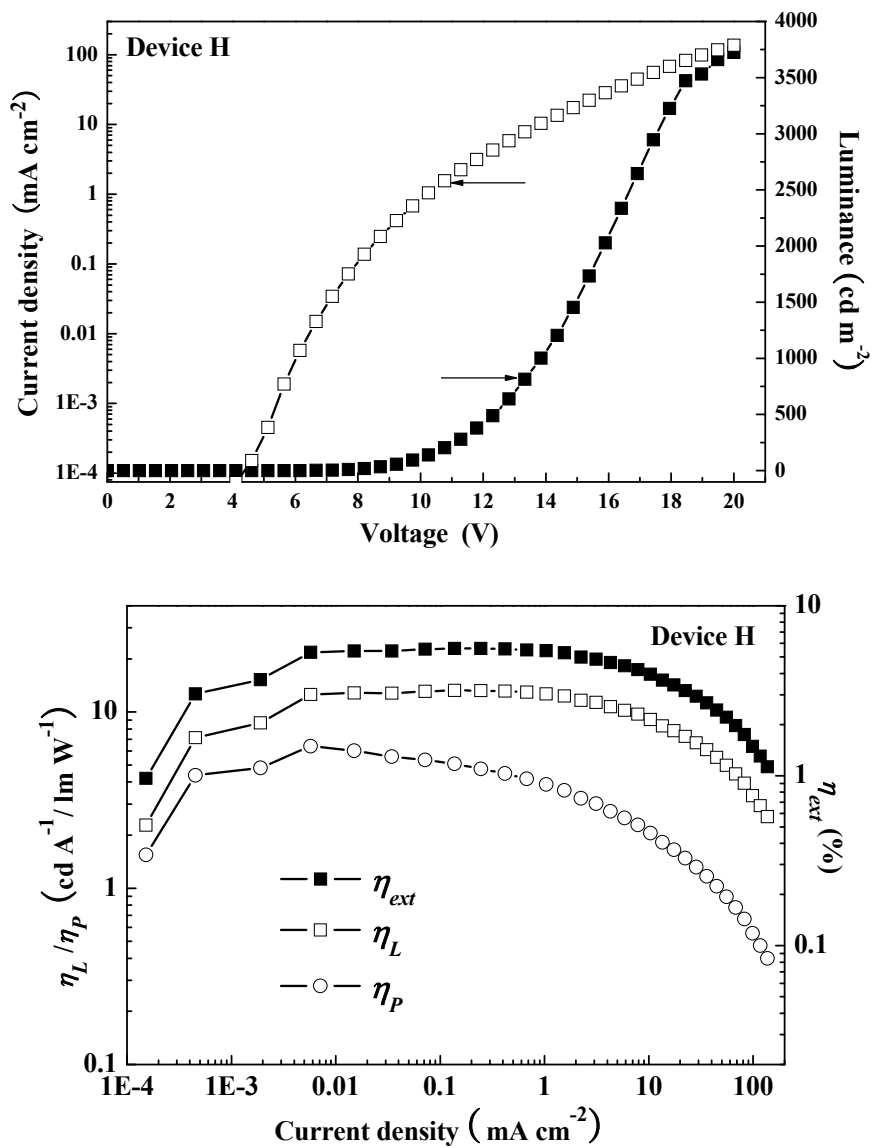


**Figure S3.** The relationship between EL efficiencies and current density for the monochromatic electrophosphorescent OLEDs A, C and D made from IrTZ1.



**Figure S4.** The general configuration for the monochromatic electrophosphorescent OLEDs made from **IrTZ2** and the molecular structures of the relevant compounds used in these devices.





**Figure S5.** The  $J$ - $V$ - $L$  curves and the relationship between EL efficiencies and current density for the device **H** made from **IrTZ2**.

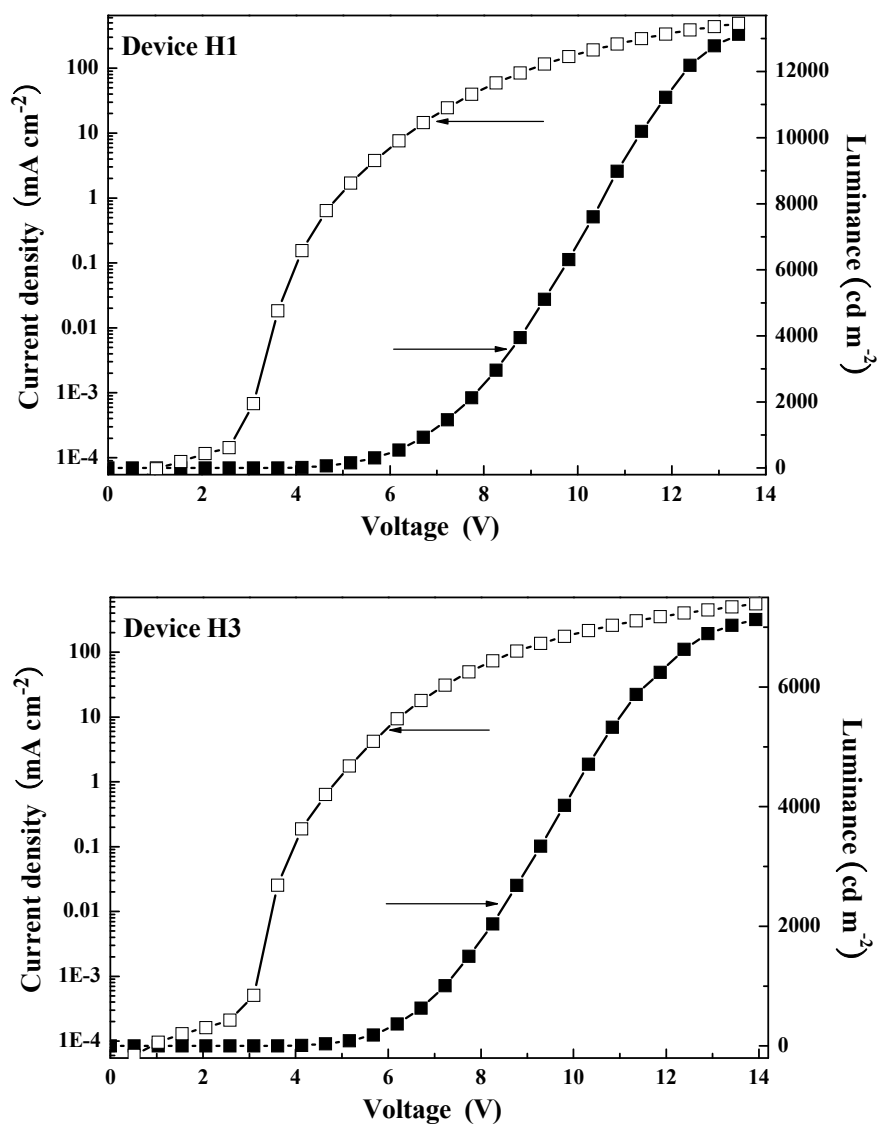
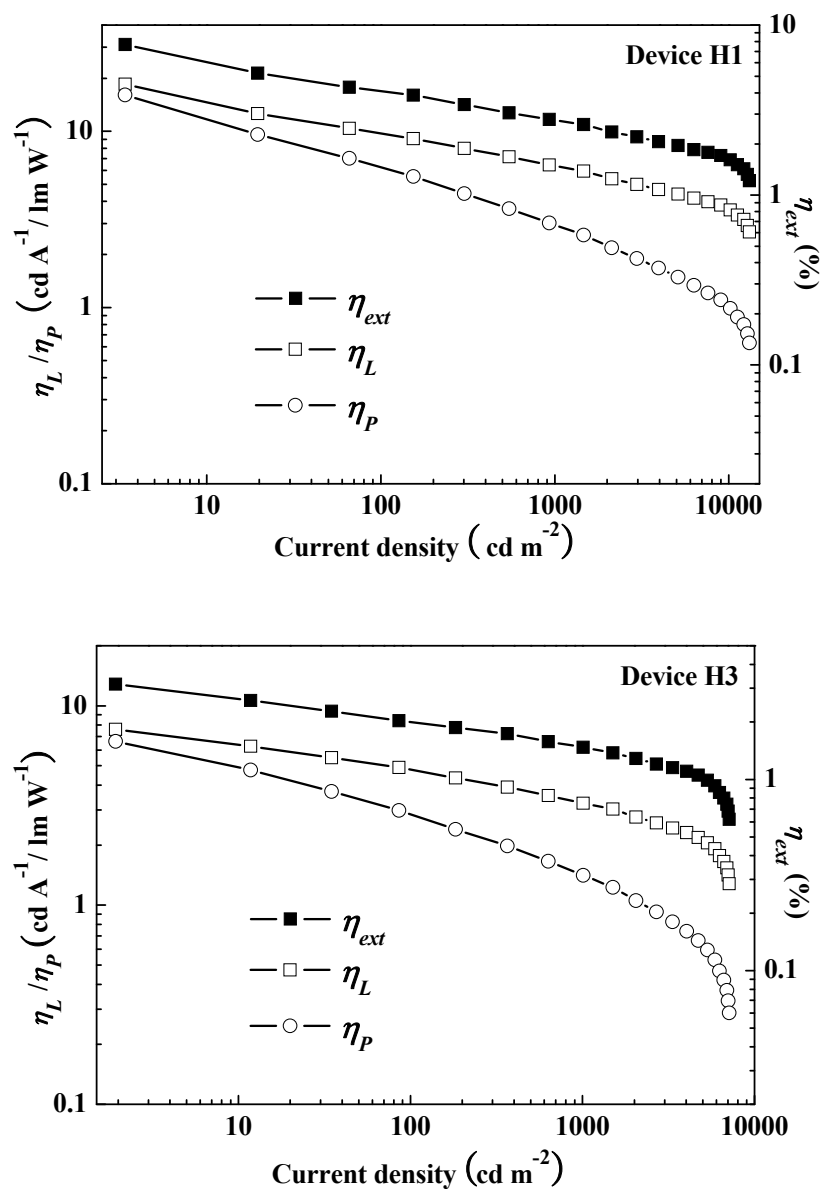
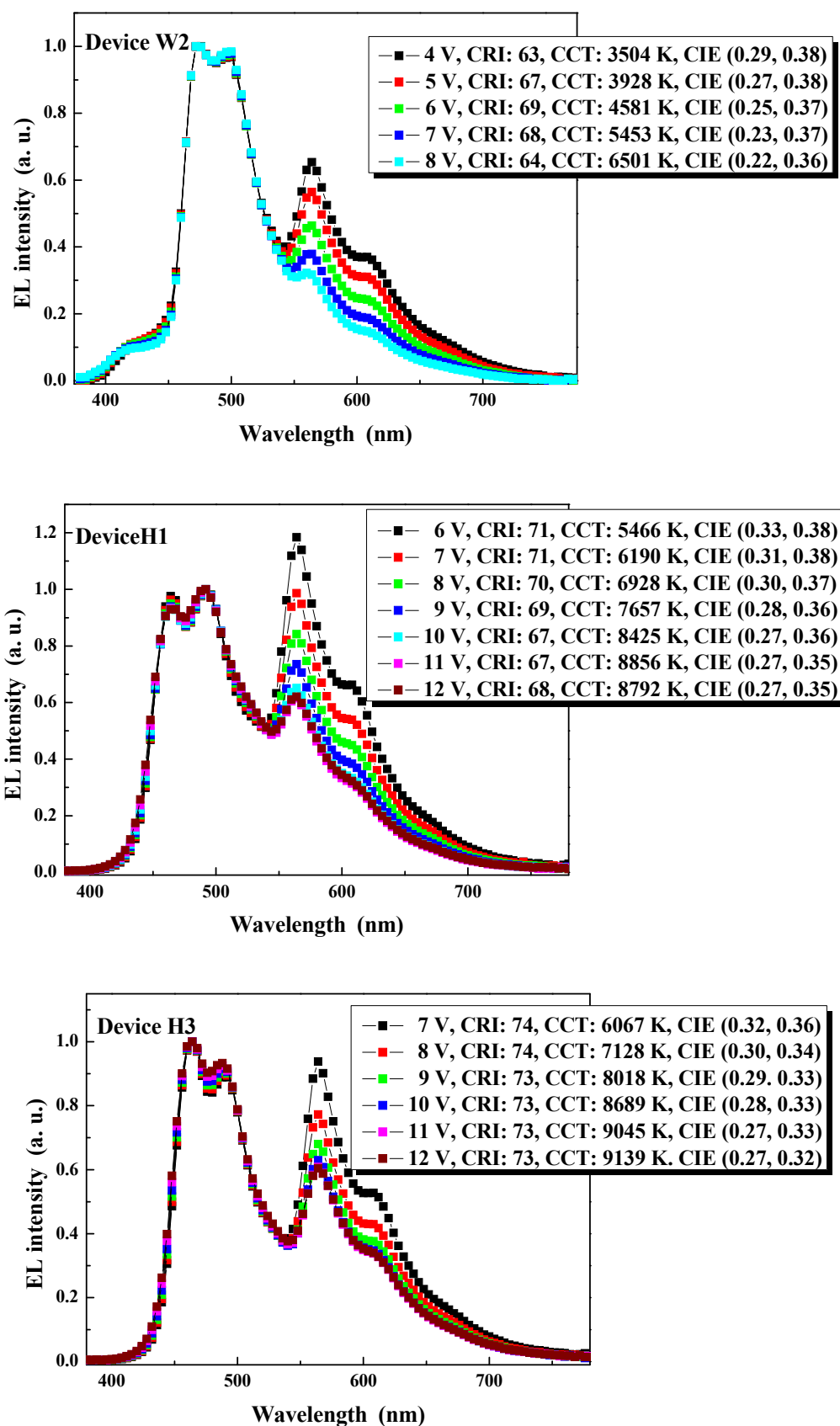


Figure S6. The  $J$ - $V$ - $L$  curves for devices H1 and H3.



**Figure S7.** The dependence between EL efficiencies and current density for devices **H1** and **H3**.



**Figure S8.** The EL spectra at different driving voltages for the WOLEDs.