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## Electronic supporting information

### Experimental

#### General information

1-Methyl-1H-imidazole, *n*-butyllithium, (2-hydroxyphenyl) boronic acid, BeSO<sub>4</sub>·4H<sub>2</sub>O and tetrakis(triphenylphosphine)palladium(0) (Pd(PPh<sub>3</sub>)<sub>4</sub>) (Aldrich Chem. Co.) were used without further purification. Tetrahydrofuran (THF) was distilled over sodium and calcium hydride.

The <sup>1</sup>H nuclear magnetic resonance (NMR), <sup>13</sup>C NMR spectra were recorded on Bruker, Avance 500 (500 MHz) spectrometer. The mass spectrometry (MS) was performed using a JEOL, JMS-AX505WA spectrometer in fast atom bombardment mode. Elemental analysis was carried out using on Flash1112, Flash2000 (CE Instrument, Italy). The <sup>1</sup>H NMR, <sup>13</sup>C NMR, mass spectrometry and elemental analysis were obtained from Seoul national university national center for inter-university research facilities. The photoluminescence spectra were recorded on a fluorescence spectrophotometer (HITACHI, F-7000) and the ultraviolet-visible (UV-Vis) spectra were obtained by means of a UV-vis spectrophotometer (Shimadzu, UV-2501PC). The highest occupied molecular orbital of the materials were determined by cycle voltammetry. Structural analysis of BeTh was performed using single crystal X-ray measurement. A BeTh single crystal grown from chloroform solution was picked up with paraton oil and mounted on a Bruker SMART CCD diffractometer equipped with a graphite-monochromated MoK $\alpha$  radiation source and a nitrogen cold stream (-100 °C). The data were corrected for Lorentz and polarization effects (SAINT), and semiempirical absorption corrections based on equivalent reflections were applied (SADABS). The structure was solved by direct methods and refined by full-matrix least-squares on F<sup>2</sup> (SHELXTL). All the non-hydrogen atoms were refined anisotropically, and hydrogen atoms were added to their geometrically ideal positions.

#### Synthesis

**2-Bromo-1-methyl-1H-imidazole.** 1-Methyl-1H-imidazole (3.00 g, 36.05 mmol) was dissolved in anhydrous THF (218 ml) under nitrogen atmosphere. The solution was stirred for 1h at -78°C and *n*-butyllithium (2.58 g, 40.19 mmol) was added dropwise slowly followed by addition of tetrabromomethane (14.54 g, 43.85 mmol) solution in anhydrous THF ( 83 ml). The solution was stirred for 2h at -78°C and for 1h at room temperature. The solution was diluted with ethylacetate and washed with ammonium chloride (15g) in distilled water (50ml). The organic layer was dried over anhydrous magnesium sulfate and evaporated in vacuo to give the crude product, which was purified by column chromatography using *n*-hexane/ethylacetate as an eluent. A brown color liquid was obtained in 67% yield.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 6.99 (s, 1H), 6.96 (s, 1H), 3.62 (s, 3H) <sup>13</sup>C NMR (500 MHz, CDCl<sub>3</sub>): δ 129.74, 122.93, 120.06, 34.51 MS (FAB) *m/z* 161 [(M+H)<sup>+</sup>].

**2-(1-Methyl-1H-imidazol-2-yl)phenol** 2-Bromo-1-methyl-1H-imidazole (4.00g, 24.14mmol), (2-hydroxyphenyl) boronic acid (4.64g, 26.56mmol), K<sub>2</sub>CO<sub>3</sub> (10.01g, 72.43mmol), Pd(PPh<sub>3</sub>)<sub>4</sub> (0.84g, 0.72mmol) were added to a mixed solvent of THF and distilled water (200 ml) in Schlenk flask. The solution was refluxed overnight under argon, and then cooled to room temperature. The solution was diluted with ethylacetate and washed with distilled water. The organic layer was dried over anhydrous MgSO<sub>4</sub> and evaporated in vacuo to give the crude product, which was purified by column chromatography using *n*-hexane/ethylacetate as an eluent. The product was obtained in 0.6g (14% yield).

<sup>1</sup>H NMR (500 MHz, DMSO): δ 12.69 (s, 1H), 7.56 (d, J=8.50 Hz, 1H), 7.28-7.24 (m, 1H), 7.09-7.08 (m, 2H), 6.91-6.88 (m, 2H), 3.93 (s, 3H) <sup>13</sup>C NMR (500 MHz, CDCl<sub>3</sub>) 157.82, 145.70, 130.00, 129.68, 125.44, 122.60, 118.31, 117.77, 113.84, 36.21 MS (FAB) *m/z* 175 [(M+H)<sup>+</sup>].

**Beryllium 2-(thiazol-2-yl)phenolate (BeTh)** To a filtered solution of 2-(thiazol-2-yl)phenol (1.40g, 7.90mmol) was added a filtered solution of BeSo<sub>4</sub>·4H<sub>2</sub>O (0.70g, 3.95mmol) and triethy lamine (3.49g, 34.52mmol) in ethanol (198 mL). The mixture was stirred at 60 °C for 3h and then was allowed to stand

at room temperature for 3 days. The yellow precipitate was filtered off, washed with ethanol. The product was obtained in 1.00g, 70% yield. The product was purified by Vacuum Sublimation Purifier.

$^1\text{H}$  NMR (500 MHz, DMSO):  $\delta$  7.71 (t,  $J=3.50$  Hz, 4H), 7.40 (s, 2H), 7.32 (t,  $J=7.50$ , 2H), 6.78 (d,  $J=8.50$  Hz, 2H), 6.71 (t,  $J=7.50$  Hz, 2H)

$^{13}\text{C}$  NMR (500 MHz, DMSO):  $\delta$  170.11, 161.06, 138.10, 133.21, 127.23, 120.67, 118.42, 115.66, 115.06

MS (FAB) *m/z* 361 [(M+H)<sup>+</sup>]. Anal. Calcd for  $\text{C}_{18}\text{H}_{12}\text{BeN}_2\text{O}_2\text{S}_2$ : C, 59.81; H, 3.35; Be, 2.49; N, 7.75; O, 8.85; S, 17.74 Found : C, 59.85; H, 3.30; N, 7.75; S, 17.70

**Beryllium 2-(oxazol-2-yl)phenolate (BeOx)** 2-(Oxazole-2-yl)phenol (0.90g, 5.58mmol) was added to a filtered solution of  $\text{BeSO}_4\cdot 4\text{H}_2\text{O}$  (0.46g, 2.79mmol) and triethylamine (2.47g, 24.40mmol) in ethanol (140 mL). The mixture was stirred at 60 °C for 3h and then was allowed to stand at room temperature for 3 days. The white precipitate was filtered off and washed with ethanol. A white product was obtained in 0.4g (44% yield). The product was purified by vacuum sublimation.

$^1\text{H}$  NMR (500 MHz, DMSO):  $\delta$  8.37 (s, 2H), 7.80 (d,  $J=8.05$  Hz, 2H), 7.39-7.36 (m, 4H), 6.79 (d,  $J=8.5$  Hz, 2H), 6.75 (t,  $J=7.50$  Hz, 2H)  $^{13}\text{C}$  NMR (500 MHz, DMSO):  $\delta$  163.68, 162.42, 139.75, 134.17, 125.58, 123.28, 120.59, 115.16, 109.63 MS (FAB) *m/z* 329 [(M+H)<sup>+</sup>]. Anal. Calcd for  $\text{C}_{18}\text{H}_{12}\text{BeN}_2\text{O}_4$ : C, 65.65; H, 3.67; Be, 2.74; N, 8.51; O, 19.43. Found : C, 65.66; H, 3.67; N, 8.58;

**Beryllium 2-(1-methyl-1H-imidazol-2-yl)phenolate (BeIm)** 2-(1-Methyl-1H-imidazol-2-yl)phenol (0.40g, 2.30mmol) was added to a filtered solution of  $\text{BeSO}_4\cdot 4\text{H}_2\text{O}$  (0.20g, 1.15mmol) and triethylamine (1.01g, 10.03mmol) in ethanol (58 mL). The mixture was stirred at 60 °C for 3h and then was allowed to stand at room temperature for 72 h. The white precipitate was filtered off and washed with ethanol. A white product was obtained in 0.3g (73% yield). The product was purified by vacuum sublimation.

$^1\text{H}$  NMR (500 MHz, DMSO):  $\delta$  7.81 (d,  $J=8.00$  Hz, 2H), 7.29 (s, 2H), 7.20-7.17 (m, 2H), 6.71 (d,  $J=8.25$  Hz, 2H), 6.66-6.62 (m, Hz, 2H), 4.03 (s, 6H)  $^{13}\text{C}$  NMR (500 MHz, DMSO):  $\delta$  163.40, 144.47, 130.80,

125.73, 124.16, 121.66, 120.81, 113.74, 113.30, 37.02 MS (FAB) *m/z* 356 [(M+H)<sup>+</sup>]. Anal. Calcd for C<sub>10</sub>H<sub>10</sub>N<sub>2</sub>O: C, 67.59; H, 5.11; Be, 2.54; N, 15.76; O, 9.00 Found C, 67.95; H, 5.79; N, 16.08; O, 9.18

## Device fabrication

Basic device structure of red, green, blue and deep blue PHOLEDs were indium tin oxide (ITO, 50 nm)/poly(3,4-ethylenedioxythiophene);poly(styrenesulfonate) (PEDOT:PSS, 60 nm)/4,4'-cyclohexylidenebis[N,N-bis(4-methylphenyl)aniline] (TAPC, 20 nm)/N,N'-dicarbazolyl-3,5-benzene (mCP, 10 nm)/emitting layer (25 nm, 5% doping)/ diphenylphosphine oxide-4-(triphenylsilyl)phenyl (TSPO1) (30 nm)/LiF (1 nm)/Al (200 nm). The mCP layer was not used in the deep blue PHOLEDs. The emitting layers were BeTh:iridium(III) bis(1-phenylisoquinoline) acetylacetonate (Ir(piq)<sub>2</sub>acac) (red), BeOx: iridium (III) tris(2-phenylpyridine) (Ir(ppy)<sub>3</sub>) (green), BeIm: iridium(III) bis((4,6-difluorophenyl)pyridine) picolinate (FIrpic) (blue) and BeIm:iridium (III) bis((3,5-difluoro-4-cyanophenyl)pyridine) picolinate (FCNIrpic) (deep blue). Doping concentration of the triplet emitters was 5%. Hole and electron only devices had the device architecture of ITO (50 nm)/PEDOT:PSS (60 nm)/TAPC (20 nm)/mCP (10 nm)/BeTh or BeOx or BeIm (25 nm)/Au (100 nm) and ITO (50 nm)/Ca (10 nm)/BeOx or BeIm (25 nm)/TSPO1 (30 nm)/LiF (1 nm)/Al (100 nm), respectively. Standard devices were also fabricated to compare the device performances of BeTh, BeOx and BeIm PHOLEDs. The standard host materials for red, green and blue were 4,4',4''-tris-(N-carbazolyl)triphenylamine, (4,4'-N,N'-dicarbazole)biphenyl and mCP, respectively.

PEDOT:PSS was spin coated on ITO glass by spin coating and baked at 150 °C for 20 min to remove residual solvent. The PEDOT:PSS coated ITO glass was transferred to vacuum chamber and organic materials were thermally deposited at a vacuum pressure of  $1.0 \times 10^{-7}$  torr. Deposition rate of organic materials was 0.1 nm/s except for the dopant materials. All devices were encapsulated with a glass lid after LiF/Al electrode deposition. All measurements were carried out after encapsulation.

## List of tables

Table S1. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for BeTh.

Table S1. Bond lengths [Å] and angles [°] for BeTh.

Be(1)-O(1)	1.573(5)
Be(1)-O(1)#1	1.573(5)
Be(1)-N(1)	1.747(5)
Be(1)-N(1)#1	1.747(5)
O(1)-C(9)	1.319(5)
N(1)-C(3)	1.314(5)
N(1)-C(1)	1.389(5)
C(1)-C(2)	1.345(7)
C(2)-S(1)	1.722(6)
S(1)-C(3)	1.734(4)
C(3)-C(4)	1.461(5)
C(4)-C(5)	1.395(6)
C(4)-C(9)	1.423(6)
C(5)-C(6)	1.386(7)
C(6)-C(7)	1.388(8)
C(7)-C(8)	1.385(6)
C(8)-C(9)	1.393(6)
O(1)-Be(1)-O(1)#1	114.3(5)
O(1)-Be(1)-N(1)	104.54(14)
O(1)#1-Be(1)-N(1)	111.17(15)
O(1)-Be(1)-N(1)#1	111.17(15)
O(1)#1-Be(1)-N(1)#1	104.54(14)
N(1)-Be(1)-N(1)#1	111.3(5)
C(9)-O(1)-Be(1)	128.0(3)
C(3)-N(1)-C(1)	112.1(3)
C(3)-N(1)-Be(1)	120.9(3)
C(1)-N(1)-Be(1)	126.7(3)
C(2)-C(1)-N(1)	115.3(4)
C(1)-C(2)-S(1)	109.5(3)
C(2)-S(1)-C(3)	90.7(2)
N(1)-C(3)-C(4)	124.3(3)
N(1)-C(3)-S(1)	112.3(3)
C(4)-C(3)-S(1)	123.4(3)
C(5)-C(4)-C(9)	120.6(4)
C(5)-C(4)-C(3)	120.4(4)
C(9)-C(4)-C(3)	119.0(3)

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C(6)-C(5)-C(4)	121.0(4)
C(5)-C(6)-C(7)	118.3(4)
C(8)-C(7)-C(6)	121.8(5)
C(7)-C(8)-C(9)	121.0(4)
O(1)-C(9)-C(8)	120.0(4)
O(1)-C(9)-C(4)	122.6(4)
C(8)-C(9)-C(4)	117.4(4)

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Figure S2. HOMO and LUMO distribution of BeTh, BeOx and BeIm.

Figure S3. Quantum efficiency-luminance curves of red, green and blue PHOLEDs fabricated by using common host materials.

Figure S4. Current density-voltage curves of BeTh (a), BeOx (b) and BeIm (C).

Figure S5. PL spectra of triplet emitter doped BeTh, BeOx and BeIm films.



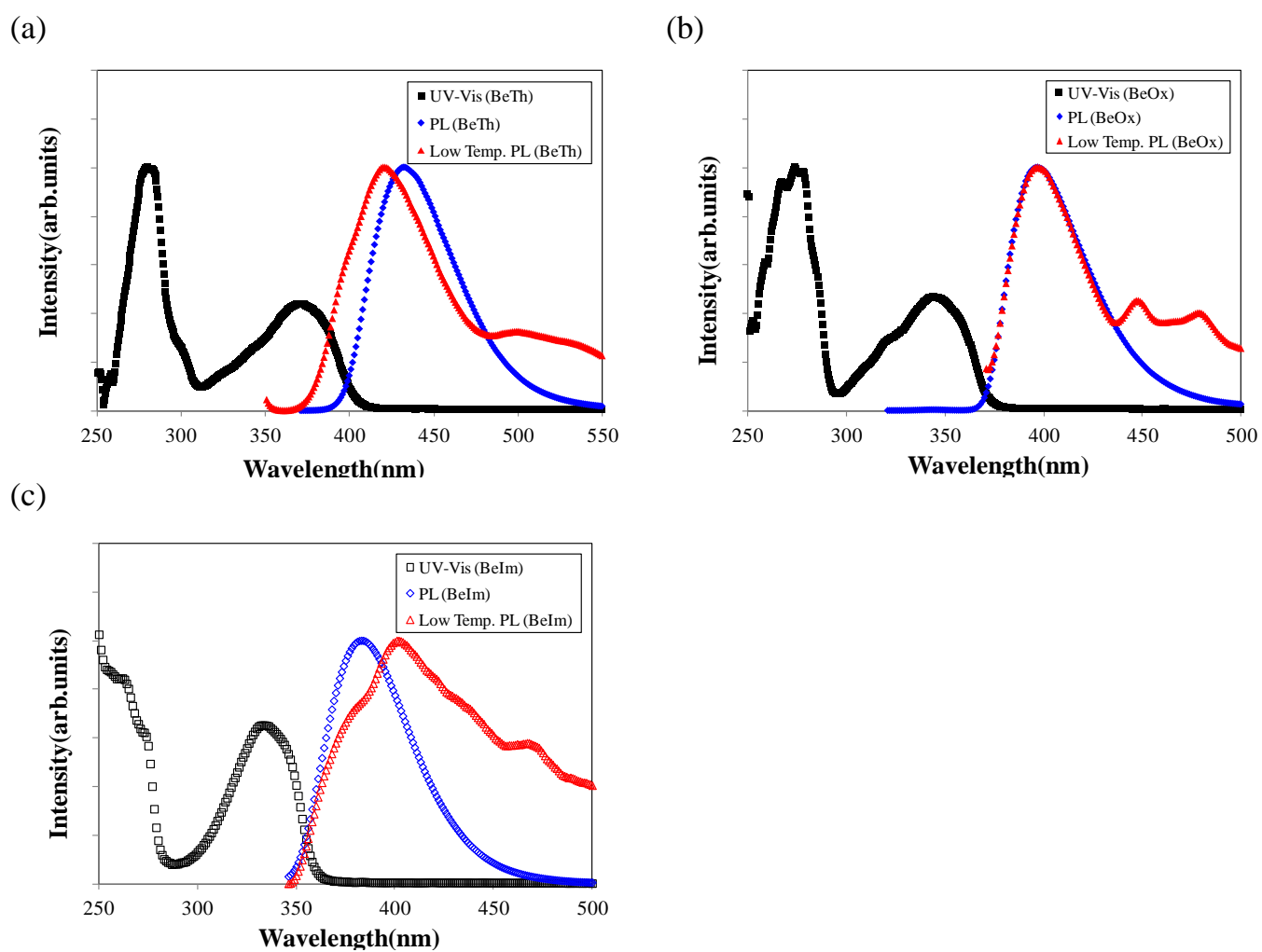


Figure S1

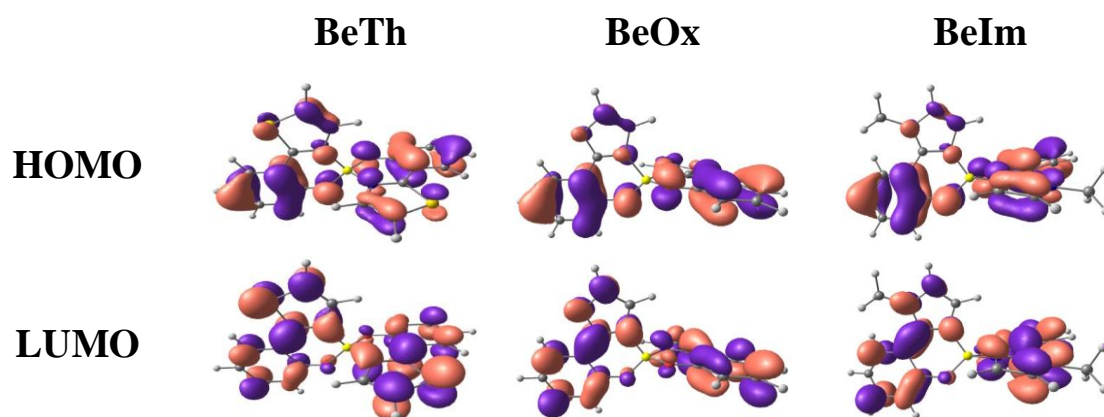


Figure S2

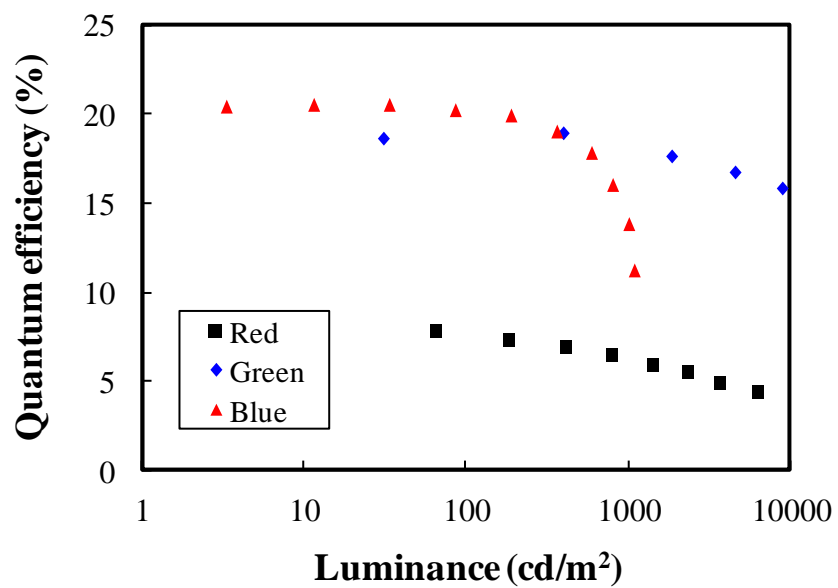


Figure S3

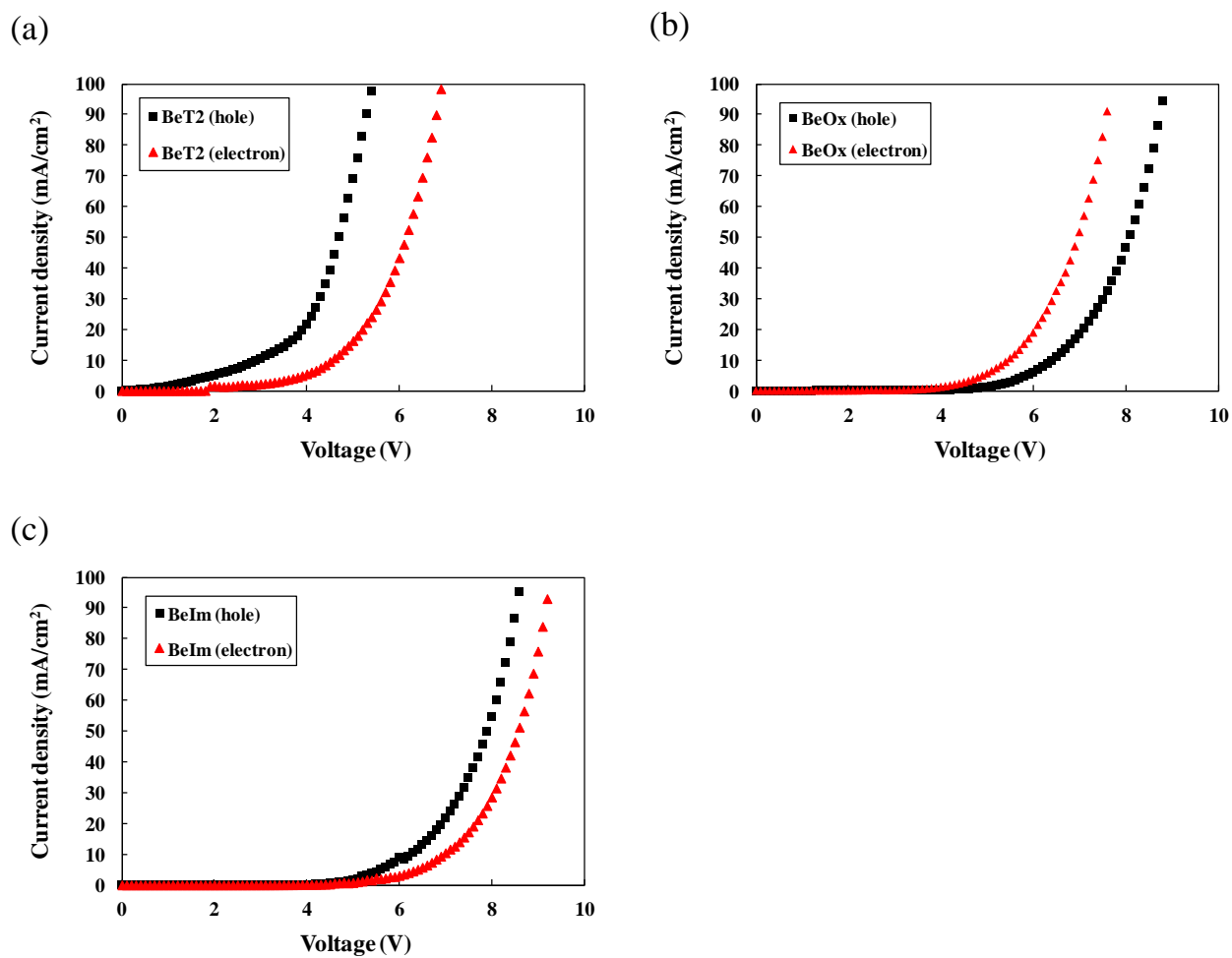


Figure S4

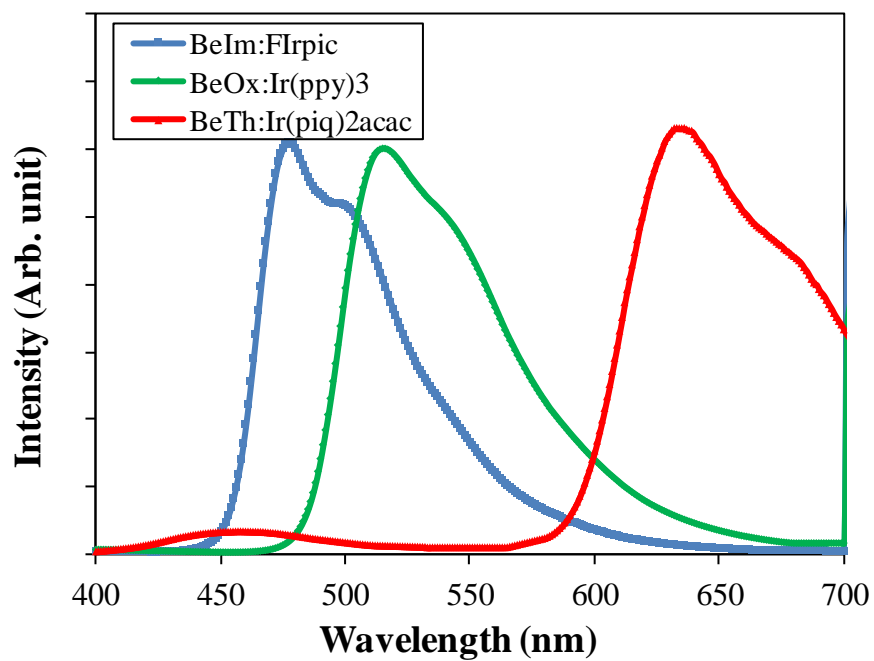


Figure S5