**Supporting Information** 

# Phosphine Oxide Jointed Electron Transporters for Reducing Interfacial Quenching in Highly Efficient Blue PHOLEDs

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#### Synthesis of 1-(4-Bromophenyl)-2-phenylbenzimidazole (PBIBr)



A mixture of PBI (9.7 g, 50 mmol), 60% sodium hydride (3.4 g, 100 mmol), 1-bromo-4-iodobenzene (42.4 g, 150 mmol), copper(I) iodide (1.9 g, 10 mmol) and 1.10-phenanthroline (2.0 g, 10 mmol) in 1,3dimethyl-2-imidazolidinone (100 mL) was heated to 190 °C and stirred for 48 h under argon. Then, the mixture was poured into water and extracted with CH<sub>2</sub>Cl<sub>2</sub> (3 × 20 mL). The organic layer was dried with anhydride Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed in *vacuo* and the residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (3:1) as the eluent to afford the product as a white powder (7.3 g, 42%). <sup>1</sup>H NMR (TMS, CDCl<sub>3</sub>, 400 MHz):  $\delta$  = 7.82-7.89 (d, *J* = 8.0 Hz, 1H), 7.81-7.83 (d, *J* = 8.8 Hz, 1H), 7.61-7.64 (d, *J* = 8.8 Hz, 1H), 7.54-7.56 (t, J = 4.0 Hz, 2H), 7.28-7.40(m, 5H), 7.18-7.24 (dd, *J*<sub>1</sub> = 16.4 Hz, *J*<sub>2</sub> = 8.4 Hz, 2H), 7.04-7.07 ppm (d, *J* = 8.8 Hz, 1H); LDI-TOF: m/z (%): 348 (100) [M<sup>+</sup>]; elemental analysis (%) for C<sub>19</sub>H<sub>13</sub>BrN<sub>2</sub>: C 65.35, H 3.75, N 8.02; found: C 65.32, H 3.77, N 8.09.

## Thermal Properties of xPBIPO



Figure S1. TGA (a) and DSC (b) curves of **xPBIPO** and **TPBI**.

## **Solid-State Optical Properties**



Figure S2. Absorption and fluorescent spectra of spin-coated films of *x*PBIPO.

#### **CV Curves**



**Figure S3.** Cyclic voltammograms of *x***PBIPO** and **TPBI**. The measurement was performed in tetrahydrofuran and dichloromethane, respectively, with tetrabutylammonium hexafluorophosphate as electrolyte at room temperature and a rate of 100 mV s<sup>-1</sup>.

### **DFT** Calculation



**Figure S4.** Contours and energy levels of the FMOs and spin density distributions of triplet states of *x***PBIPO** and **TPBI**.

## **Device Structure and Energy Level of Blue PHOLEDs**



**Scheme S1.** Energy level diagram of blue-emitting FIrpic-based devices and chemical structures of TAPC and *m*CP.

## **Device Efficiency Repeatability**



Figure S5. Efficiency range of five blue PHOLEDs with the error bars for *x*PBIPO, TPBI and TmPyPB.

#### References

- [1] a)J.-X. Cai, T.-L. Ye, X.-F. Fan, C.-M. Han, H. Xu, L.-L. Wang, D.-G. Ma, Y. Lin, P.-F. Yan, J. *Mater. Chem.* 2011, 21, 15405; b)H. Xu, D.-H. Yu, L.-L. Liu, P.-F. Yan, L.-W. Jia, G.-M. Li, Z.-Y. Yue, J. Phys. Chem. B 2010, 114, 141; c)H. Xu, Z.-F. Xu, Z.-Y. Yue, P.-F. Yan, B. Wang, L.-W. Jia, G.-M. Li, W.-B. Sun, J.-W. Zhang, J. Phys. Chem. C 2008, 112, 15517.
- [2] A. D. Becke, J. Chem. Phys. 1993, 98, 5648.
- [3] C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* 1988, 37, 785.
- M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, J. T. Vreyen, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Octhterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, A. L. G. Liu, P. Piskorz, I. Komaromi, R. L.Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, *Gaussian 03, Revision D.02, Gaussian Inc., Pittsburgh, PA* 2004.
- [5] J. Lee, N. Chopra, S.-H. Eom, Y. Zheng, J. Xue, F. So, J. Shi, *Appl. Phys. Lett.* 2008, 93, 123306.
- [6] C. W. Lee, J. Y. Lee, *Adv. Mater.* **2013**, *25*, 5450.