Supplementary Information

A Weak Electron Transporting Material with High Triplet Energy and Thermal Stability via Super Twisted Structure for High Efficient Blue Electrophosphorescent Devices

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The lowest unoccupied molecular orbital (LUMO) level was estimated to be 3.0 eV, as measured by cyclic voltammetry (CV) with a three-electrode configuration as shown in Figure S1. The LUMO of TemPPB is -3.0 eV from the CV plot, i.e., LUMO = -4.8 + 1.8 = -3.0 (eV), and the HOMO is -7.0 eV, i.e., HOMO = LUMO – E_g = -3.0 - 4.0 = -7.0 (eV).

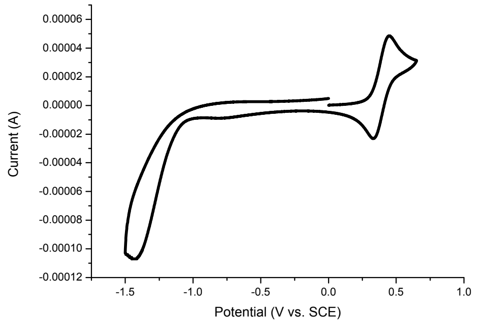

Fig.S1. CV plot of TemPPB film on Pt electrode in CH_3CN containing 0.1 M of *n*-Bu_4NClO_4 as the supporting electrolyte with ferrocene as the inner-reference with a HOMO at -4.8 eV.[1]

The low temperature phosphorescence spectrum was measured in a frozen solution (2-methyl tetroTHF). The phosphorescence spectrum is shown Figure S2. The triplet energy is calculated from the onset of phosphorescence spectrum as B3PyPB reported by Kido.[2] The onset of phosphorescence of TemPPB is 390 nm, according to 3.2 eV of triplet energy.

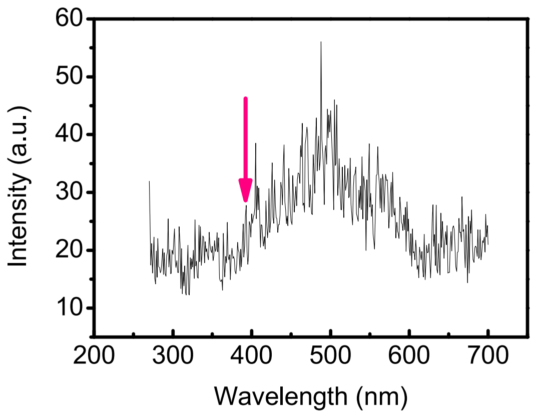

Fig. S2 Phosphorescence spectrum of TemPPB at low temperature. The triplet energy was calculated from the onset of phosphorescence peak (390 nm, 3.2 eV).

The electron mobility was measured with time-of-flight (TOF) method. A thin film of TemPPB was evaporated on the ITO substrate and then Al was deposited on the film as cathode. When a beam of pulsed laser (337 nm) was injected from the ITO side, exciton could be generated and separated to hole and electron. The electron would transport in TemPPB film if there was a bias voltage between ITO and Al. The mobility can be obtained by recording the time of electron flight in the film and the formula as following equation

$$\mu = L / t_\tau E$$

in which μ is the electron mobility, L is the thickness of TemPPB film, t_τ is the time of flight, E is the electric field intensity (which can be calculated by dividing bias voltage U and L, in our sample, L=1000 nm, U=100 V).

Fig. S3 shows the electron transporting situation under a bias of 100 V. To find the time of flight more conveniently, we change the coordinate into double-log form as shown in the inset of Fig. S3 according to the literature [3], from which we can estimate μ is about 3×10^{-7} $cm^2/(V\cdot S)$.

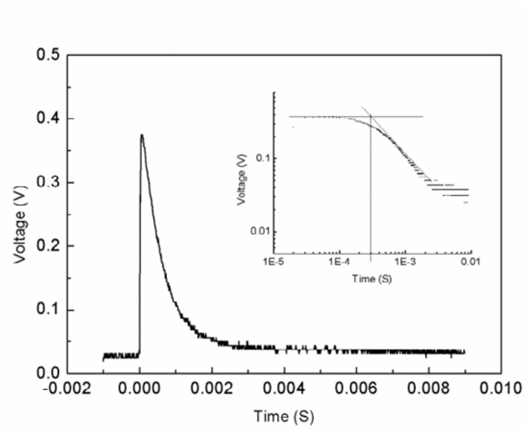

Fig. S3 TOF plot of TemPPB.

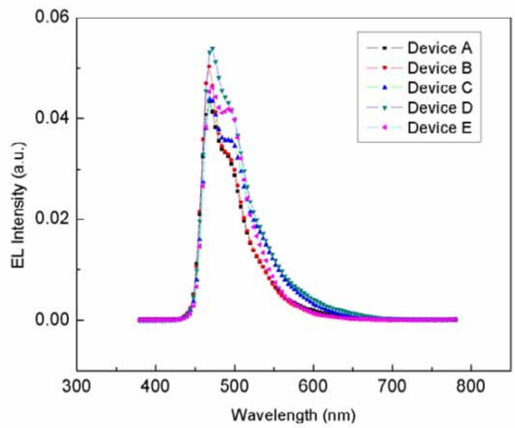

Fig. S4 EL spectra of devices.

References

1. S. Kong, L. Xiao, Y. Liu, Z. Chen, B. Qu, Q. Gong, *New J. Chem*. 2010, **34**, 1994.

2. H. Sasabe, E. Gonmori, T. Chiba, Y.-J. Li, D. Tanaka, S.-J. Su, T. Takeda, Y.-J. Pu, K. I, Nakayama, J. Kido, Chem. Mater. 2008, **20**, 5951.