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New Strategy for Developing Deep Blue TADF Materials with Narrow FWHM and CIE_v<0.06 Employing Host Materials as Donors

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1. General methods

All reagents are purchased directly from the relevant merchants without further purification. All the solvents used in the measurement have undergone deoxygenation treatment, and the rest of the solvents have not been purified. All reactions are carried out under an inert atmosphere. ¹H-NMR and spectra were measured on Bruker avance III NMR spectrometer (400MHz) in CDCl₃. The mass spectra were performed by GCT premier TOF mass spectrometer. The UV-Vis absorption spectra were record on TU-1901 UV-Vis spectrophotometer with range of 200-800 nm. The fluorescence spectra and low-temperature phosphorescence spectra were measured at 77 K by a FLS 920 spectrometer manufactured from Einburgh Corporation. The thermal decomposition (T_d) temperature and thermogravimetric analysis curves are measured under nitrogen atmosphere with a heating rate of 10 °C/min from 50 to 800 °C. The T_d of the three emitters were measured by an

HCT-2 thermogravimetric analyzer. Cyclic voltammetry (CV) was carried out in 0.1 mol L⁻¹ dichloromethane solution of supporting electrolyte, tetrabutylammonium hexafluorophosphate, measured on the RST 3100 electrochemical workstation. Ferrocene acted as the internal standard and the scan rate of the CV curve of the target molecule is 50 mV s⁻¹.

100K a) 100k b) 200k 200K 300k 300K 10 DCBTRZ PPCTRZ 10 10³ Count Counts 10² 10 10¹ 10¹ 10⁰ 10 15000 5000 10000 15000 5000 2000 20000 10000 Time (ns) Time (ns)

2. Photoluminescence transient decay characteristics

Fig.S1. Temperature-dependent transient PL (100,200,300 K) decay curves of a) DCBTRZ and b)
PPCTRZ in CBP host (10 wt% doped film).

3. Device fabrication and characterization

The ITO glass used in electroluminescent measurement is cleaned and pretreated to ensure its surface is smooth and clean. All the materials and metal electrodes which used to fabricate OLED devices were based on evaporator template for vacuum evaporation with vacuum degree below 2×10^{-4} Pa. The deposition rate of organic layer, LiF layer and Al is 2-3 Å/s,0.1 Å/s, and > 6 Å/s, respectively. When all the materials are deposited, the device

must be completely cooled and then encapsulated with UV curing glue. The corresponding electroluminescence and current density-voltage-luminance characteristics of the devices were measured with a source meter (Keithley Model 2400) and a luminance meter/spectrometer (PhotoResearch PR655).

4. NMR
 IR and Mass Spectra



Fig.S2. ¹H NMR spectrum of 4-CZTRZ.



Fig.S3. IR spectrum of 4-CZTRZ.



Fig.S4. ¹H NMR spectrum of DCBTRZ.



Fig.S5. TOF-MS spectrum of DCBTRZ.



Fig.S6. ¹H NMR spectrum of PPCTRZ.



Fig.S7. TOF-MS spectrum of PPCTRZ.