ELECTRONIC SUPPLEMENTARY INFORMATION

Deep Blue-Emissive Bifunctional (Hole-Transporting + Emissive) Materials with CIEy ~ 0.06 Based on 'U'-Shaped Phenanthrene Scaffold for Application in Organic Light-Emitting Diodes

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EXPERIMENTAL SECTION

General Aspects.¹H NMR spectra were recorded on JEOL (400/500 MHz) spectrometers in CDCl₃ as a solvent. ¹³C NMR spectra were recorded on JEOL-Lambda (100/125 MHz) spectrometers with complete proton decoupling. ESI and EI mass spectra analyses were carried out on Waters ^QTOF and GCT premier mass spectrometers, respectively. Melting points were determined with a JSGW melting point apparatus. IR spectra were recorded on a Bruker Vector 22 FT-IR spectrophotometer. The TGA and DSC measurements were carried out using Mettler-Toledo and SDT Q600 instruments, respectively, at 10 ^oC/min under a nitrogen gas atmosphere. UV-vis absorption spectra were recorded on a Shimadzu UV-1800 spectrophotometer. PL measurements in solution and solid state were carried out using FluoroMax-4; FM4-3000 spectrofluorimeter, Horiba Scientific. Cyclic voltammetry measurements were performed using CHI610E electrochemical work-station (CH instruments, Texas, USA). All solvents were distilled prior to use, and HPLC grade solvents used for UV-vis and PL measurements were procured from Merck. Column chromatography was conducted with a silica gel of 100-200µ mesh.

Materials. ITO-coated glass slides of thickness 0.7 mm and resistance 11 Ω , and materials such as NPB, *m*CP, TmPyPB, TPBI, BCP, LiF and Al, which were employed for device fabrications, were procured from commercial sources. Solvents were distilled prior to use and HPLC grade solvents were employed for cleaning of the ITO-coated glasses and carrying out other measurements in solution state.



Scheme S1. The Premise for the Choice of Phenanthrene Core.

Fig. S1. Normalized absorption (a) and fluorescence (b) spectra of PCZL, PDPA and PTPA in the thin film state.



Fig. S2. Phosphorescence spectra of PCZL, PDPA and PTPA in 2-MeTHF (ca. 1×10^{-5} M) at 77 K.



Fig. S3.CV profiles of PCZL, PDPA and PTPA.



Fig. S4.TGA profiles of PCZL, PDPA and PTPA.



Fig. S5. DSC profiles of PCZL, PDPA and PTPA.



Fig. S6. Current density vs voltage (a) and luminance vs voltage (b) profiles for the devices of configurations A and B.



Fig. S7. EL spectra captured for **PCZL**, **PDPA** and **PTPA** in devices of configurations A and B. Note the difference in the EL spectra of **PTPA** in configurations A and B, cf. text for discussion.



Fig. S8. Plots of external quantum efficiency vs current density (a), external quantum efficiency vs luminance (b), luminous efficiency vs current density (c), luminous efficiency vs luminance (d), power efficiency vs current density (e) and power efficiency vs luminance (f) for the devices of configuration A, refer to text.



Fig. S9. Current density vs voltage (a) and luminance vs voltage (b) profiles for the devices of configurations C and D.



Fig. S10. Plots of external quantum efficiency vs current density (a), external quantum efficiency vs luminance (b), luminous efficiency vs current density (c), luminous efficiency vs luminance (d), power efficiency vs current density (e) and power efficiency vs luminance (f) for the devices of configurations C and D, refer to text.



Fig. S11. ¹H (400 MHz) NMR spectrum of 3,6-dibromophenanthrenein CDCl₃.



Fig. S12. ¹H (400 MHz) and ¹³C (125 MHz) NMR spectra of PCZL in CDCl₃.



Fig. S13. ¹H (500 MHz) and ¹³C (125 MHz) NMR spectra of PDPA in CDCl₃.



Fig. S14.¹H (400 MHz) and ¹³C (125 MHz) NMR spectra of PTPA in CDCl₃.