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## Diphenylamine/triazine hybrids as bipolar hosts for phosphorescent organic lightemitting diodes

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## **General Information**

All chemicals, reagents, and solvents were used as received from commercial sources without further purification. All reactions were carried out under nitrogen and anhydrous conditions unless noted otherwise. <sup>1</sup>H NMR (400MHz) and <sup>13</sup>C NMR (100 MHz) spectra were measured on a Bruker Ascend 400 spectrometer using CDCl<sub>3</sub> as a solvent and the spectral data were reported in ppm relative to tetramethylsilane (TMS) as an internal standard. Molecular weights were measured with a Bruker Autoflex III MALDI-TOF mass spectrometer. Elemental analyses of carbon, hydrogen, and nitrogen were performed on a Vario EL III microanalyzer. UV-vis absorption spectra were recorded on a PG TU-1901 recording spectrophotometer. Photoluminescence (PL) spectra were measured on a Hitachi F-7000 fluorescence spectrophotometer and phosphorescence spectra at 77 K were recorded on a Perkin-Elmer LS 50B spectrofluorometer. The absolute PL quantum yields were measured using a Hamamatsu C9920-02G integrating sphere system coupled with a 150 W xenon lamp and a PMA-12 photonic multichannel analyzer. Differential scanning calorimetry (DSC) was performed on a Mettler Toledo DSC1 STARe system with nitrogen flow at 20 ml/min. Samples were preheated to above their melting points, and then cooled down to -30 °C at -100°C/min before the second heating and cooling scans were recorded at 10 °C/min. Thermogravimetric analysis (TGA) was undertaken with a TA instrument Q600 at a scanning rate of 10 °C/min under nitrogen. Cyclic voltammetry (CV) was carried out using nitrogen-purged anhydrous tetrahydrofuran (THF) for the reduction and dichloromethane for the oxidation scan at room temperature with a CHI voltammetric analyzer. Tetrabutylammonium hexafluorophosphate  $(TBAPF_6)$  (0.1 M) was used as the supporting electrolyte. The conventional three-electrode configuration consists of a platinum working electrode, a platinum wire auxiliary electrode, and an Ag wire pseudo-reference electrode with ferrocenium–ferrocene (Fc<sup>+</sup>/Fc) as the internal standard. Cyclic voltammograms were obtained at a scan rate of 100 mV/s. Formal potentials are calculated as the average of cyclic voltammetric anodic and cathodic peaks. The onset potential was determined from the intersection of two tangents drawn at the rising and background current of the cyclic voltammogram. The geometrical and electronic properties of the three hosts were performed with the Gaussian 09 program package. The calculation was optimized by means of B3LYP with the 6-31G(d) atomic basis set. The molecular orbitals were visualized using Gaussview.

## **Device Fabrication and Measurement**

The fabricated devices were grown on clean glass substrates pre-coated with a 180-nm thick layer of indium tin oxide (ITO) with a sheet resistance of 15~20  $\Omega$ /sq. The ITO surface was treated with oxygen plasma for 2 min, following a degrease in an ultrasonic solvent bath, and then was dried at 120 °C before it was loaded into an evaporator. All layers were grown in succession by thermal evaporation at a pressure below 5 × 10<sup>-4</sup> Pa without breaking vacuum. The thickness of each layer was determined by a quartz thickness monitor. Current–brightness–voltage characteristics were measured using Keithley source measurement units (Keithley 2400 and Keithley 2000) with a calibrated silicon photodiode. The EL spectra were measured using a SpectraScan PR650 spectrophotometer. External quantum efficiencies were calculated from the luminance, current density, and EL spectrum, assuming a Lambertian distribution. All the measurements were carried out in an ambient atmosphere.



Fig. S1 Fluorescence spectra in toluene at 77 K of DPA-TRZ, DDPA-TRZ, and TDPA-TRZ.



**Fig. S2** Transient PL decay curves in doped mCP film at a concentration of 10 wt% for DPA-TRZ, DDPA-TRZ, and TDPA-TRZ.

## <sup>1</sup>H NMR spectroscopy







<sup>13</sup>C NMR spectroscopy



