

Supporting Information

Highly Efficient Deep-Blue OLED with an Extraordinary Narrow FWHM of 35 nm and Y Coordinate < 0.05 Based on a Fully Twisting Donor-Acceptor Molecule

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S-1 Detailed Synthesis of TPA-PIM

All the reagents and solvents used for the syntheses were purchased from Aldrich or Acros and used as received. All reactions were performed under a dry nitrogen atmosphere.

2-(4-bromophenyl)-1,4,5-triphenyl-1H-imidazole (M1)

A mixture of aniline (10.0 mmol), benzil (2.0 mmol), 4-bromobenzaldehyde (2.0 mmol), ammonium acetate (8.0 mmol), and acetic acid (15 mL) was refluxed under nitrogen in an oil bath. After 2h, the mixture was cooled and filtered. The solid product was washed with an acetic acid/water mixture (1:1, 30 mL) and water. Then it was dried in the vacuum and used directly for the next step without further purification and characters. ¹H NMR (500 MHz, DMSO) δ 7.50 (t, $J = 7.4$ Hz, 4H), 7.37 – 7.22 (m, 14H), 7.19 (t, $J = 7.3$ Hz, 1H). MS (ESI): MW 451.4, m/z 450.6 (M⁺).

N,N-diphenyl-4'-(1,4,5-triphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-amine (TPA-PIM)

A mixture of N,N-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (200 mg, 0.54 mmol) (synthesized by: n-butyllithium added into 4-bromo-N,N-diphenylaniline at -78 °C, then 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane added, and stirred for 24h at room temperature), M1 (225 mg, 0.5 mmol), sodium carbonate (424 mg, 4.0 mmol), toluene (3 mL) and distilled water (2 mL), with Pd(PPh₃)₄ (30mg) acting as catalyst was refluxed at 90°C for 48h under nitrogen. Then some water was added to the resulting solution and the mixture was extracted with chloroform for several times. The organic phase was dried over anhydrous magnesium sulfate. After filtration and solvent evaporation, the liquid was purified by column chromatography using petroleum ether/CH₂Cl₂ as the eluent to afford a white solid (yield 65%). ¹H NMR (500 MHz, DMSO) δ 7.58 (dd, $J = 16.2, 8.7$ Hz, 4H), 7.50 (d, $J = 7.2$ Hz, 2H), 7.43 (d, $J = 8.5$ Hz, 2H), 7.35 (dd, $J = 7.3, 4.0$ Hz, 4H), 7.30 (dd, $J = 8.0, 5.2$ Hz, 7H), 7.25 (t, $J = 6.3$ Hz, 4H), 7.18 (d, $J = 7.4$ Hz, 2H), 7.10 – 7.02 (m, 6H), 6.99 (d, $J = 8.7$ Hz, 2H). MS (ESI): MW 615.8, m/z 615.8 (M⁺). Elemental analysis calculated [%] for C₄₅H₃₃N₃: C, 87.77; H, 5.40; N, 6.82,

found: C, 87.86; H, 5.21; N, 7.15.

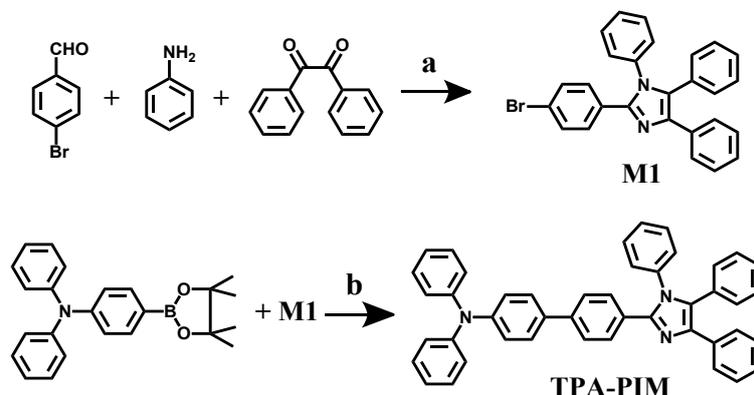


Figure S1. The synthesis route of TPA-PIM (a. in CH_3COOH and ammonium acetate, refluxed for 2h, yield: 75%; b. $\text{Pd}(\text{PPh}_3)_4$, sodium carbonate in Toluene and distilled water, refluxed for 48h under nitrogen, yield: 65%.)

S-2. Characterization and Measurement

The ^1H NMR spectra were recorded on AVANCZ 500 spectrometers at 298 K by utilizing deuterated dimethyl sulfoxide (DMSO) as solvents and tetramethylsilane (TMS) as a standard. The compounds were characterized by a Flash EA 1112, CHNS–O elemental analysis instrument. The MALDI-TOF-MS mass spectra were recorded using an AXIMA-CFRTM plus instrument. UV-vis absorption spectra were recorded on a UV-3100 spectrophotometer. Fluorescence measurements were carried out with a RF-5301PC. The differential scanning calorimetry (DSC) analysis was determined using a NETZSCH (DSC-204) instrument at $10\text{ }^\circ\text{C min}^{-1}$ under nitrogen flushing. Cyclic voltammetry (CV) was performed with a BAS 100W Bioanalytical Systems, using a glass carbon disk ($\Phi=3\text{ mm}$) as the working electrode, a platinum wire as the auxiliary electrode with a porous ceramic wick, Ag/Ag^+ as the reference electrode, standardized for the redox couple ferricinium/ferrocene. All solutions were purged with a nitrogen stream for 10 min before measurement. The procedure was performed at room temperature and a nitrogen atmosphere was maintained over the solution during measurements.

The EL devices were fabricated by vacuum deposition of the materials at 10^{-6} Torr onto ITO glass with a sheet resistance of $25\ \Omega\ \text{square}^{-1}$. All of the organic layers were

deposited at a rate of 1.0 \AA s^{-1} . The cathode was deposited with LiF (1 nm) at a deposition rate of 0.1 \AA s^{-1} and then capping with Al metal (100 nm) through thermal evaporation at a rate of 4.0 \AA s^{-1} . The electroluminescence (EL) spectra and Commission Internationale De L'Eclairage (CIE) coordination of these devices were measured by a PR650 spectra scan spectrometer. The luminance-current and density-voltage characteristics were recorded simultaneously with the measurement of the EL spectra by combining the spectrometer with a Keithley model 2400 programmable voltage-current source. All measurements were carried out at room temperature under ambient conditions.

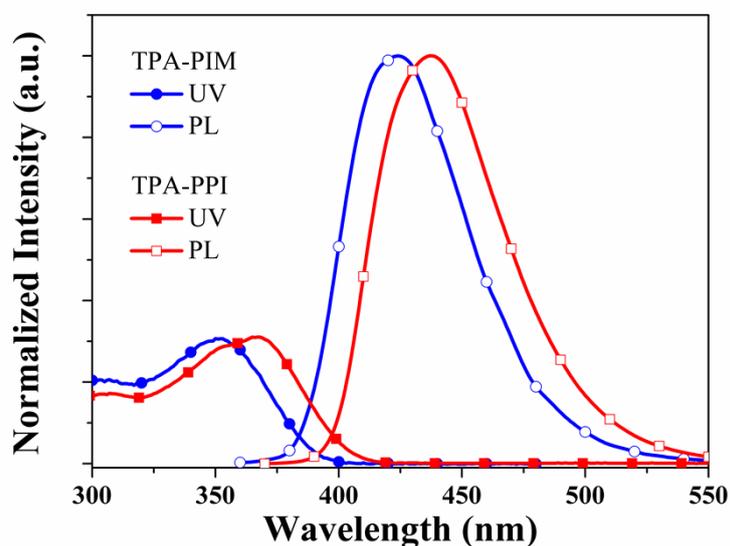


Figure S2. The UV and PL spectra of TPA-PIM and TPA-PPI in the tetrahydrofuran solution at the concentration of 10^{-5} M

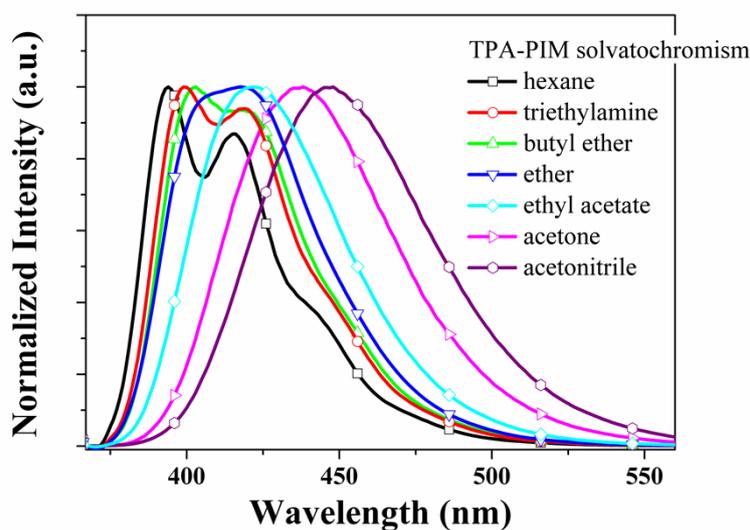


Figure S3. PL spectra of TPA-PIM measured in different solvents with increasing

polarity (hexane 0.0012, triethylamine 0.048, butyl ether 0.096, ether 0.167, ethyl acetate 0.200, acetone 0.284, and acetonitrile 0.305).

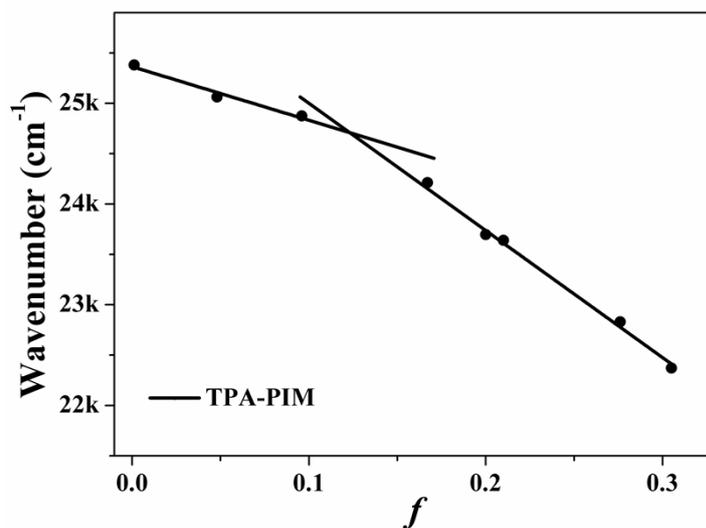


Figure S4. Linear correlation of orientation polarization (f) of solvent media with maximum wavenumber for TPA-PIM. (the line in the highly and lowly polar region were fitted by the points with $f \geq 0.2$ and ≤ 0.1 respectively)

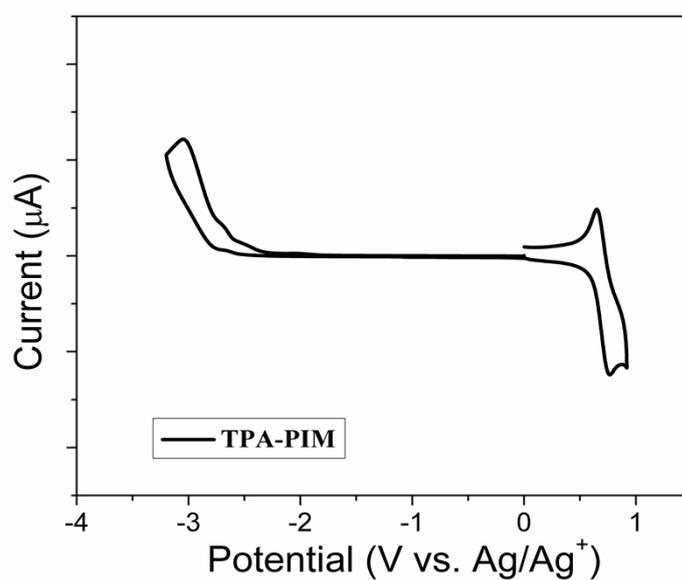


Figure S5. The CV measurement of TPA-PIM

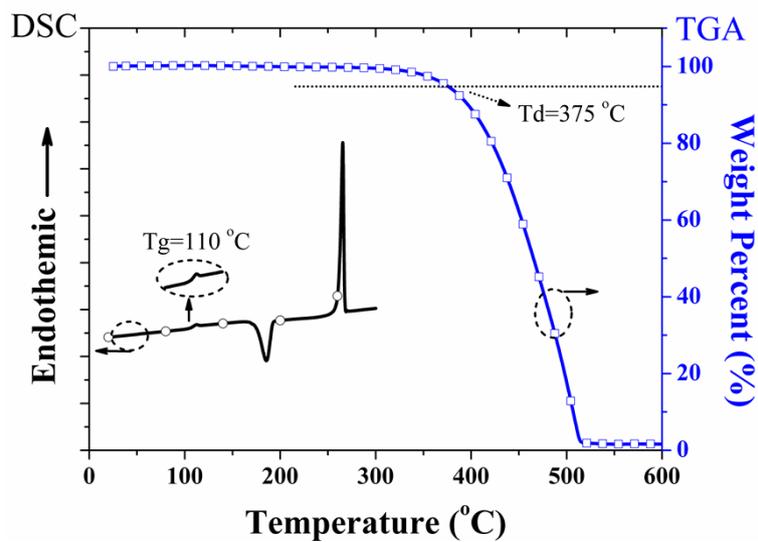


Figure S6. The DSC and TGA graphs of TPA-PIM

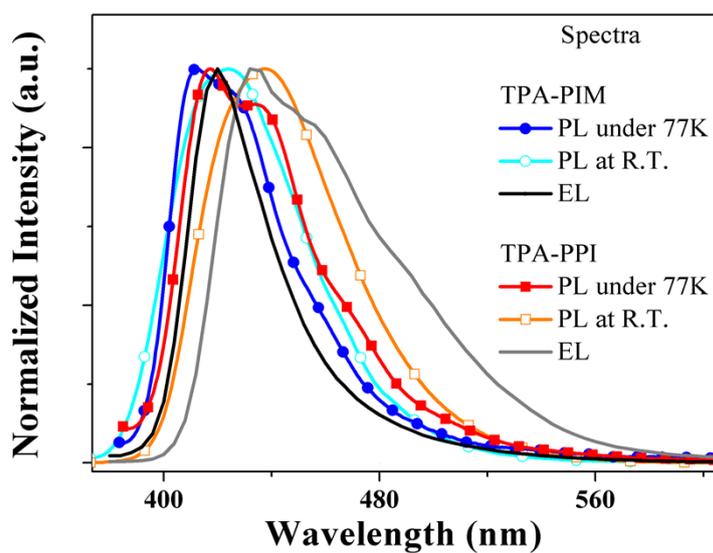


Figure S7. The PL spectra of TPA-PIM and TPA-PPI under 77K and at room temperature (R.T.) in the tetrahydrofuran solution at the concentration of 10^{-5} M as well as their respective EL spectra

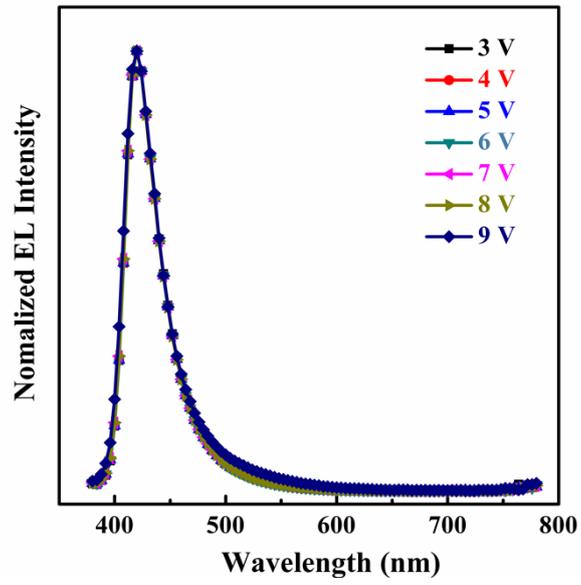


Figure S8. The EL spectra of TPA-PIM based OLED at different driving voltages