Electronic Supplementary Information

Pyridine based *meta*-linking deep-blue emitter with high conjugation extent and electroluminescent efficiencies

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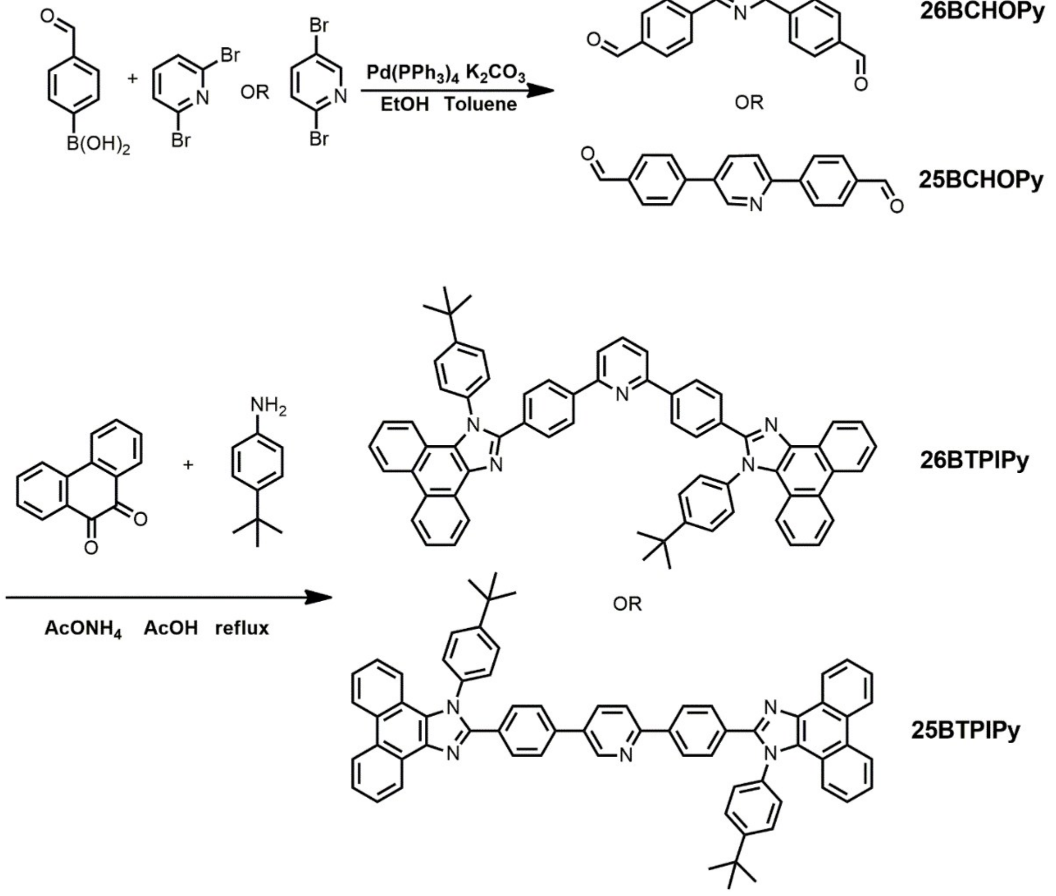

Scheme S1 Synthetic procedures of **26BTPIPy** and **25BTPIPy**.

Synthetic procedures

The synthesis of 4,4'-(pyridine-2,6-diyl)dibenzal-dehyde (26BCHOPy) and 4,4'-(pyridine-2,5-diyl)dibenzaldehyde (25BCHOPy) was proceeded following reported procedures.[1]

26BTPIPy: 9,10-phenanthrenequinone (0.92 g, 4.4 mmol), 2,6-BCHOPy (0.57 g, 2 mmol), 4-*tert*-butylbenzenamine (0.66 g, 4.4 mmol), and ammonium acetate (2.31 g, 30.0 mmol) were added into glacial acetic acid (30 mL).The mixture was refluxed for 24 h under an argon atmosphere. After cooling to room temperature, an orange-yellow mixture was obtained and poured into methanol under stirring. The crude product was separated by filtration, washed with methanol, and dried under vacuum. The product was purified by column chromatography (silica gel) using eluent of petroleum ether/dichloromethane (V/V) 1/4 to give a pale solid, with a 70% yield (1.3 g). ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.86 (d, J = 7.9 Hz, 2H), 8.80 (d, J = 8.4 Hz, 2H), 8.75 (d, J = 8.4 Hz, 2H), 8.10 (d, J = 8.2 Hz, 4H), 7.86 (t, J = 7.7 Hz, 1H), 7.76 (t, J = 7.8 Hz, 8H), 7.69 (dd, J = 8.1, 6.2 Hz, 6H), 7.52 (dd, J = 8.3, 6.3 Hz, 6H), 7.30 (t, J = 7.6 Hz, 2H), 7.21 (d, J = 8.3 Hz, 2H), 1.47 (s, 18H). MS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{67}H_{54}N_5$: 929.17. Found: 929.0. Anal. Calcd for $C_{67}H_{53}N_5$: C, 86.70; H, 5.76; N, 7.54; found: C, 86.78; H, 5.71; N, 7.49.

25BTPIPy: The synthetic procedures were similar to that of **26BTPIPy**. Yield: 55.5 %.^{1}H NMR (300 MHz, CD_2Cl_2) δ 8.85 (d, J = 1.5 Hz, 1H), 8.81 (d, J = 8.2 Hz, 3H), 8.76 (d, J = 8.3 Hz, 2H), 7.81 – 7.74 (m, 4H), 7.73 – 7.64 (m, 10H), 7.58 (d, J = 2.3 Hz, 1H), 7.55 (t, J = 2.5 Hz, 1H), 7.52 (d, J = 2.2 Hz, 3H), 7.49 (d, J = 2.0 Hz, 2H), 7.37 – 7.25 (m, 8H), 1.47 (s, 18H). MS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{67}H_{54}N_5$: 929.17. Found: 928.9. Anal. Calcd for $C_{67}H_{53}N_5$: C, 86.70; H, 5.76; N, 7.54; found: C, 86.75; H, 5.77; N, 7.46.

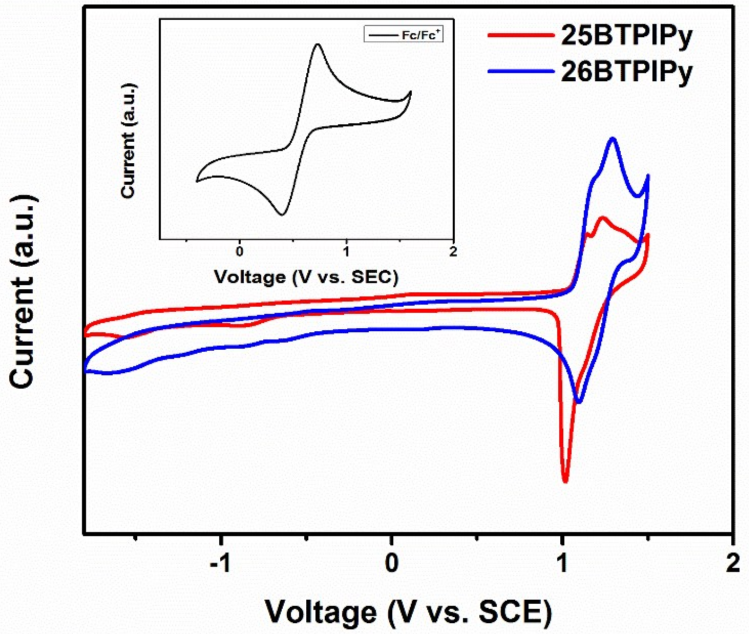

Fig. S1 Positive CV scans of **26BTPIPy** and **25BTPIPy** (inset: ferrocene) against saturated calomel electrode (SCE)

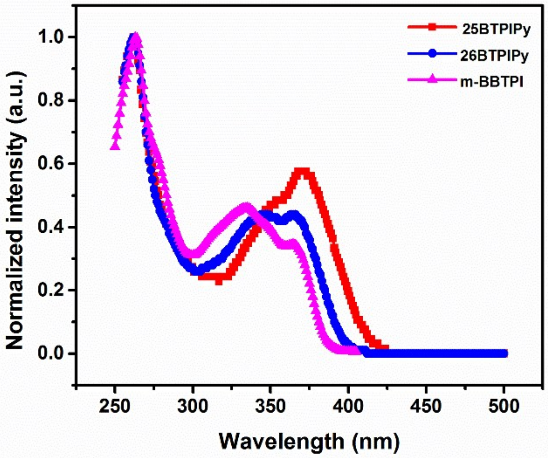

Fig. S2 Absorption spectra of *m*-BBTPI, **26BTPIPy** and **25BTPIPy** in DCM.

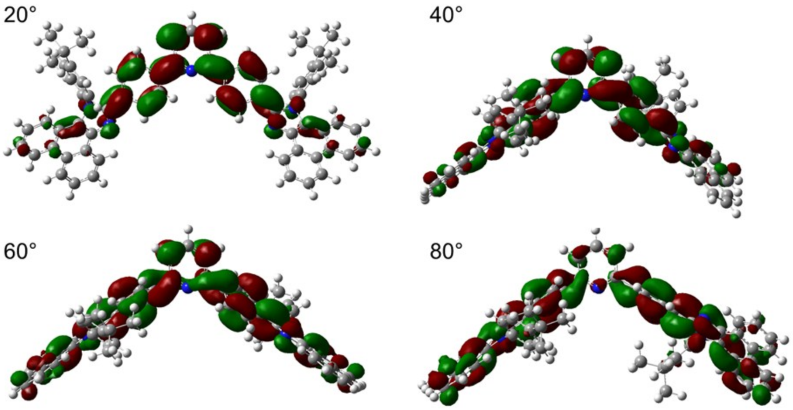

Fig. S3 Calculated LUMO distributions of **26BTPIPy** with arbitrary fixed twisting angle between the pyridine ring and two connected benzene rings.

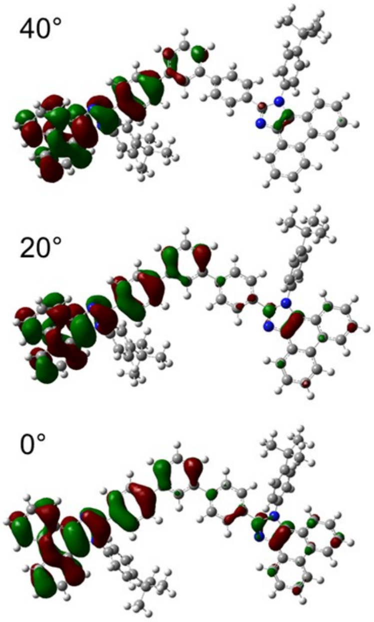

Fig. S4 Calculated HOMO distributions of *m*-BBTPI with arbitrary fixed twisting angle between the central benzene ring and two connected benzene rings.

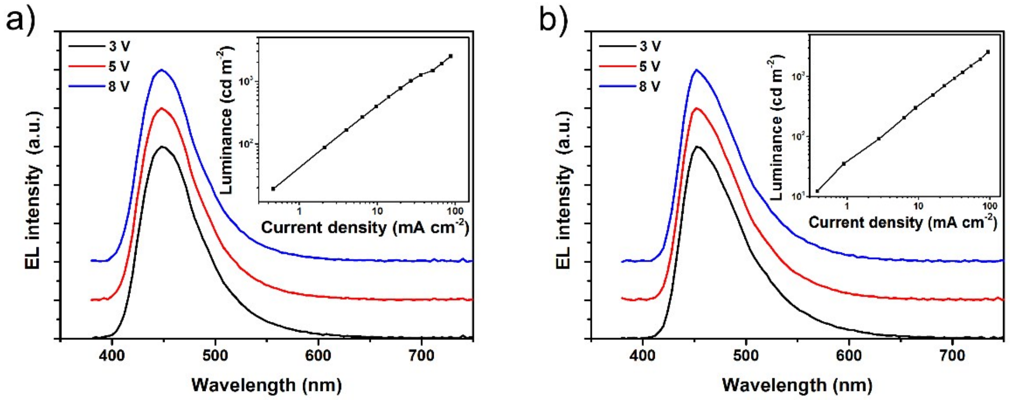

Fig. S5 EL spectra at different voltages (inset is luminescence-current density plot) of a) **26BTPIPy** and b) **25BTPIPy**-based bilayer devices

References:

1. a) N. Kuhnert, C. Patel and F. Jami, *Tetra. Lett.*, 2005, **46**, 7575-7579; b) A. Suzuki and H. C. Brown, *Organic Syntheses via Boranes: Suzuki Coupling*, Aldrich Chemical Company, 2003.