Electronic Supplementary Information for:

2-Phenylpyrimidine skeleton-based electron-transport materials for extremely efficient green organic light-emitting devices

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General Procedures. The optimized structures and single-point energies (HOMO, LUMO energies) were calculated by Gaussian03[1] at the RB3LYP 6-31G(d) and 6-311+G(d,p) levels, respectively. ^{1}H NMR spectra were recorded on JEOL 400 (400 MHz) spectrometer. Mass spectra were obtained using a JEOL JMS-K9 mass spectrometer. Differential scanning calorimetry (DSC) was performed using a Perkin-Elmer Diamond DSC Pyris instrument under nitrogen atmosphere at a heating rate of 10°C min^{-1}. Thermogravimetric analysis (TGA) was undertaken using a SEIKO EXSTAR 6000 TG/DTA 6200 unit under nitrogen atmosphere at a heating rate of 10°C min^{-1}. UV-Vis spectra were measured using a Shimadzu UV-3150 UV-vis-NIR spectrophotometer. Photoluminescence spectra were measured using a FluroMax-2 (Jobin-Yvon-Spex) luminescence spectrometer. HOMO levels were determined by photoelectron yield spectroscopy (OPTEL). The phosphorescent spectra were measured by using a streak camera (C4334 from Hamamatsu Photonics) at 4.2 K. The current density–luminance–voltage characteristics of the OLEDs were measured by Keithley source meter 2400 and Konica Minolta CS-200, respectively. Electroluminescence (EL) spectra were taken by an optical mutichannel analyzer, Hamamatsu PMA 11.

(1) M. J. Frisch et al. Gaussian 03; Gaussian Inc.: Pittsburgh, PA 2003.

Synthesis of 3. 3,5-Dichlorophenyl boronic acid (5.03 g, 26.4 mmol) and **2** (2.70 g, 12.0 mmol) were added to a round bottom flask. Acetonitrile (190 mL) and aqueous Na_2CO_3 (1 M, 60 mL) were added and nitrogen bubbled through the mixture for 1 hour. Then, $PdCl_2(PPh_3)_2$ (0.42 g, 0.60 mmol) was added and the resultant mixture was stirred for 9 hours at 70 ˚C under N_2 flow. The precipitate was filtered, and washed with water and methanol. The resulting off-white solid was dissolved in reflux toluene 450 mL, filtered through silica-gel pad (50 cc) and washed with toluene 50 mL. After the clear filtrate was concentrated to 50 mL, the precipitate was collected, washed with hexane, dried in vacuo to afford **3** (3.75 g, 70%) as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77–8.64 (m, 2H) 8.15 (d, *J*=1.4 Hz, 4H), 7.86 (s, 1H), 7.58–7.53 (m, 5H) ppm; MS: m/z 446 $[M]^+$.

Synthesis of 1. 3-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine (16.5 g, 80.4 mmol) and **3** (3.0 g, 6.7 mmol) were added to a round bottom flask. 1,4-Dioxane (85 mL) and aqueous K_3PO_4 (1.35 M, 35 mL) were added and nitrogen bubbled through the mixture for 1 hour. Then, $Pd_2(dba)_3$ (0.73 g, 0.80 mmol) and PCy_3 (0.54 g, 1.92 mmol) were added and the resultant mixture was vigorously stirred for 30 hours at reflux temperature under N_2 flow. The precipitate was filtered, and washed with water and methanol. The resulting off-white solid was purified by chromatography on silica gel (eluent: $CHCl_3/CH_3OH$ = 100:2, 100:2.5, 100:4 to 100:10 v/v) to afford **1a** (3.43 g, 83%) as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.03 (d, 4H, J=2.3 Hz), 8.76–8.69 (m, 6H) 8.51 (d, 4H, J=1.4 Hz), 8.17 (s, 1H), 8.05 (dt, 4H, J=2.3, 7.8 Hz), 7.93 (t, 2H, J=1.4 Hz), 7.61–7.56 (m, 3H), 7.48 (dd, 4H, J=4.8, 7.8 Hz) ppm; MS: *m/z* 617 $[M]^+$; Anal. Calcd for $C_{42}H_{28}N_6$: C, 81.80; H, 4.58; N, 13.63%. Found: C, 81.54; H, 4.37; N, 13.64%. UV-vis (film): λ_{max} = 260, 323 nm. For **1b**: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.79 (dd, 8H, J=1.8, 4.6 Hz), 8.75 (dd, 2H, J=1.8, 5.0 Hz), 8.57 (d, 4H, J=1.8 Hz), 8.15 (s, 1H), 8.03 (t, 2H, J=1.8 Hz), 7.68 (dd, 8H, J=1.8, 4.6 Hz), 7.60–7.59 (m, 3H) ppm; MS: *m/z* 617 $[M]^+$. Anal. Calcd for $C_{42}H_{28}N_6$: C, 81.80; H, 4.58; N, 13.63%. Found: C, 81.90; H, 4.37; N, 13.72%. UV-vis (film): λ_{max} = 263, 320 nm.

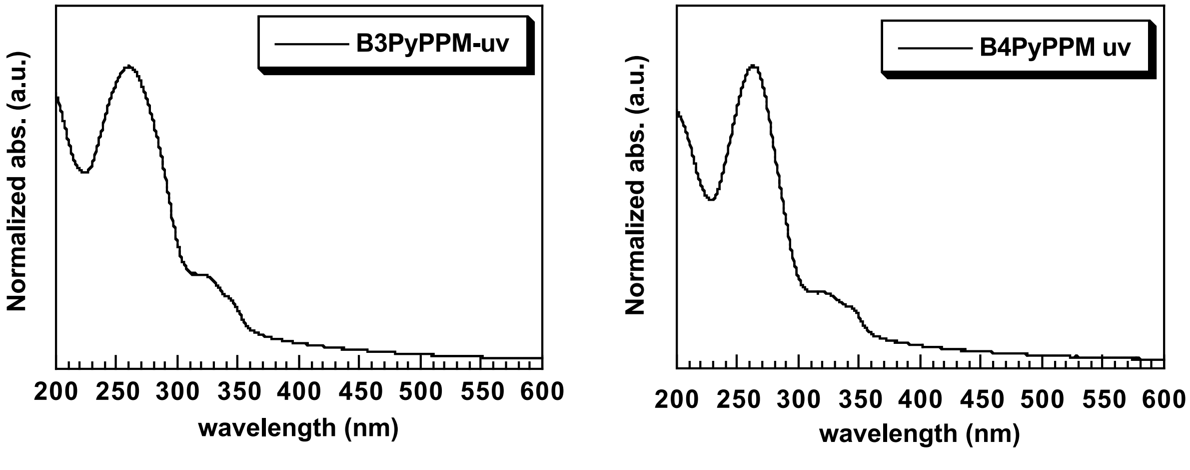

Figure S-1. UV–vis spectra of vacuum deposited film of **1**. No emission was observed from vaccum deposited film of **1** (λ_{ex} = 250 nm).

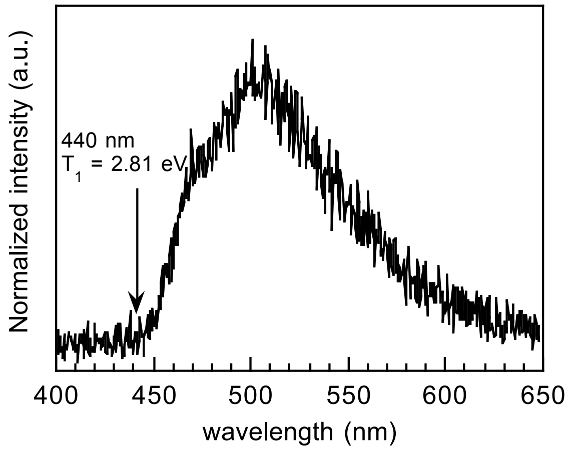

Figure S-2. Phosphorescent spectrum of vacuum-deposited film of **1a** at 4.2 K, measured by streak camera with a N_2 gas laser (337 nm) as an excitation light.

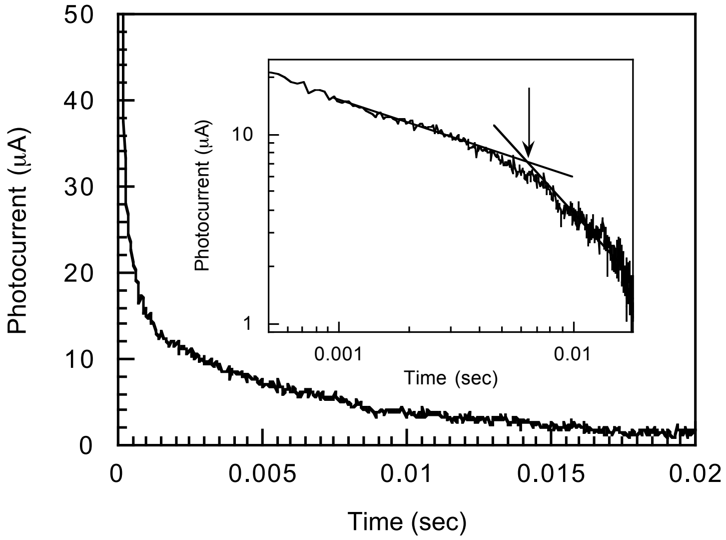

Figure S-3. Transient photocurrent profile for **1a** measured at room temperature. Electric field ($E^{1/2}$) was 624 $[V/cm]^{1/2}$. Sample thickness was 8.8 μm. Inset: Double logarithmic plot.

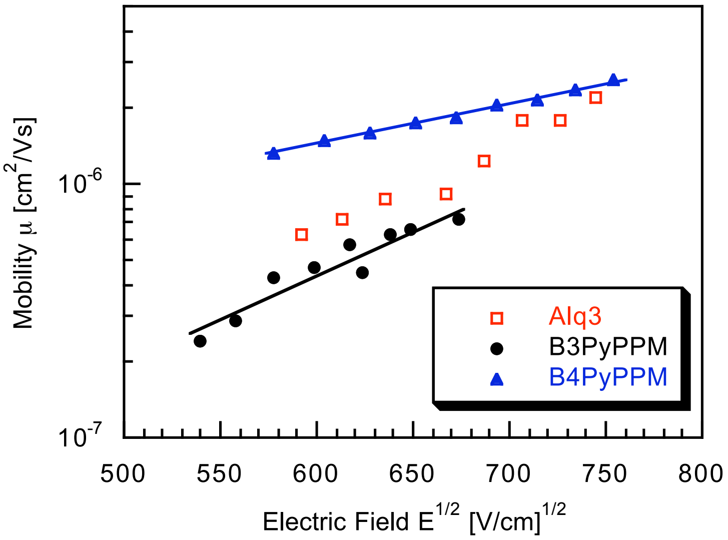

Figure S-4. Electron mobility of BPyPPM derivatives and Alq_3.