



Supporting Information

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Simple Carbazole/Oxadiazole Hybrid Molecule: Excellent Bipolar Host for Green and Red Phosphorescent OLEDs

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Experimental Section

General Information: ^1H NMR and ^{13}C NMR spectra were measured on a MERCURY-VX300 and MERCURY-VX600 spectrometer, respectively. Elemental analyses of carbon, hydrogen, and nitrogen were performed on a Vario EL III microanalyzer. Mass spectra were measured on a ZAB 3F-HF mass spectrometer. UV-Vis absorption spectra were recorded on a Shimadzu UV-2500 recording spectrophotometer. PL spectra were recorded on a Hitachi F-4500 fluorescence spectrophotometer. Differential scanning calorimetry (DSC) was performed on a NETZSCH DSC 200 PC unit at a heating rate of $10\text{ }^\circ\text{C min}^{-1}$ from 30 to $300\text{ }^\circ\text{C}$ under argon. The glass transition temperature (T_g) was determined from the second heating scan. Thermogravimetric analysis (TGA) was undertaken with a NETZSCH STA 449C instrument. The thermal stability of the samples under a nitrogen atmosphere was determined by measuring their weight loss while heating at a rate of $15\text{ }^\circ\text{C min}^{-1}$ from 25 to $600\text{ }^\circ\text{C}$. Cyclic voltammetry (CV) was carried out in nitrogen-purged anhydrous DMF (reduction scan) and dichloromethane (oxidation scan) at room temperature with a CHI voltammetric analyzer. Tetrabutylammonium hexafluorophosphate (TBAPF₆) (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^+/Fc) as the internal standard. Cyclic voltammograms were obtained at scan rate of 100 mV s^{-1} . 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.

Device fabrication and measurement: The hole-injection MoO₃, hole-transporting material NPB (1,4-bis(1-naphthylphenylamino)-biphenyl), hole-blocking BCP (2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline) and electron-transporting materials Alq₃ (tris(8-hydroxyquinoline)aluminum) were commercially available. Commercial indium tin oxide (ITO) coated glass with sheet resistance of 10 Ω/□ was used as the starting substrates. Before device fabrication, the ITO glass substrates were pre-cleaned carefully and treated by UV/O₃ for 2 min. Then the sample was transferred to the deposition system. 10 nm of MoO₃ was firstly deposited to ITO substrate, followed by NPB, emissive layer, 10 nm BCP, and 30 nm Alq₃. Finally, a cathode composed of 1 nm of lithium fluoride and 100 nm of aluminum were sequentially deposited onto the substrate in the vacuum of 10⁻⁶ Torr to construct the device. The L-V-J of EL devices was measured with a Keithley 2400 Source meter and a Keithley 2000 Source multimeter equipped with a calibrated silicon photodiode. The EL spectra were measured by JY SPEX CCD3000 spectrometer. All measurements were carried out at room temperature under ambient conditions.

Synthesis of 2,5-bis(2-(9H-carbazol-9-yl)phenyl)-1,3,4-oxadiazole (o-CzOXD): A mixture of carbazole (0.668 g, 4 mmol), 2,5-bis(2-fluorophenyl)-1,3,4-oxadiazole^[1]

(0.516g, 2 mmol), and K_2CO_3 (12 mmol, 1.4 g) in 6 ml of DMSO was stirred at 150 °C for 12 h under argon condition. After cooled to room temperature, the mixture was poured into water, filtered, then purified by recrystallization in $CHCl_3/C_2H_5OH$ twice to give a white solid. Yield: 0.916 g, (83 %), mp: 245 °. 1H NMR (300 MHz, $CDCl_3$, δ): 8.15-8.12 (m, 4H), 7.64 (t, $J = 7.8$ Hz, 2H), 7.51 (d, $J = 7.5$ Hz, 2H), 7.32 (t, $J = 8.1$ Hz, 2H), 7.32-7.20 (m, 10H), 6.87-6.82 (m, 4H). ^{13}C NMR (600 MHz, $CDCl_3$, δ): 161.9, 141.7, 135.7, 133.0, 131.0, 130.7, 129.1, 126.3, 123.8, 123.1, 120.5, 120.1, 109.6. Anal. Calcd. for $C_{38}H_{24}N_4O$ (%): C 82.59, H 4.38, N 10.14; Found: C 82.68, H 4.25, N 9.94. MS (ESI): m/z : 552.3 (M^+).

X-ray Crystallographic Details: Colorless crystals of *o*-CzOXD suitable for X-ray diffraction studies were grown by slow evaporation of its solution in CH_2Cl_2 /hexane at room temperature. Crystallographic measurements were obtained on a Bruker SMART CCD area-detector diffractometer. The structure was performed at 273 K using graphite monochromated Mo-K α radiation ($\lambda = 0.71073$ Å). The data were corrected for absorption using the SADABS program. The structures were solved by direct methods using SHELXS-97 program. Non-hydrogen atoms were refined with anisotropic thermal parameters by full-matrix least-squares calculations on F2 using SHELXL-97. Hydrogen atoms were directly obtained from Difference Fourier Maps and several DFIX commands were applied on hydrogen atoms. Drawings were produced using Diamond 3.0 and Mercury 1.4.1 software. Crystal data for *o*-CzOXD: $C_{38}H_{24}N_4O$, F. W. = 552.61, monoclinic, $P2(1)/n$, $a = 13.9314(10)$ Å, $b = 11.2500(8)$ Å, $c = 18.6444(14)$ Å, $\beta = 109.8420(10)^\circ$, $V = 2748.6(3)$ Å³, $Z = 4$, 16150 reflections

were collected of which 5685 were unique ($R_{int}=0.0171$), final $R_1[I>2\sigma(I)]=0.0345$, $\omega R_2(\text{all data})=0.0821$. The crystallographic data of *o*-CzOXD (excluding structure factors) has been deposited to the Cambridge Crystallographic Data Centre with the deposition number CCDC-693979. This data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

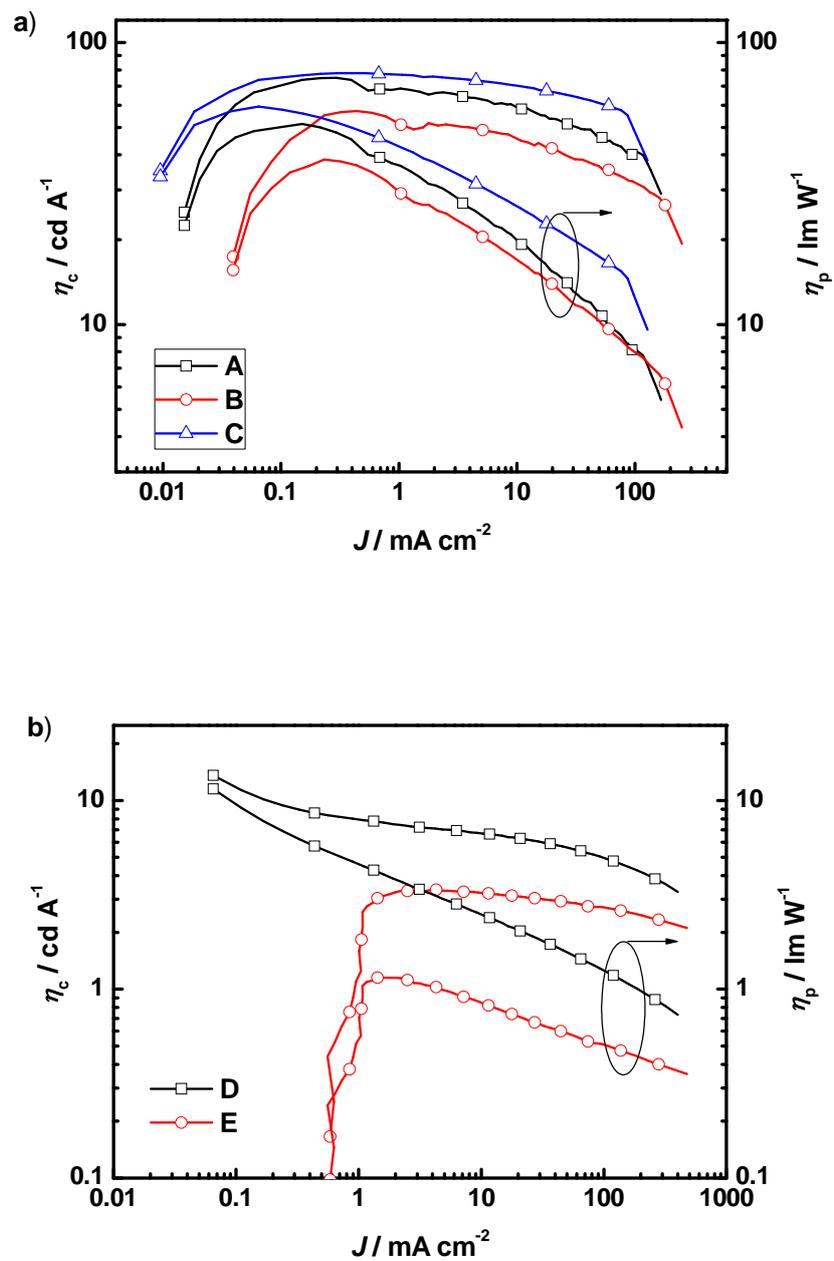


Figure S 1. Efficiency versus current density (J) curves a): Device A-C; b): Device D and E.

Reference:

[1] X. M. Zheng, Z. Li, Y. L. Wang, W. D. Chen, Q. C. Huang, C. X. Liu, G. H. Song. *J. Fluor. Chem.* **2003**, *123*, 163.