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Electronic Supplementary Information

Highly Efficient Single-layer Organic Light-emitting Devices Based on a Bipolar Pyrazine/Carbazole Hybrid Host Material

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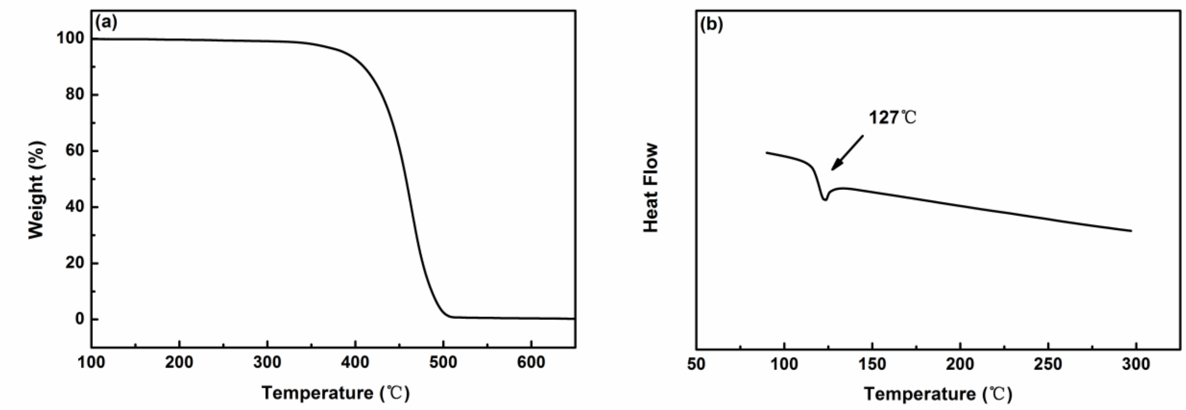

Fig. S1 (a) TGA thermograms recorded at a heating rate of 10 °C min^{-1}; (b) DSC traces recorded at a heating rate of 10 °C min^{-1}.

Table S1 Summary of the Physical Measurements of 26PyzCz.

Compound	T_g [a]	T_d [a]	λ_{abs} [b]	λ_{em} [b]	λ_{ph} [c]	E_g [d]	E_T [e]	HOMO/LUMO [f]
	(°C)	(°C)	(nm)	(nm)	(nm)	(eV)	(eV)	(eV)
26PyzCz	127	410	293, 319	418	494	3.03	2.51	5.83/2.80

[a] T_g: glass transition temperatures. [b] Measured in dichloromethane solution at room temperature. [c] Measured in 2-MeTHF glass matrix at 77 K. [d] E_g: The band gap energies were estimated from the optical absorption edges of UV-Vis absorption spectra of the film. [e] E_T: The triplet energy was estimated from the onset peak of the phosphorescence spectra. [f] HOMO and LUMO estimated from the UPS and the optical band gap from the absorption spectra.

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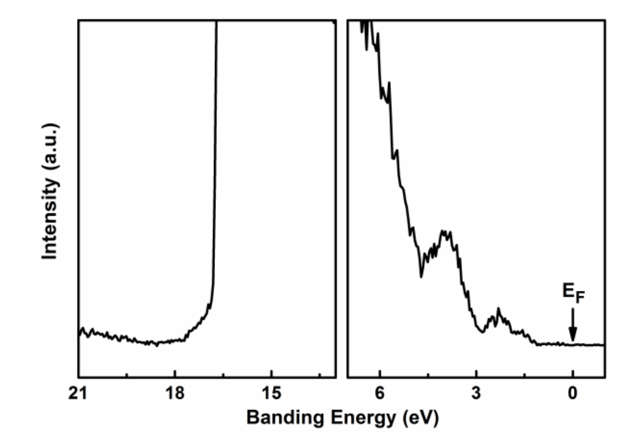

Fig. S2 UPS spectrum of 26PyzCz thin film prepared by thermal evaporation.

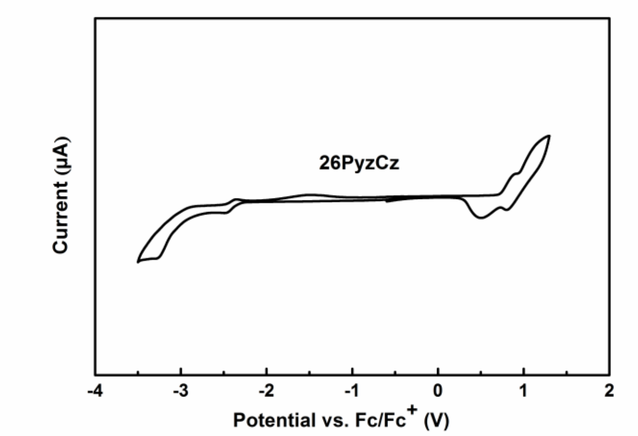

Fig. S3 Cyclic voltammogram of 26PyzCz in DCM and DMF for oxidation and reduction scan.

The electrochemical properties of the 26PyzCz were determined by cyclic voltammetry (CV) as shown in Fig. S3. The measurements were performed in DCM and DMF for oxidation and reduction scans with ferrocene as the internal reference. The compound undergoes both reversible oxidation and reduction to approbate the formation of stable cation and anion radicals, suggesting a bipolar transporting property of 26PyzCz. The reversible oxidation peak around 0.81 V is attributed to the oxidation of carbazole, whereas the reversible reduction peak, observed about -2.35 V, is associated with the electron injection into the pyrazine.

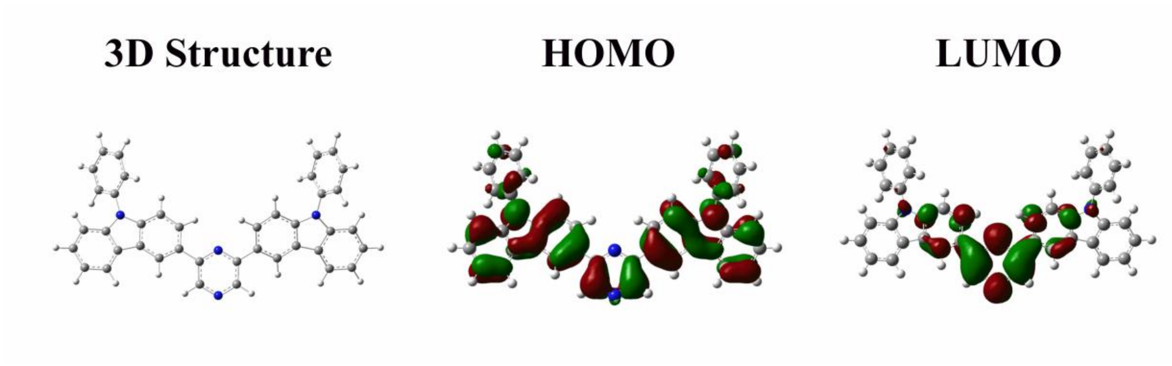

Fig. S4 3D structure and frontier molecular orbital surfaces of 26PyzCz.

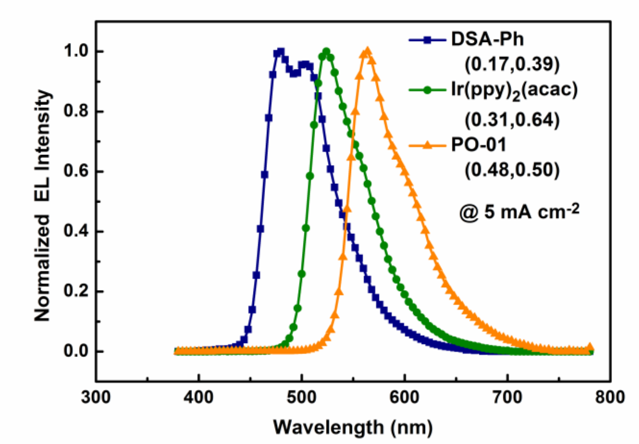

Fig. S5 The EL spectra of blue, green and orange emission SL devices at 5 mA cm^{-2}.

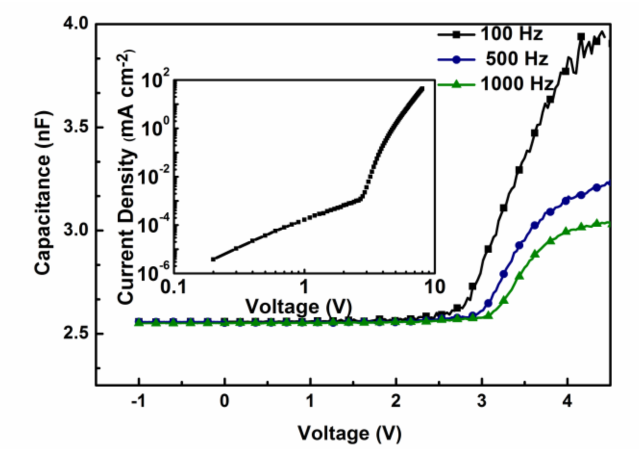

Fig. S6 Capacitance-voltage characteristics of the device measured at 100 Hz, 500 Hz and 1000 Hz; The inset is the current density-voltage characteristic of the device.

Fig. S6 shows the measured capacitance-voltage (*C*-*V*) characteristics under various frequencies. At negative and low bias, the capacitance maintains a constant value of about 2.5 nF, which is attributed to the geometrical capacitance and chemical capacitance of the intrinsic layers. When the voltage is larger than V_{bi} (the built-in voltage due to the contact potential difference between the ITO and Al electrode), the capacitance is dominated by a chemical capacitance (C_n). This is related to the excess minority carriers that alter the occupancy of electrons in the LUMO of the materials, as follows[1, 2]

$$C_n = e^2 \frac{dn}{dE_{Fn}} \qquad (1)$$

Here the capacitance is given per unit volume, e corresponds to the positive elementary charge, n accounts for the free electron concentration, and E_{Fn} stands for the electron quasi-Fermi level. The result demonstrates that the electron can be effectively injected into the device over 2.5 V, which is consistent with the current density-voltage (*I*-*V*) characteristics.

Notes and references

1. J. Bisquert, D. Cahen, G. Hodes, S. Ruhle, A. Zaban, *J. Phys. Chem. B,* 2004, **108**, 8106.

2. G. Garcia-Belmonte, A. Munar, E. M. Barea, J. Bisquert, I. Ugarte, R. Pacios, *Org. Electron.*, 2008, **9**, 847.