Design and synthesis of fluorene-based block polymer host materials for efficient electroluminescence

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Main Experimental Reagents and Testing Instruments

In the experiment, all reactants such as 4-hydroxycarbazole, bisphenol fluorene, benzophenone, cesium carbonate, potassium carbonate, silica gel, etc., were purchased and used directly. Reagents such as dimethyl sulfoxide (DMSO), 1,6-dibromohexane, acetone, ethanol, etc., were also used directly otherwise specified. Other solvents like petroleum ether and dichloromethane were purchased as analytical grade and used directly.

Testing Instruments: ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE 500 spectrometer. The glass transition temperature (Tg) of samples was measured using a DSC 2910 differential scanning calorimeter at a heating rate of 10 ℃ min^{-1} under an N^{2} atmosphere. A UV-2450 UV-Visible spectrophotometer was used to measure absorption intensity and transmittance of samples; fluorescence emission spectra in solution state were measured using a HORIBA FLUOROMAX-4 fluorescence spectrophotometer. Cyclic voltammetry (CV) was conducted using a voltammetry analyzer with a glassy carbon working electrode, a platinum wire counter electrode, and a silver wire reference electrode. The excitation energies of singlet and triplet states were obtained using the TD-DFT method based on optimized ground-state molecular structures. For solution measurements, all samples were prepared at a concentration of 10^{-5} M in toluene. For thin film measurements, the films were spin-coated from 15 mg/mL solutions in 1,2-dichloroethane onto pre-cleaned quartz substrates at 2000 rpm, resulting in uniform films with thickness of 80. The excitation wavelength was 350 nm for all PL measurements, with slit widths of 5 nm for both excitation and emission monochromators. All quantum chemical calculations were performed using the Gaussian 09 software package. Geometry optimization was carried out using the B3LYP functional with the 6-31G(d,p) basis set. Low-lying excited singlet and triplet states were computed using the optimized structures with time-dependent density functional theory (TD-DFT) at the same level.

Preparation and Characterization of OLED Devices

The preparation process can be briefly described as follows: First, the glass substrates coated with ITO were rinsed with deionized water, followed by ultrasonic treatment in acetone, ethanol, and isopropanol sequentially. Before device fabrication, the substrates were treated in a UV-ozone oven for 20 minutes. The hole transport layer (PEDOT:PSS) was then spin-coated onto the ITO substrate at a speed of 3000 rpm and annealed at 150℃ for 10 minutes. Subsequently, the substrate was transferred to a nitrogen glove box, where a 1,2-dichloroethane solution containing the emissive layer was spin-coated onto the PEDOT:PSS layer and annealed at 80℃ for 10 minutes. TPBi was used as the electron transport layer, Cs_2CO_3 as the hole transport layer, and Al as the cathode. After vacuum deposition, the devices were tested and characterized under ambient conditions without protective encapsulation. The combination of a Photo Research PR655 SpectraScan and a Keithley 2400 Sourcemeter was used to record the electroluminescence (EL) spectra, device brightness, and current density-voltage characteristics.

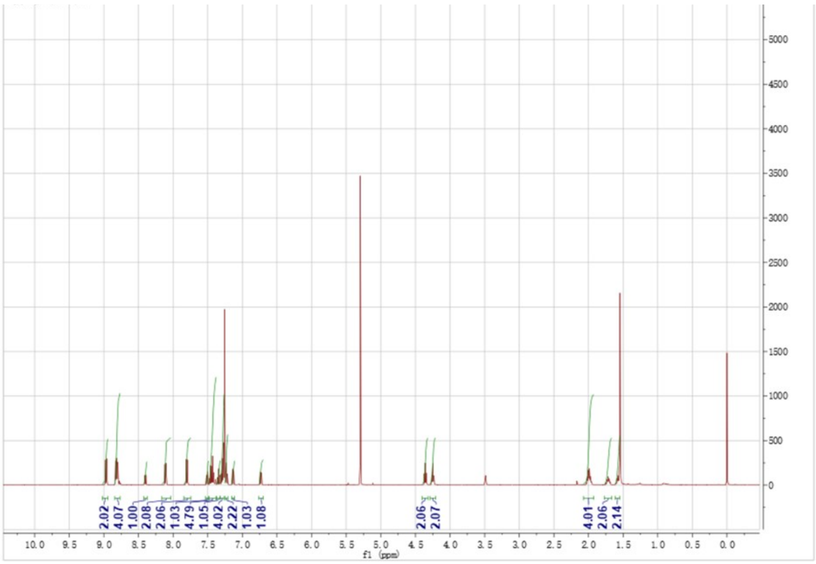

Fig. S1 ^{1}H NMR spectra of 4,4'-(((((9H-fluorene-9,9-diyl)bis(4,1-phenylene))bis(oxy))bis(hexane-6,1-diyl))bis(oxy))bis(9H-carbazole)(M_2)

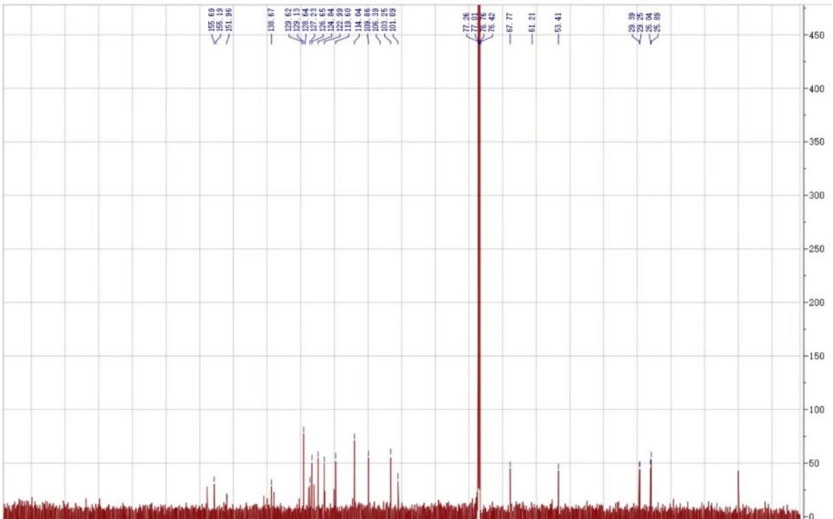

Fig. S2 ^{13}C NMR spectra of 4,4'-(((((9H-fluorene-9,9-diyl)bis(4,1-phenylene))bis(oxy))bis(hexane-6,1-diyl))bis(oxy))bis(9H-carbazole)(M_2)

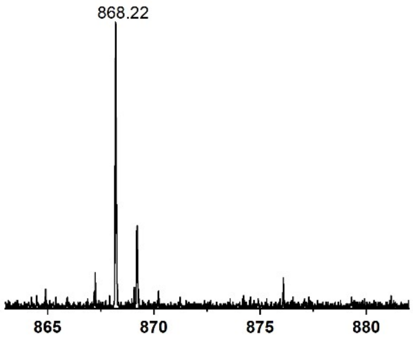

Fig. S3 MS spectra of 4,4'-(((((9H-fluorene-9,9-diyl)bis(4,1-phenylene))bis(oxy))bis(hexane-6,1-diyl))bis(oxy))bis(9H-carbazole)(M_2)

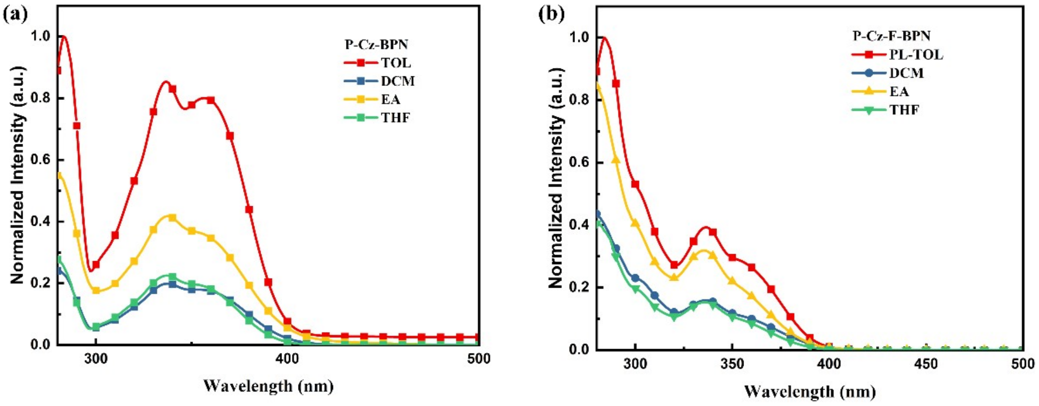

Fig S4 UV-Vis absorption spectra of P-Cz-BPN (a) and P-Cz-F-BPN (b) in different solvents

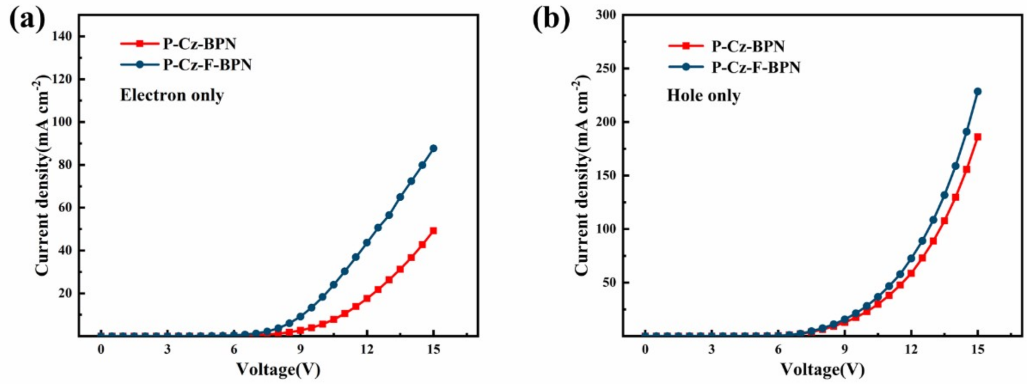

Fig S5 The hole-only and electron-only devices of P-Cz-BPN and P-Cz-F-BPN