

High efficiency and low driving voltage blue/white electrophosphorescence enabled by the synergistic combination of singlet and triplet energy of bicarbazole derivatives



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ABSTRACT

New host materials (BCz–DBT and BCz–DBF) are synthesized by regrouped 3,3-bicarbazole (BCz) and dibenzothiophene (DBT)/dibenzofuran (DBF). Their thermal, electrochemical, electronic absorption and photoluminescent properties are also carefully investigated. The materials exhibit high glass transition temperatures (T_g) of 134 °C and 139 °C, respectively. This kind of molecular design can effectively achieve high triplet energies and suitable highest occupied molecular orbital and lowest unoccupied molecular orbital (HOMO/LUMO) energy levels. High external quantum efficiencies (EQE) of sky blue (EQE = 25%) and three-color white (EQE = 21.4%) phosphorescent OLEDs have been achieved by using BCz–DBF as the host material.

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1. Introduction

Organic light-emitting diodes (OLEDs) have been actively touted as promising candidates for solid-state light and full-color display [1]. The need to improve performance for commercial applications has become more and more urgent in recent years. Furthermore, materials and device design for OLEDs is crucial to device performance [2]. More particularly, through diligent molecular design, 75% of triplet excitons can be harnessed in emission by direct or indirect transition from T_1 state to S_0 state [3–7]. To suppress the triplet–triplet annihilation (TTA) and triplet-polaron quenching (TPQ), emitters should be homogeneously dispersed within compatible host materials for state-of-the-art OLEDs [8–11]. Therefore, developing appropriate host materials is as important as preparing efficient emitters for OLEDs.

Recently, the design principle of appropriate host materials for highly efficient devices is increasingly clear [12]. In general, the bipolar molecules containing both p-type and n-type moieties can facilitate high performance even in the most challenging blue phosphorescent OLEDs (PhOLEDs). By choosing reasonable linkage, the resulted materials with both electron

donating/withdrawing groups can minimize intramolecular charge transfer (ICT) and thus gain high triplet energy (E_T) level as well as matched HOMO/LUMO levels for carrier injections [13–18]. For example, Lee's group reported a new bipolar host molecule CbBPCb ($E_T = 2.77$ eV), which can achieve very high EQE of 30.1% in sky-blue PhOLEDs [19]. Our group also synthesized a novel bipolar host material POSTF ($E_T = 2.80$ eV) with spiro-structure, which obtained 26.8% in sky-blue emission and 27.2% in white emission [20]. Because of the success of bipolar hosts in blue phosphorescence, the research on traditional unipolar hosts gradually fades out due to their inferior performance in device. By understanding and absorbing the essence in designing bipolar materials, however, it can be anticipated that unipolar hosts could rejuvenate if suitable building blocks be carefully selected [21–25].

In this communication, we designed and prepared two new unipolar host materials BCz–DBT and BCz–DBF, which are regrouped by 3,3-bicarbazole (BCz) and dibenzothiophene (DBT)/dibenzofuran (DBF) to confirm this conjecture. It is critical to know that the DBT and DBF are both p-type moieties but possess relative low-lying LUMO levels [26–28]. Combined with BCz, a typical hole-transport moiety with suitable HOMO level, [29] the separation in frontier molecular orbitals could be expected. What's more, T_1 state will be localized at the BCz because of the ortho-meta linkage, thus high T_1 energy could obtain simultaneously.

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Though all of the three units are electron-rich groups, these features resemble that of bipolar system. The consequently blue PhOLEDs exhibited EQE of 23.5% and 25.0% for BCz–DBT and BCz–DBF (B1 and B2), respectively. Additionally, we further utilized BCz–DBF in three-color RGB white PhOLEDs. The resulting WOLEDs showed three evenly separated peaks and a high EQE of 21.4%.

2. Results and discussions

BCz–DBT and BCz–DBF were prepared by classic Suzuki coupling reaction according to Scheme 1. The detailed synthetic procedure and characterizations are described in the Experimental Section and Supporting Information. Both compounds were characterized by ^1H NMR and ^{13}C NMR spectroscopies, mass spectrometry.

In differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) measurements (Figs. 1 and 2), both BCz–DBT and BCz–DBF exhibited good thermal stabilities. Decomposition temperatures (T_d), which correspond to 5% weight loss upon heating during TGA, were measured to be 424 and 415 °C for BCz–DBT and BCz–DBF, respectively. In addition, BCz–DBT and BCz–DBF also have high T_g of 139 and 134 °C, respectively, which are summarized in Table 1. These tiny differences T_d or T_g might stem from the different atomic sizes of sulfur and oxygen. The UV/vis absorption, photoluminescence (PL) and low low-temperature PL spectra (Fig. 3) of BCz–DBT and BCz–DBF were measured to investigate their photophysical properties. The optical energy gaps (E_g) estimated from the onset absorption wavelength of BCz–DBT and BCz–DBF were 3.38 and 3.31 eV, respectively. BCz–DBT and BCz–DBF also show the similar PL emission peaks at 3.06 and 3.16 eV, respectively. The E_T s of BCz–DBT and BCz–DBF obtained from the highest energy vibronic and of the low-temperature PL spectrum at 77 K were calculated as 2.69 and 2.68 eV, respectively. The PL emission peaks of BCz–DBT and BCz–DBF are almost identical to that of the parent BCzPh molecule. More importantly, the emission peaks of the two new hosts exhibit only ~ 0.04 eV bathochromic shift as compared to that of BCzPh. This proved that introducing DBT or DBF units into BCz fragments did not decrease the E_T of

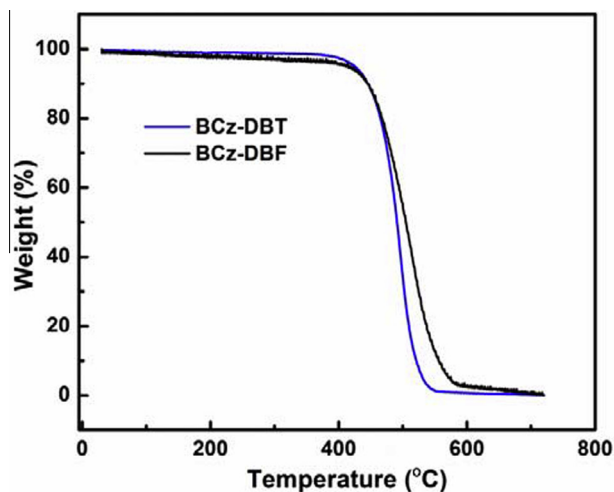
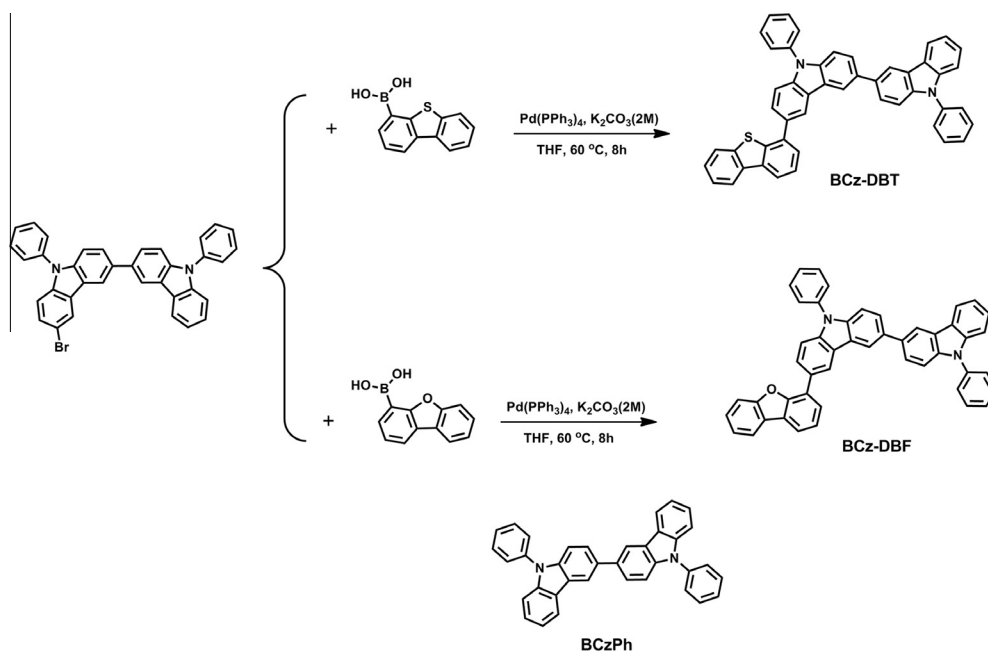


Fig. 1. DSC traces of BCz–DBT and BCz–DBF recorded at a heating rate of 10 °C/min.

BCzPh. The HOMO levels of thin films of BCz–DBT and BCz–DBF were measured by ultraviolet photoemission spectroscopy (UPS) as -5.74 and -5.84 eV, respectively (Figs. S1 and S2). The LUMO levels of -2.36 and -2.53 eV for BCz–DBT and BCz–DBF were subsequently estimated according to the equation of $E_{\text{LUMO}} = E_{\text{HOMO}} + E_g$, where E_g is the optical band gap. In comparison with BCzPh (HOMO = -5.64 eV; LUMO = -2.36 eV), the HOMO and LUMO levels of the two hosts are efficiently modulated. Density Functional Theory (DFT) calculations (B3LYP/6–311G(d)) were carried out to elaborate the structure–property relationship of BCz–DBT, BCz–DBF and BCzPh. As shown in Fig. 4, the HOMOs of BCz–DBT and BCz–DBF are spread over the BCz backbone with little contribution from DBT and DBF moieties, whereas the LUMOs are mainly localized at the DBT or DBF moieties. This spatial separation of HOMOs and LUMOs should be beneficial for hole and electron injection and lead to low driving voltages. The HOMO and LUMO levels were tuned by 0.11 and 0.16 eV, respectively. Additionally, we carried out a Mülliken population analysis to depict the spin density distribution of unpaired electrons in the triplet state.



Scheme 1. Synthetic route and chemical structures of the host materials.

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