



Fine-tuning the balance between carbazole and oxadiazole units in bipolar hosts to realize highly efficient green PhOLEDs

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ABSTRACT

A series of new bipolar hosts **C101**, **C201**, and **C102** comprising hole-transporting carbazole as donor (D) and electron-transporting oxadiazole as acceptor (A) have been designed and synthesized to tune D/A ratio with a view for getting in-depth information about structure–property–performance relationship. The D/A ratio exerts subtle influences on absorption spectra and energy levels. Time-of-flight (TOF) measurements reveal that the increment of donor units effectively increase the hole mobility. The appropriate energy levels and triplet energies along with promising morphological and thermal stability of these molecules bring out them as suitable hosts to realize green PhOLEDs with (PBi)₂Ir(acac) and (PPy)₂Ir(acac) emitters. Green phosphorescent devices hosted by **C101**, **C201**, and **C102** achieved maximum external quantum efficiencies of 20.7%, 20.4%, and 17.3%, respectively. These results indicate that carbazole/oxadiazole hybrid molecule with one carbazole and oxadiazole each is a better candidate for highly efficient green PhOLEDs.

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1. Introduction

Phosphorescent OLEDs (PhOLEDs), known for effectively utilizing both singlet and triplet excitons to achieve a 100% internal quantum efficiency (IQE), have received great research attentions both from academia and industrial [1,2]. To realize highly efficient electrophosphorescence, transition metal-based emitters are usually dispersed into a suitable host material for suppressing triplet–triplet annihilation and self-quenching of phosphors [3]. As host materials essentially manage both charge transport and recombination functions and also play a vital role to confine emissive excitons within the emitting layer, the molecular design of host material becomes a crucial issue. Efficient host materials should possess properties such as good morphological and thermal stability for retaining

the amorphous thin film quality, balanced charge transport characters to afford sufficient charge flux, high triplet energy (E_T) for preventing exciton quenching, and suitable energy levels relative to the neighboring layers for giving low operation voltage [4]. The design of bipolar host materials configured with electron-donating structures as donors (D) and electron-deficient groups as acceptors (A) seems to be the most appealing strategy in recent years [5]. Among the hole-transporting components reported in the literature, carbazole has found and will continue to find extensive use in a myriad of material context for PhOLEDs due to their good hole-transporting ability and sufficiently high E_T [6]. On the other hand, 1,3,4-oxadiazole [7] and other electron-withdrawing groups such as phosphine oxide [8], triazine [9], and benzimidazole [10], have been utilized as efficient electron-transporting acceptors. Their low-lying LUMOs are well matched to the neighboring electron-transport layer (ETL), diminishing electron-injection barrier and effectively transporting electrons to emitting layer. Due to the intrinsic dual-transport property, hole and electron mobilities and even energy levels could

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be individually tuned via given different donor and acceptor in one bipolar host material [11]. In addition, the physical properties of bipolar host materials and eventually the performance of device adopting them are closely governed by the number of hole- (HT) and electron- (ET) transporting moieties and their linking topology. For example, Lee et al. reported a series of bipolar materials comprised of different numbers of carbazole and diphenylphosphine oxide [12] where the HOMO and the LUMO can be suitably tailored to align with their neighboring active layers. In addition, the charge mobilities of bipolar molecules evidently vary along with the D/A ratio. Consequently, under the same device structure, the host material with lower D/A ratio gave higher current density, which can be directly attributed to the better electron transport property and lower ETL/EML energy barrier [13]. Because the charge balance is highly related to the inherent carrier mobility of functional materials and the interfacial charge injection barriers, this result revealed a facile way to modulate and balance the charge fluxes, giving an excellent example of structure–property–performance relationship of bipolar host materials. Considering the promising physical properties and good performance of carbazole- and oxadiazole-containing OLED materials, we reported in this paper the synthesis, properties and device characteristics of a series of bipolar host materials **C101**, **C201**, and **C102** comprising of different combinations of D (carbazole) and A (oxadiazole). The energy levels as well as carrier mobility of the bipolar host materials can be manipulated through altering the D/A ratio, while maintaining sufficiently high E_T to confine emissive excitons within the emitting layer. The devices gave the maximum external quantum efficiency (η_{ext}) of 20.7%, 20.4%, and 17.2% as **C101**, **C201**, and **C102** were adopted as hosts for green phosphor (PPy)₂Ir(acac), respectively. These results revealed that bipolar host **C101** containing equal number of HT and ET components gave the most efficient device due to better interfacial energy alignment and smaller charge injection barrier.

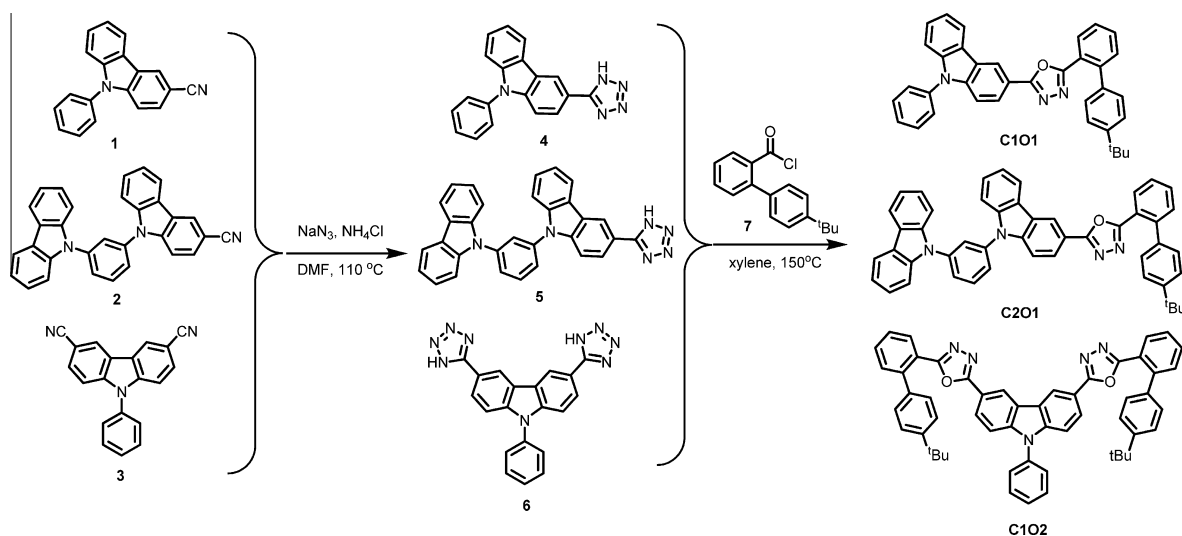
2. Results and discussions

2.1. Synthesis

Scheme 1 depicts the synthesis of the title compounds **C101**, **C201**, and **C102**. Starting from the CN-substituted carbazole derivatives **1** [14], **2** [15], and **3** [16], which were converted to their corresponding tetrazole intermediates **4**, **5**, and **6** in excellent yields by treating with NaN₃ and NH₄Cl. The tetrazoles were reacted with biphenyl acid chloride **7**, which was prepared from its corresponding acid [17], to give the desired bipolar host materials **C101**, **C201**, and **C102** with excellent isolated yields. Their structural identities and purities were confirmed by satisfactory spectroscopic data and elemental analysis (see **Supporting information**). The resulting bipolar molecules were configured with the electron-accepting oxadiazole group attaching to the C3 position of electron-donating carbazole group. In addition, the peripheral oxadiazole was capped by a phenyl group together with a bulky 4-*tert*-butylphenylene at the *ortho* position to bring in steric hindrance and highly twisted conformation for improving morphological stability.

2.2. Crystal structures

The molecular structures of **C101** and **C102** were unambiguously verified from single-crystal X-ray diffraction analysis (**Fig. 1**). The highly twisted manner between the 4-*tert*-butylphenyl group and end-capping phenyl group can be obviously observed with dihedral angles of 61.11° for **C101** (C21–C26–C27–C32) and 73.47° for **C102** (C13–C18–C19–C24). Therefore, the introduction of twisted phenyl rings as peripheral blocking groups can enhance the morphological stability by efficiently preventing the molecules from stacking. In addition, the carbazole and oxadiazole moieties in these two materials are nearly coplanar as evidenced by the small dihedral angles of 2.31° for **C101** (C7–C2–C1–N1) and 4.90° for



Scheme 1. Synthetic routes of **C101**, **C201**, and **C102**.

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