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Bipolar type indolocarbazole host for green phosphorescent organic light-emitting diodes

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ABSTRACT

A bipolar host designed using indolocarbazole as a bipolar moiety was developed by coupling two indolocarbazole moieties via a phenyl linker. The indolocarbazole derived hosts could carry holes and electrons in the emitting layer, functioning as bipolar hosts in the green phosphorescent organic light-emitting diodes. The linker based molecular design was superior to the directly coupled molecular design to match carrier balance for high quantum efficiency in the green phosphorescent devices.

Introduction

Since the first demonstration of phosphorescent emission from Ir based triplet emitters, phosphorescent organic light-emitting diodes (PHOLEDs) have been in the main stream of device technology due to their benefit of high external quantum efficiency (EQE). [1–3] Theoretical calculation predicted internal quantum efficiency (IQE) of 100% in the PHOLEDs in comparison with 25% in the traditional fluorescent organic light-emitting diodes (OLEDs). [4]

The EQE of the PHOLEDs is typically dominated by carrier balance and radiative transition efficiency which are dominated by hosts and phosphorescent emitters, respectively. [5,6] As the EQE can be optimized by carrier balancing hosts along with highly efficient triplet emitters, the host adjusting the number of holes and electrons is one of key components of the emitting layer. [7] The carrier adjusting role of the host can be accomplished by adopting either bipolar charge transport unit or combination of hole and electron transport unit in the host backbone. [8–13] The second approach has been widely used, but the first approach has not been extensively explored because of limited number of bipolar unit in spite of excellence as the host. Therefore, investigation of the bipolar unit derived hosts should be carried out.

Herein, we report a host material based on indolo[3,2,1-*jk*] carbazole (IC) bipolar unit as the host of green phosphorescent emitter encouraged by both hole and electron transporting capability of the IC unit. 1,3-Bis(indolo[3,2,1-*jk*]carbazol-2-yl) benzene (ICphIC) was synthesized as the IC bearing bipolar host for application in green PHOLEDs. It was described that the phenyl linker included ICphIC host is favored to increase the EQE of the PHOLEDs by reaching high EQE of 14.5% compared to 12.8% of the IC derived host without the phenyl linker due to balanced carrier density.

Results and discussion

The IC unit was chosen as the main skeleton of the host encouraged by the highest occupied molecular orbital (HOMO)/lowest unoccupied molecular orbital (LUMO) levels of −5.56/−1.25 eV by Gaussian molecular simulation (B3LYP 6-31G). The HOMO of IC was shallower than that of a common carbazole and the LUMO was deeper than that of carbazole. The shallow HOMO level suggests good electron donating character for hole generation and the deep LUMO level indicates good electron accepting character for electron generation. [14] Therefore, the IC unit can be a good bipolar charge transport unit.

The ICphIC host was prepared by coupling two IC units through meta- position of a phenyl unit. Br substituted IC unit was converted into boronic ester functionalized IC unit using a Pd $(OAc)_2$ catalyst assisted by X-phos in 1,4-dioxane solvent, and then coupling of the 1,3-diiodobenzene and boronic ester substituted IC yielded ICphIC. The ICIC was prepared according to the procedure reported in the literature. [15] Detailed chemical analysis data and synthesis are summarized in Scheme 1 and experimental section.

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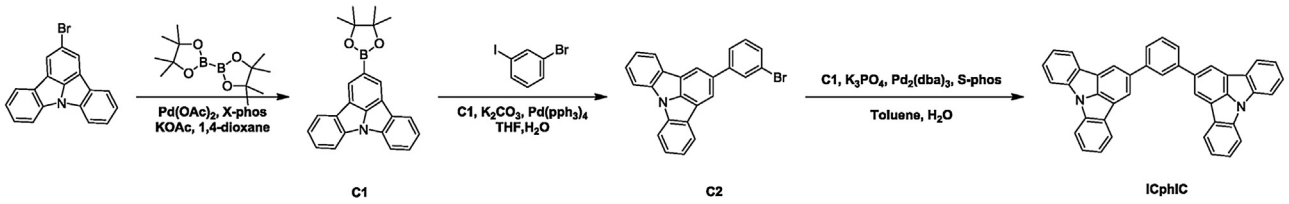

Scheme 1. Synthetic scheme of ICphIC.

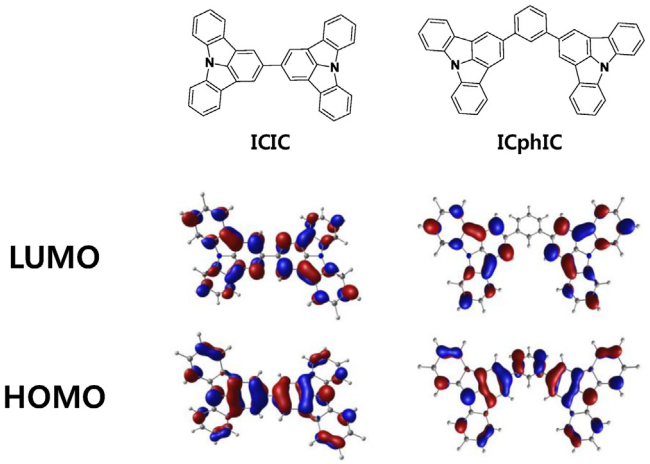

Fig. 1. HOMO and LUMO distribution of ICphIC and ICIC.

The bipolarity of the ICphIC host was investigated by orbital analysis and single carrier transport properties. Molecular orbital analysis was performed by comparing the HOMO and LUMO calculation results in Fig. 1. Geometry optimization and frontier orbital calculation by B3LYP 6-31G basis set of Gaussian 09 program showed full picture of the HOMO and LUMO distribution. Uniform distribution of the HOMO in the whole backbone structure and dominant LUMO distribution mostly in the IC unit was observed in the ICphIC host. Both HOMO and LUMO were dispersed in the IC unit, suggesting that the IC unit can be a hole transport unit as well as an electron transport unit.

Single carrier device data were also used to confirm the calculated bipolarity of the ICphIC host. Hole and electron only device data of the ICphIC host are plotted in Fig. 2. Device data of the ICIC host were also plotted for comparison. The hole current density of the ICphIC hole only device was quite analogous to that of the ICIC device, but the electron current density of the ICphIC device was higher than that of the ICIC device, proposing strengthened electron transport character of ICphIC. Bipolar character was reinforced in the ICphIC host relative to the ICIC host.

The physical parameters of the ICphIC host were collected by ultraviolet–visible (UV–vis) and photoluminescence (PL) measurements. Fig. 3 is a picture showing the UV–vis absorption, fluorescent emission and phosphorescent emission of the ICphIC host. In the UV–vis absorption data, strong absorption below 300 nm and weak absorption between 300 and 385 nm by the IC interlinked backbone structure were observed. In the PL analysis data, fluorescent emission at a peak wavelength of 389 nm and a phosphorescent emission with the first peak wavelength of 438 nm were observed using toluene solution at room temperature and at

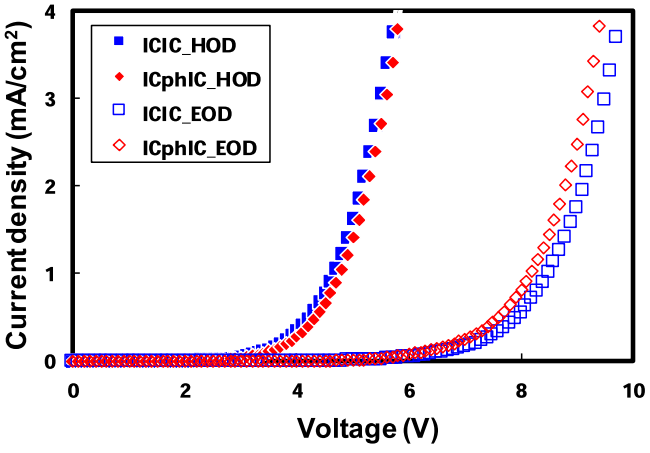

Fig. 2. Current density–voltage data of hole and electron only devices of ICphIC and ICIC.

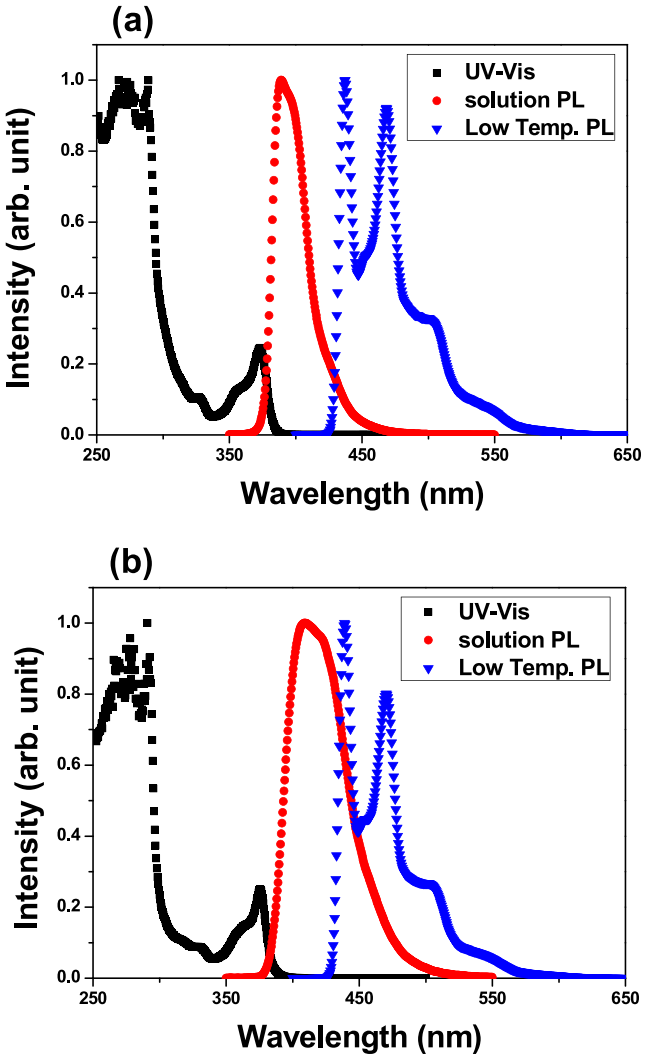

Fig. 3. UV–vis, solution PL and low temperature PL spectra of ICphIC (a) and ICIC (b).

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