



Pyridazine derived bipolar host materials for phosphorescent organic light-emitting diodes



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ABSTRACT

Two organic materials incited by electron deficiency of a pyridazine moiety were designed for application as bipolar host materials of phosphorescent organic light-emitting diodes. Modification of the pyridazine moiety with carbazole and pyrrolocarbazole hole transport units provided 3,6-bis(2-(9H-carbazol-9-yl)phenyl)pyridazine (CzPd) and 3,6-bis(2-(3-phenylpyrrolo[3,2-a]carbazol-10(3H)-yl)phenyl)pyridazine (PCzPd) as bipolar host materials. The 3,6-bis(2-(9H-carbazol-9-yl)phenyl)pyridazine and 3,6-bis(2-(3-phenylpyrrolo[3,2-a]carbazol-10(3H)-yl)phenyl)pyridazine were high triplet energy hosts by ortho-substitution of the hole transport units. Based on the triplet energy of the host materials, green phosphorescent organic light-emitting diodes were devised and the green devices presented high quantum efficiency of 15.5%

1. Introduction

The design and development of bipolar host materials have been the dominant material technology to improve the external quantum efficiency (EQE) of phosphorescent organic light-emitting diodes (PhOLEDs) because they are ideal as host materials balancing hole and electron carriers for exciton formation [1–4]. There have been many bipolar host materials which have been effective to optimize the hole and electron recombination in the PhOLEDs.

The most common hole transport unit of the bipolar host materials was carbazole [5–9], while popular electron transport units were diphenylphosphine oxide, diphenyltriazine, pyridine, and five membered hetero aromatic moieties [10–12]. The diphenylphosphine oxide unit was favored for high triplet energy by the tetrahedral geometry of the diphenylphosphine oxide [13,14], and the diphenyltriazine unit was good for the design of stable host materials [15,16]. Pyridine and five-membered hetero aromatic moieties were also diversely used in many bipolar host materials design [17–21]. However, there have not been many electron transport units for application in bipolar host materials and new electron transport units are to be developed to expand the design platform of the host materials.

In this work, a pyridazine moiety was selected as the electron transport unit to build the bipolar host materials along with carbazole and pyrrolocarbazole hole transport units. Two hosts, 3,6-bis(2-(9H-carbazol-9-yl)phenyl)pyridazine (CzPd) and 3,6-bis(2-(3-phenylpyrrolo[3,2-a]carbazol-10(3H)-yl)phenyl)pyridazine (PCzPd), were derived

from the pyridazine moiety and were employed as the hosts in the green PhOLEDs. The CzPd and PCzPd hosts substantiated the applicability of the pyridazine moiety as the electron transport unit by demonstrating bipolar carrier transport properties and high EQE in the green PhOLEDs.

2. Results and discussion




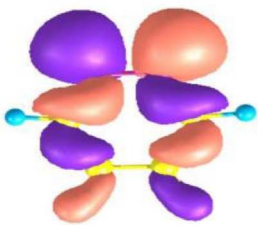
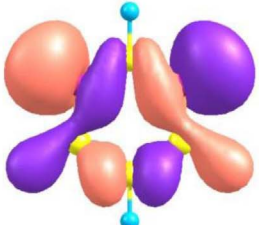
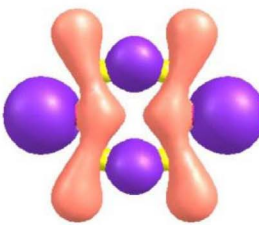
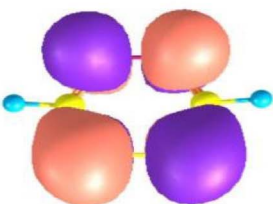
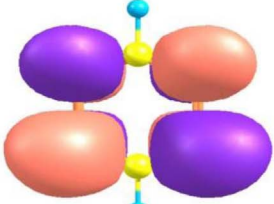
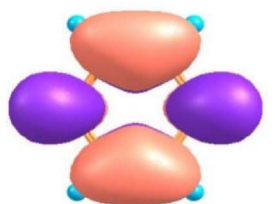
Pyridazine moiety has two sp² [2] N units in the six-membered aromatic structure and shows electron deficiency by the higher electronegativity of N than C. It is similar to pyrimidine and pyrazine with two sp² [2] N units in the heteroaromatic ring although the position of N is dissimilar. Therefore, the pyridazine moiety is expected to carry and inject electrons as well as the pyrimidine and pyrazine moieties which have been already demonstrated to be good electron transport units.

As the pyridazine moiety has similar molecular structure to pyrimidine and pyrazine, molecular simulation results of the three heteroaromatic units with two N atoms were compared in Table 1. Comparing the three heteroaromatic moieties, pyridazine is similar to pyrazine and better than pyrimidine in terms of electron accepting properties judging from the LUMO. The pyrimidine and pyrazine were already proven as the electron transport unit of host materials [20,21], so it is conjectured that pyridazine would behave as an electron transport unit of hosts. Therefore, two hosts with the pyridazine electron transport unit was designed by expanding the pyridazine core with hole transport phenylcarbazole and phenylpyrrolocarbazole units. The

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Table 1
Electronic orbital simulation results of pyridazine, pyrimidine, and pyrazine.

	Pyridazine	Pyrimidine	Pyrazine
Structure			
Singlet energy	3.62	4.35	4.03
Triplet energy	2.75	3.78	3.26
	-6.37	-6.93	-6.83
HOMO			
	-1.40	-1.16	-1.42
LUMO			

carbazole and pyrrolocarbazole were introduced at ortho- position of the phenyl unit to obtain high triplet energy. Synthesis of the pyridazine compounds was carried out by two-step chemical reactions of Suzuki coupling and NaH assisted amination of dichloropyridazine as shown in Scheme 1. Detailed synthesis is explained in experimental section.

Frontier orbital of CzPd and PCzPd hosts was investigated to predict photophysical behavior and energy levels of the hosts. Fig. 1 shows the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) of CzPd and PCzPd. As intended in the molecular design, the HOMO and LUMO were positioned in the hole transport carbazole or pyrrolocarbazole unit, and electron transport pyridazine unit, respectively. The HOMO and LUMO were apparently separated by the donor-acceptor type backbone structure. Triplet energy was also estimated from the molecular simulation and the calculated triplet energy of CzPd and PCzPd was 2.71 eV.

The frontier orbital analysis results predict that the HOMO and LUMO would be governed by the carbazole or pyrrolocarbazole, and central diphenylpyridazine units, which was confirmed by the HOMO and LUMO measurement using cyclic voltammetry (CV). The CV analysis data in Fig. 2 provide the HOMO/LUMO values of $-6.14/-3.17$ and $-5.87/-3.07$ eV in CzPd and PCzPd, respectively. Both the HOMO and LUMO of PCzPd were deeper than those of CzPd because of strong electron donor character of the pyrrolocarbazole moiety. The pyrrolocarbazole moiety has an additional pyrrole unit attached to the

carbazole and shows strong electron donating properties, which made the HOMO of PCzPd shallow. The strong donor character of the pyrrolocarbazole also altered the LUMO because the central diphenylpyridazine unit is directly linked to the pyrrolocarbazole moiety.

Ultraviolet-visible (UV-vis) absorption and PL emission of the CzPd and PCzPd hosts were analyzed using UV-vis spectrometer and fluorescence spectrometer. UV-vis absorption and solid PL emission spectra of CzPd and PCzPd are presented in Fig. 3. UV-vis absorption of CzPd and PCzPd was extended to 350 nm by absorption of the main diphenylpyridazine core and donor moieties. Both room temperature PL (fluorescence) and low temperature PL (phosphorescence) emission of CzPd and PCzPd were measured. Fluorescence emission of CzPd and PCzPd was observed at 432 nm and 434 nm, respectively, but phosphorescence was not clearly observed due to too weak phosphorescent emission. It is projected from the molecular simulation results that the triplet energy of CzPd and PCzPd would be high enough for energy transfer to a green triplet emitter by the ortho-connection between donors and a phenyl linker.

The energy transfer in the CzPd: tris[2-phenylpyridinato-C²,N]iridium(III) (Ir(ppy)₃) and PCzPd:Ir(ppy)₃ films was analyzed by transient PL measurements (Fig. 4). The typical decay curve of Ir(ppy)₃ was observed in the CzPd and PCzPd films, demonstrating efficient energy transfer from the hosts to Ir(ppy)₃.

Thermal properties reflected in glass transition temperature (T_g)

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