



Spatially separated donor-acceptor design of host materials for independent control of photophysical properties and carrier transport properties



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ABSTRACT

Triplet host materials with spatially separated donor and acceptor moieties were synthesized and the effect of the spatial separation of the donor and acceptor moieties via aromatic linkage on the photophysical properties of the host materials was elucidated. It was revealed that the aromatic linkage had weak influence on the absorption and triplet energy of the donor-acceptor type host materials with completely separated donor and acceptor moieties. Charge transport properties and device performances were found to be changed by the type of the aromatic linkage. Therefore, the spatially separated donor-acceptor design was proven to independently control photophysical properties and charge transport properties.

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1. Introduction

Organic materials with donor and acceptor moieties in the backbone structure have been popular as the host materials of phosphorescent organic light-emitting diodes (PHOLEDs) because of bipolar carrier transport properties which have beneficial effect on driving voltage and external quantum efficiency (QE) of the PHOLEDs [1–7].

Low driving voltage can be realized by good hole injection from a hole transport layer to the donor moiety of the host and by good electron injection from an electron transport layer to the acceptor moiety of the host. The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) gap of the host material is narrowed by the donor-acceptor structure and the energy barrier for hole and electron injection is reduced, resulting in low driving voltage.

External QE enhancement is another merit of using donor-acceptor type host materials. As hole and electron injection is boosted simultaneously by the donor-acceptor structure, holes and electrons can recombine with minimal loss of carriers and the external QE can be increased. Generally, bipolar host materials with the donor-acceptor moieties demonstrated high external QE

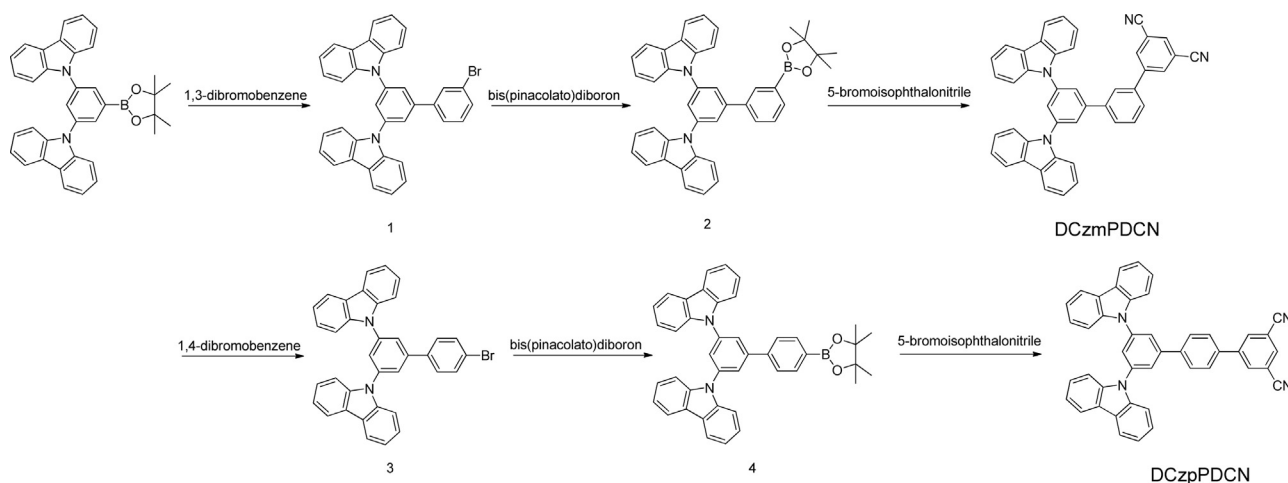
compared to unipolar host materials with only donor moieties or acceptor moieties [8–18].

In the typical design of the donor-acceptor type host materials, donor and acceptor moieties were linked directly or via a linkage made up of an aromatic unit or non-aromatic unit. The aromatic linkage has merits of good thermal stability, narrow HOMO-LUMO gap and good carrier transport properties, but decrease of the triplet energy is accompanied by the extensively conjugated molecular structure [8–11]. The non-aromatic linkage does not degrade the triplet energy, but loss of π -orbital character destabilizes the molecule and carrier transport is degraded [19–23]. Therefore, an ideal design of the host materials would be to link donor and acceptor moieties through an aromatic linkage without sacrificing the triplet energy of the host materials.

In this work, a novel molecular design with a spatially separated donor and acceptor moieties via an aromatic linkage was developed to independently manage the photophysical properties and carrier transport properties. It was established that a molecular design with completely localized HOMO and LUMO on the donor and acceptor moieties had weak influence on the absorption spectra and triplet energy of the host materials irrespective of the geometrical structure of the linkage. The linkage mostly affected the carrier transport properties without any effect on the QE.

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Scheme 1. Synthetic scheme of DCzmpPCDN and DCzpPCDN.

2. Experimental

2.1. General information

1,3,5-Tribromobenzene, 1,3-dibromobenzene and 1,4-dibromobenzene were purchased from Alfa Aesar. Co. and tetrakis(triphenylphosphine) palladium (0), 1,1'-bis(diphenylphosphino) ferrocene, bis(pinacolato) diboron and 5-bromoisophthalonitrile were purchased from P&H Co. Copper(I) cyanide, 1,10-phenanthroline, 9H-carbazole and potassium acetate were products of Aldrich Co. All solvents were purchased from Duksan Sci. Co. and these chemicals were used without additional purification. Tetrahydrofuran (THF) was distilled over calcium hydride and sodium. General

characterization of the synthesized materials was performed according to the method described in our previous work [15].

2.2. Synthesis

9,9'-(3'-Bromo-[1,1'-biphenyl]-3,5-diyl) bis(9H-carbazole) (**1**) 9,9'-(5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3-phenylene) bis(9H-carbazole) (4.30 g, 8.05 mmol), 1,3-dibromobenzene (9.50 g, 40.2 mmol), and tetrakis(triphenylphosphine) palladium (0) (0.28 g, 0.24 mmol) were dissolved in anhydrous THF (90 mL) with stirring under a nitrogen atmosphere, and then 2 M K_2CO_3 solution (30 mL) was added to reaction mixture. The mixture was heated to reflux for 6 h and cooled to room

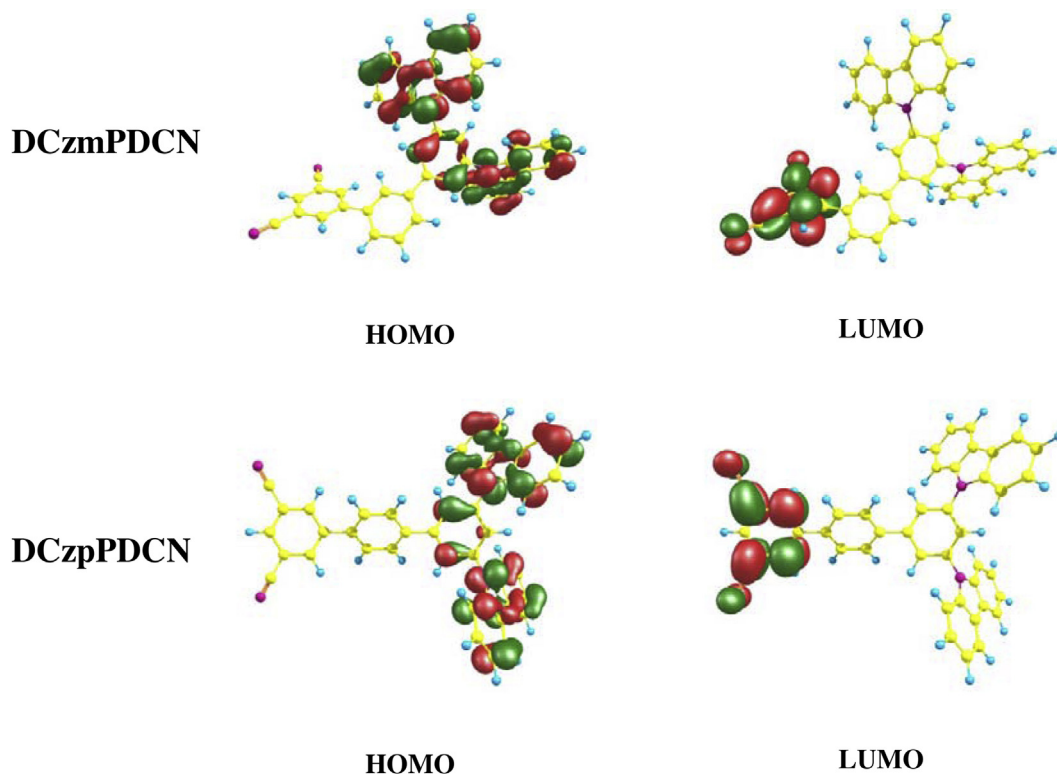


Fig. 1. Calculated HOMO and LUMO distribution of DCzmpPCDN and DCzpPCDN.

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