



Manipulating the LUMO distribution of quinoxaline-containing architectures to design electron transport materials: Efficient blue phosphorescent organic light-emitting diodes

Xiaojun Yin^a, Hengda Sun^b, Weixuan Zeng^a, Yepeng Xiang^a, Tao Zhou^a, Dongge Ma^{b, **}, Chuluo Yang^{a, *}

^a Hubei Collaborative Innovation Center for Advanced Organic Chemical Materials, Hubei Key Lab on Organic and Polymeric Optoelectronic Materials, Department of Chemistry, Wuhan University, Wuhan 430072, People's Republic of China

^b State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, People's Republic of China

ARTICLE INFO

Article history:

Received 2 May 2016

Received in revised form

16 July 2016

Accepted 16 July 2016

Available online 26 July 2016

Keywords:

Electron transport materials
Organic light emitting diodes
Phosphorescence
Quinoxaline

ABSTRACT

A series of new quinoxaline-containing compounds, namely, 2,3,6,7-tetrakis(3-(pyridin-3-yl)phenyl)quinoxaline (**Tm3PyQ**), 2,3,6,7-tetrakis(3-(pyridin-4-yl)phenyl)quinoxaline (**Tm4PyQ**), 1,4-bis(2,3-dimethyl-7-(pyridin-3-yl)quinoxalin-6-yl)benzene (**3PyDQB**), and 1,4-bis(2,3-dimethyl-7-(pyridin-4-yl)quinoxalin-6-yl)benzene (**4PyDQB**) were designed and synthesized as electronic transporting materials. The lowest unoccupied molecular orbital (LUMO) distributions of these compounds vary with the locations of quinoxaline moieties, which result in adjustable intermolecular charge-transfer integrals. All the compounds exhibit favorable electron affinity (2.73–2.88 eV) and good thermostability (glass transition temperatures in the range of 112–148 °C). Using these compounds as electron transport layers, the bis(4,6-(difluorophenyl)pyridinato-*N,C*^{2'})picolinate iridium(III) (Firpic)-based blue phosphorescent organic light emitting diodes (PhOLEDs) achieve good performances with a maximum current efficiency ($\eta_{c,max}$) of 30.2 cd A⁻¹ and a maximum external quantum efficiency ($\eta_{ext,max}$) of 14.2%. Moreover, these efficiencies reveal small roll-offs at high luminance.

© 2016 Elsevier B.V. All rights reserved.

1. Introduction

Charge transport is of significant importance in organic light-emitting diodes (OLEDs) [1–6], since the generation of light in OLED is the consequence of the recombination of holes and electrons injected from the electrodes to the emitting layer [7–12]. A balanced charge carrier injection and transport in OLED is considered to be essential for achieving high performance [13–16]. However, the hole mobility is generally 2–3 orders of magnitude higher than that of electron in the OLED due to the electron trapping [17–20]. Developing new electron-transporting materials (ETMs) with enhanced electron mobility (μ_e) to alleviate such contradiction is of significance [21–25]. Several strategies have been adapted to promote the μ_e of the ETMs, such as extending the

π -conjugation of the molecule [26–30] or utilizing the intra-/intermolecular hydrogen bonds [31–34]. Beyond that, manipulating the lowest unoccupied molecular orbital (LUMO) distributions of the molecule to afford effective LUMO overlaps between neighboring molecules is also a feasible way [35–37], because the effective LUMO overlaps could enlarge the intermolecular charge-transfer integrals, and then facilitate the electron transfer from one molecule to another [38,39].

Nitrogen-embedded monocyclic compounds such as pyridine and pyrimidine are generally recognized as desired electron-transporting units in constructing new ETMs with both high triplet energy level (E_T) and high μ_e [40–44]. For example, the well-known ETM of 1,3,5-tri(*m*-pyrid-3-yl-phenyl)benzene (TmPyPB) has a E_T of 2.75 eV and a μ_e of 1.0×10^{-3} cm² V⁻¹ s⁻¹ simultaneously [45]. Nevertheless, their thermal stabilities are often undesirable, which may lead to a poor morphological stability in the OLED and hence resulting in inferior device performance at high brightness [46–49]. In order to enhance the glass transfer temperature (T_g) of the compounds, extended π -conjugation of the aza-aromatics such

* Corresponding author.

** Corresponding author.

E-mail addresses: md1014@ciac.jl.cn (D. Ma), clyang@whu.edu.cn (C. Yang).

as quinoline, quinoxaline, naphthyridine, etc., have been incorporated into the π -conjugated skeleton [50–54].

In this article, four new quinoxaline-based ETMs, namely, **Tm3PyQ**, **Tm4PyQ**, **3PyDQB** and **4PyDQB** were designed and synthesized (Scheme 1). The *ortho*-linkage is intended to decrease the π -extension, and thus maintain a high E_T of the molecule (Fig. 1). Density functional theory (DFT) simulation reveals that their LUMO distributions can be manipulated by adjusting the location of quinoxaline units. All these ETMs exhibit favorable electron affinities (2.73–2.88 eV) and desirable T_g s (>112 °C). The *bis*(4,6-(difluorophenyl)pyridinato-*N,C*^{2'})picolinate iridium(III) (Firpic)-based blue phosphorescent OLEDs employ them as electron transport layers (ETLs) achieved good performance, with a maximum current efficiency ($\eta_{c,max}$) of 30.2 cd A⁻¹ and a maximum external quantum efficiency ($\eta_{ext,max}$) of 14.2%.

2. Experimental

2.1. Instrumentation

¹H NMR and ¹³C NMR spectra of the compounds were recorded on a Varian MERCURY-VX300 spectrometer. The molecular weights were evaluated by VJ-ZAB-3F or Waters ZQ2000 LC/MS Mass spectrometer. Elemental analyses of C, H and N were performed on a Perkin-Elmer 204B microanalyzer. UV–Vis absorption spectra and photoluminescence (PL) spectra were obtained on Shimadzu UV-2500 spectrophotometer and Hitachi F-4600 fluorescence spectrophotometer, respectively. Thermodynamic investigation of

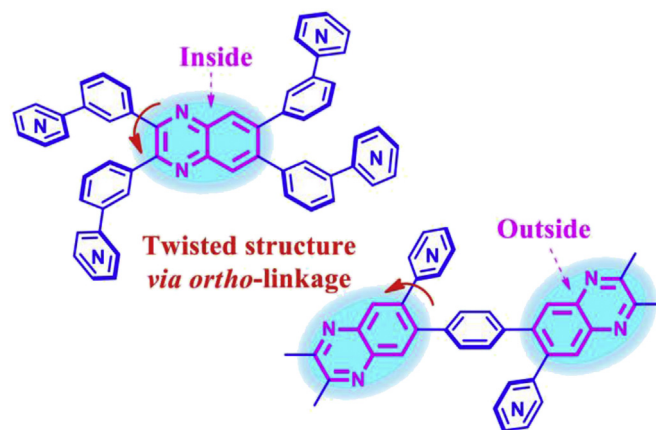
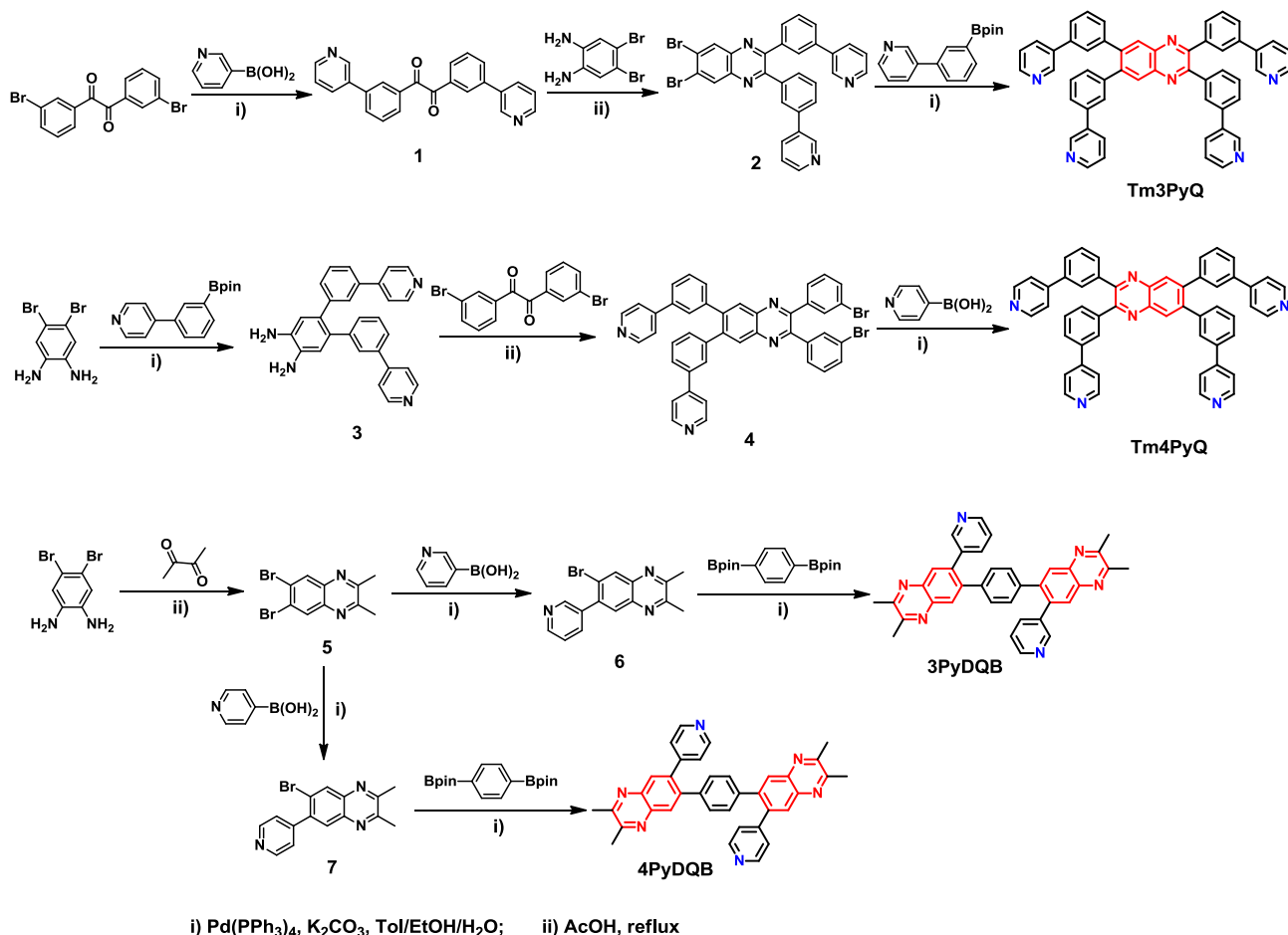


Fig. 1. Molecular design strategy of the quinoxaline-based compounds.

thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) of the compounds were undertaken with a NETZSCH STA 449C instrument and NETZSCH DSC 200 PC unit, respectively. Cyclic voltammetry (CV) measured in nitrogen-purged dimethyl formamide (DMF) solution by using a CHI voltammetric analyzer. The Bu₄NPF₆ (0.1 M) was used as the supporting electrolyte with ferrocenium-ferrocene (Fc/Fc⁺) was identified as the internal standard, and scan rate was 100 mV s⁻¹. The lowest unoccupied molecular orbital (LUMO) energy level (eV) of the samples were



Scheme 1. Synthetic routes of the quinoxaline-containing compounds.

Download English Version:

<https://daneshyari.com/en/article/1264705>

Download Persian Version:

<https://daneshyari.com/article/1264705>

[Daneshyari.com](https://daneshyari.com)