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Efficient violet non-doped organic light-emitting device based on a pyrene derivative with novel molecular structure

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ABSTRACT

A novel pyrene derivative 1,6-bis[2-(3,5-diphenylphenyl)phenyl]pyrene (DPPP) was successfully designed and synthesized. X-ray analysis shows the pyrene core in this compound is fully protected by the introduced 3,5-diphenylphenyl groups, resulting no π–π stacking between pyrene units, and the dihedral angle between pyrene ring and adjacent benzene ring is as large as 80.1°. This structure character leads to DPPP achieving a violet emission both in solution and as a thin solid film. Furthermore, DPPP exhibits high thermal properties due to its non-coplanar structure and large molecular size. The non-doped electroluminescence device employing DPPP as emitting layer shows a stable and efficient violet emission with a maximum external quantum efficiency of 2.2% and a CIE coordinate of (0.16, 0.04), which is remarkable in reported violet devices.

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1. Introduction

Organic light-emitting devices (OLEDs) have attracted much attention because of their applications in flat-panel displays and solid-state lightings [1]. Efficient violet emitting materials play an important role in OLEDs since violet emitters can be utilized to generate light emission over the whole visible region and white light emission [2–9]. Moreover, high-efficiency short-wavelength emission can effectively reduce the power consumption of full-color OLEDs [10]. In fact, violet OLEDs are also of great importance in other fields, such as high-density information storage [11]. Although many short-wavelength (blue-violet/violet) OLEDs have been reported in recent years [12–25], violet OLEDs with emission peak below 400 nm and high color purity are still very rare to date [22–24]. The molecular design of organic materials capable of efficient violet emission in OLEDs is highly challenging. To achieve a violet emission, the extent of conjugation in molecule must be confined, which in turn would usually impose constraints in molecular size. However, the resultant limited molecular size normally reduce the thermal stability of organic molecules and renders it more difficult to form stable and uniform amorphous thin films, which are detrimental for device operation. Furthermore, the confined conjugation length will cause decrease of charge-transporting ability and fluorescent quantum yield for organic molecules [26,27].

As a large conjugated aromatic system, pyrene not only has highly efficient violet emission around 390 nm, but also has high carrier mobility and excellent hole injection ability [28–30]. Nevertheless, pyrene itself is not suitable to act as violet-emitter in OLEDs due to its strong tendency to crystallize and form excimers by π–π stacking, which leads to a red-shifted emission above 480 nm as well as the decrease of fluorescence efficiency and make it incapable of forming stable amorphous thin film [28,29]. To suppress the π–π stacking, bulky groups generally are introduced to pyrene backbone at various positions, such as 1- and 6-positions, 2- and 7-positions, or 1-, 3-, 6-, and 8-positions [25,28,31–36]. In addition, incorporating pyrene with other chromophores also is a common strategy to design light-emitting materials for OLEDs [28,37–41]. As far as we know, numerous pyrene based light-emitting materials have been prepared through above mentioned methods, but only one violet OLED using pyrene derivative as

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emitting layer was reported by Kaafarani and co-workers, and this device exhibits a low efficiency of 0.04 cd/A [12]. The important reasons may be (i) introducing bulky rigid groups to pyrene backbone increases the extent of conjugation in molecule resulting in a longer emission wavelength, (ii) interactions between pyrene units have not been fully suppressed in solid state, which leads to pyrene derivatives exhibiting a obviously red-shifted emission in solid state compared with in solution.

In this paper, we designed and synthesized a novel violet-light-emitting material 1,6-bis[2-(3,5-diphenylphenyl)phenyl]pyrene (DPPP) employing pyrene as the chromophore (Scheme 1). In this compound, two 3,5-diphenylbenzene groups are connected with pyrene backbone by two benzene rings, respectively, and the bulky 3,5-diphenylbenzene group and pyrene unit locate at the adjacent positions of benzene ring. The structural characteristic of DPPP has significant advantages. Firstly, it can increase the dihedral angles between pyrene ring and adjacent benzene rings to confine the extent of conjugation in molecule through improving steric hindrance. Secondly, the bulky 3,5-diphenylbenzene groups can cap the pyrene core from both sides to prohibit the strong interactions between pyrene units. In addition, the bulky substituents at pyrene backbone can increase the molecular size to improve the high thermal stability. We characterized the structure and physical properties of DPPP, as we desired, it exhibits high-efficiency violet emission and high thermal stability. The non-doped electroluminescence device using DPPP as emitting layer achieved an efficient and stable violet emission (λ_{max} = 396 nm, EQE_{max} = 2.2%).

2. Experimental

2.1. General information

Commercially available reagents were used without purification unless otherwise stated. The ^1H NMR spectra and ^{13}C NMR spectrum were recorded on Bruker Avance 400 spectrometer. Elemental analysis was performed on a Vario III elemental analyzer. Mass spectra were obtained on a Bruker Microflex spectrometer. The absorption and photoluminescence spectra were recorded on a Hitachi U-3010 UV–Vis spectrophotometer and a Hitachi F-4500 fluorescence spectrophotometer, respectively. Photoluminescence quantum yield of solid film was measured by a combined measurement system for infrared fluorescence (Nanolog^R FluoroLog-3-2-iHR320) equipped with F-3018 integrating sphere. Cyclic voltammetry was performed on a CHI620C electrochemical analyzer, and the electrolytic cell is a conventional three-electrode cell consisting of a Pt working electrode, a Pt wire counter electrode and an Ag/AgCl reference electrode. Thermal gravimetric analysis (TGA) and differential scanning calorimetry (DSC) were performed on a TA instrument TGA2050 and a TA instrument DSC2910, respectively, with a heating rate of 10 °C/min under the nitrogen atmosphere. DFT calculations were performed using Gaussian 03 with the B3LYP/6-31G(d) method [42].

2.2. Synthesis

2.2.1. Compound 3

1-Iodo-2-bromobenzene **2** (1.41 g, 5.0 mmol), 3,5-diphenylphenyl boronic acid **1** (1.37 g, 5.0 mmol), and tetrakis(triphenylphosphine)palladium [$Pd(PPh_3)_4$] (80 mg) were mixed in toluene (35 ml), then Na_2CO_3 (2 M, 10 mL) and ethanol (10 mL) were added under the nitrogen atmosphere. The mixture reacted at 80 °C under the nitrogen atmosphere over night. After cooling, the resulting solution was extracted with CH_2Cl_2 three times, then the combined organic solution was dried over anhydrous $MgSO_4$ and evaporated with a rotary evaporator. The crude product was puried by column chromatography (eluent = petroleum ether 60–90 °C) to give a white powder (yield: 1.56 g, 82%). ^1H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.83 (1H, s), 7.72–7.69 (5H, m), 7.63 (2H, s), 7.48–7.44 (5H, t, J = 8.0), 7.35–7.40 (3H, q, J = 6.7), 7.24 (1H, s). TOF-MS: 384.126.

2.2.2. Compound 4

n-Butyl lithium (1.6 M, 1.5 mL) was added dropwise to the solution of compound **3** (1.5 g, 4 mmol) in anhydrous THF (20 mL) at −80 °C over half an hour, and the mixture was stirred for another 1 h at this temperature. Then trimethylborate (0.6 mL, 5.2 mmol) was added to the reaction mixture at −80 °C, and stirred for 12 h at room temperature. Then HCl (2 M, 10 mL) was added, and stirred for 1 h. The resulting solution was extracted with CH_2Cl_2 three times, then the combined organic solution was dried over anhydrous $MgSO_4$ and evaporated with a rotary evaporator. The crude product was puried by column chromatography (eluent = dichloromethane/petroleum ether, 1:3 v/v) to give a white powder (yield: 0.82 g, 58%). ^1H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.94 (1H, d, J = 8.0), 7.85 (1H, s), 7.65–7.68 (4H, m), 7.62 (2H, s), 7.28–7.52 (9H, m), 4.66 (2H, s).

2.2.3. DPPP

1,6-Dibromopyrene (0.36 g, 1 mmol), compound **3** (0.77 g, 2.2 mmol) and tetrakis(triphenylphosphine)palladium [$Pd(PPh_3)_4$] (25 mg) were mixed in toluene (15 ml), then Na_2CO_3 (2 M, 3 mL) and ethanol (5 mL) were added under the nitrogen atmosphere. The mixture reacted at 110 °C under the nitrogen atmosphere over night. After cooling, the resulting solution was extracted with CH_2Cl_2 three times, then the combined organic solution was dried over anhydrous $MgSO_4$ and evaporated with a rotary evaporator. The crude product was puried by column chromatography (eluent = dichloromethane/petroleum ether, 1:8 v/v) to give a white powder (yield: 0.37 g, 46%). ^1H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.20 (1H, d, J = 4), 8.15–8.07 (4H, m), 8.04–7.98 (3H, m), 7.81 (1H, d, J = 4), 7.76 (1H, d, J = 8), 7.68–7.65 (3H, m), 7.61–7.56 (3H, m), 7.51–7.48 (3H, m), 7.42 (1H, d, J = 8), 7.33 (1H, S), 7.24 (4H, s), 7.17–7.13 (7H, m), 7.08–7.04 (4H, m), 6.96–6.94 (6H, m). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 142.12, 141.97, 141.09, 141.05, 141.02, 140.09, 140.00, 137.60, 132.08, 130.49, 130.21, 129.91, 128.82, 128.57, 128.48, 128.27, 127.72, 127.22, 127.15, 127.07, 127.03, 125.62, 124.55, 124,27. TOF-MS: 811.232. Anal. Calcd. for $C_{64}H_{42}$: C, 94.78; H, 5.22. Found: C, 94.62; H, 5.26.

2.3. X-ray structure determination

The single crystal suitable for X-ray diffraction analysis was obtained by slowly evaporating the $CDCl_3$ solution of DPPP. Crystal data were collected on a Bruker SMART APEX-II CCD diffractometer with Mo Kα radiation (λ = 0.071073 Å) at 296 K. The data were corrected for Lorentz-polarization factors as well as for absorption. Structures were solved by direct methods and refined by full-matrix least squares methods on F^2 with the SHELX-97 program. All nonhydrogen atoms were refined anisotropically, while hydrogen atoms were placed in geometrically calculated positions. Crystal data for DPPP: $C_{64}H_{42}$, M = 810.98, Monoclinic, P2(1)/c, a = 9.201(4) Å, b = 11.487(5) Å, c = 21.142(10) Å, $\alpha = \gamma = 90°$, β = 94.410(6)°. V = 2228.1(18) Å^3, Z = 2, D_{Calc} = 1.209 Mg/m^3, 16535 reflections measured, 4128 unique reflections with $I > 2\sigma(I)$, R_1 = 0.0459, wR_2 = 0.1049. CCDC 1008121.

2.4. OLED fabrication and measurements

Indium-tin-oxide (ITO) coated glass substrates were cleaned with isopropyl alcohol and deionized water, then dried in an oven

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