



Novel tetraarylsilane-based hosts for blue phosphorescent organic light-emitting diodes

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ABSTRACT

Two highly twisted tetraarylsilane derivatives containing carbazole and benzimidazole were designed and synthesized with high triplet energy level (E_T) as hosts for blue phosphorescent organic light-emitting diodes (PHOLEDs). The thermal, photophysical, electrochemical properties and geometry optimization of materials were studied. The central silicon atom effectively disconnected the electronic interactions among the three functional units in a molecule, resulting in high E_T and relatively wide band gap (E_g) (≥ 3.5 eV). Finally, the blue PHOLED devices using 3,3'-(phenyl(4-(9-phenyl-9H-carbazol-2-yl)phenyl)silanediy)bis(4,1-phenylene) bis(9-phenyl-9H-carbazole) (TCzSi) as host material achieved a maximum current efficiency of 25.5 cd A⁻¹, a maximum power efficiency of 18.15 lm W⁻¹, a maximum luminance of 6285 cd m⁻² and a maximum external quantum efficiency (EQE) of 13.32%. This study showed a molecular design strategy to develop novel tetraarylsilane-based compounds for blue hosts.

1. Introduction

Phosphorescent organic light-emitting diodes (PHOLEDs) have attracted great attention because they can theoretically achieve 100% internal quantum efficiency by harvesting both singlet and triplet excitons through intersystem crossing (ISC) [1–3]. However, phosphorescent heavy metal complexes have relatively long lifetime about microsecond level, which may cause competitive factors such as triplet-triplet annihilation and concentration quenching. To achieve highly efficient electrophosphorescence, the heavy-metal phosphors are normally homogeneously dispersed into a host matrix at a low concentration to reduce these competitive factors [4]. The guest phosphor acts as the emitter, and the host material is used for carrier transport and energy transfer in the doped device [5]. Therefore, it's very critical to design appropriate host materials.

In general, several requirements have to be considered when designing novel host materials. Firstly, as a host for blue phosphor, its triplet energy level (E_T) must be higher than that of dopant material to avoid reverse energy transfer from the guest back to the host and

confine the triplet excitons within the emission layer [6]. Secondly, to reduce the hole and electron injection barrier and the turn-on voltage of devices, the highest occupied molecular orbital (HOMO) level and the lowest unoccupied molecular orbital (LUMO) level of host materials should match well with adjacent functional layers. Thirdly, the hosts should have proper and balanced carrier-transporting properties that would be beneficial to balance the hole-electron transfer and obtain relatively wide area of carrier recombination [7]. Finally, it is desirable that host materials have high thermal and morphological stability to guarantee the device's operational stability [5].

Carbazole-based compounds have attracted intense interest because of their high E_T and outstanding hole-transporting ability [8–11]. For example, carbazole-based host for efficient phosphorescent emitters named 1,3-bis(9H-carbazol-9-yl)benzene (mCP) possesses wide band gap (E_g) and high E_T (2.9 eV). Another carbazole derivative 4,4'-bis(9-carbazolyl)-biphenyl (CBP) with the biphenyl bridge has been widely utilized as the host material for blue PHOLEDs, with a relative low E_T (2.6 eV). The E_T is slightly lower than iridium (III) bis (4,6-(difluorophenyl) pyridine-N, C2') picolinate (Flrpic, 2.65 eV), a common

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dopant used as blue phosphor iridium complex, and the efficiency of devices used CBP as hosts is low [1]. In addition, Chen et al. synthesized several carbazole-based phosphorescent host materials with better OLED performance due to their good thermal stability [12]. Therefore, several strategies consisting of improving the thermal stability, reducing the conjugative effect between carbazole and adjacent groups, and appropriately reducing the planarity are presented for the development of carbazole-based host materials.

Tetraarylsilane compounds with wide band-gap and high thermal stability also have been reported as host materials for deep blue electrophosphorescence [13–15], but their poor carrier-transporting ability and high hole-injecting barrier hampered excitons recombination in the emitting layer lead to high turn-on voltage of PHOLEDs.

Therefore, p-type tetraarylsilane compounds combining silane with electron-donating carbazole can meet the requirements of the ideal host material for blue PHOLED [16–18]. Furthermore, benzimidazole as electron-accepting moiety can also be introduced into the tetraarylsilane compounds [19–21].

Likewise, in this study, we designed and synthesized two highly twisted tetraarylsilane derivatives as the high triplet energy hosts for blue PHOLEDs. A tetraarylsilane was introduced as the central core, linking carbazoles or benzimidazole with benzene through Suzuki coupling reaction. 3,3'-((phenyl(4-(9-phenyl-9H-carbazol-2-yl)phenyl)silanediy) bis(4,1-phenylene))bis(9-phenyl-9H-carbazole) (TCzSi) contained three electron-donating carbazoles, but 9-phenyl-2-(4-(phenyl(4'-(1-phenyl-1H-benzo[d]imidazole-2-yl)-[1,1'-biphenyl]-4-yl)(4-(9-phenyl-9H-carbazol-3-yl)phenyl)silyl)phenyl)-9H-carbazole (DCzMzSi) included two carbazoles and an electron-withdrawing benzimidazole. The typical tetrahedral geometry owing to the coordination of silicon was effective in ensuring the separation of the three functional units in a molecule. The highly twisted structure resulted in relatively high singlet and triplet energy, and the tetraarylsilane increased the E_T and thermostability. The TCzSi showed outstanding thermal, photophysical, and electrochemical properties and is suitable for blue PHOLEDs as hosts.

2. Experimental section

2.1. General information

All chemicals and solvents were purchased from local suppliers or TCI and used without further purification.

Nuclear magnetic resonance (^1H NMR) and (^{13}C NMR) spectra were collected with a Bruker DMX-400 Spectrometer. The ESI-TOF-MS mass spectra were performed under a TripleTOF 4600 mass spectrometer. Elemental analyses were performed by a PerkinElmer 2400 II elemental analyzer. The thermogravimetric analysis (TGA) was performed on a Perkin-Elmer TG/DTA thermal analysis instrument at a scanning rate of $10\text{ }^\circ\text{C min}^{-1}$ under nitrogen. Differential scanning calorimetry (DSC) was performed on a Mettler Toledo DSC 822 system at a heating rate of $10\text{ }^\circ\text{C min}^{-1}$ under a nitrogen atmosphere. The UV-vis absorption spectra were measured by a Perkin-Elmer Lambda 950 spectrophotometer. Photoluminescent (PL) spectra were measured on a Fluoromax-4 fluorescence spectrophotometer in solution of 10^{-5} mol/L and film, respectively. The DFT calculations were performed with the Gaussian 03 series of programs using the B3LYP hybrid functional and 6-31G(d, p) basis set. Electrochemical cyclic voltammetry (CV) was performed to measure the highest occupied molecular orbital (HOMO) level in anhydrous acetonitrile with 0.1 M tetrabutylammonium hexafluorophosphate (TBAPF₆) at a scan rate of 100 mV/s.

2.2. Synthetic procedures

2.2.1. Syntheses of tris (4 - bromide) phenyl silicone (T(4-Br)PSi) and 9-phenyl-9H-carbazol-3-ylboronic acid (CzB(OH)₂)

To a solution of 1,4-dibromobenzene (4.25 g, 18 mmol) in anhydrous

diethyl ether (100 ml) was added dropwise n-butyllithium (8.3 ml, 2.4 M, 19.8 mmol, 1.1 equiv) at $-78\text{ }^\circ\text{C}$ under nitrogen atmosphere. The mixture was stirred for 3 h at that temperature. Then, phenyltrichlorosilane (1 ml, 6 mmol) was added to the mixture. The reaction mixture was further stirred overnight at room temperature. After the reaction completed, the mixture was quenched by addition of water (60 ml), and then extracted with ether. The combined organic layers were washed with water, and dried over anhydrous Na₂SO₄. After filtration and evaporation, the crude product was recrystallized from ethanol to afford T(4-Br)PSi as a white solid (yield = 2.5 g, 75.6%). ^1H NMR (400 MHz, CDCl₃) δ 7.53–7.52 (6H, d, J = 8.20 Hz), 7.49–7.45 (3H, m), 7.41–7.39 (2H, d, J = 7.41 Hz), 7.37–7.35 (6H, d, J = 7.72 Hz).

CzB(OH)₂ was synthesized according to the reported literature [22].

2.2.2. Synthesis of 3,3',3''-((phenylsilanetriyl)tris(benzene-4,1-diy))tris(9-phenyl-9H-carbazole) (TCzSi) and 3,3'-((4-bromophenyl)(phenyl)silanediy)bis(4,1-phenylene))bis(9-phenyl-9H-carbazole) (DCzBrPSi)

Tris (4-bromide) phenyl silicone (T(4-Br)PSi) (2.29 g, 4 mmol), 9-phenyl-9H-carbazol-3-ylboronic acid (CzB(OH)₂) (2.3 g, 8 mmol), *Trans*-Dichlorobis(triphenyl-phosphine)Palladium(II) (0.05 g, 0.07 mmol) and toluene (40 ml) were sequentially added to a 250 ml round-bottom flask. The mixture was stirred 10 min under nitrogen atmosphere until it became clear. Then 2 M Na₂CO₃ (10 ml) was added to the reaction mixture. The mixture was stirred at $105\text{ }^\circ\text{C}$ for 10 h. After cooled down to room temperature, the mixture was extracted with dichloromethane twice. The combined organic layers were washed with water, and dried over anhydrous Na₂SO₄. After filtration the organic layer was stored and evaporated under reduced pressure. Then, the crude product was purified by column chromatography on silica gel (petroleum ether: dichloromethane = 5:1, v/v) to afford TCzSi as a white solid (yield = 1.1 g). TCzSi: ^1H NMR (400 MHz, CDCl₃) δ 8.42 (s, 3H), 8.19 (d, 3H, J = 7.65 Hz), 7.82–7.76 (m, 14H), 7.70 (d, 3H, J = 8.40 Hz), 7.63–7.60 (m, 12H), 7.50–7.42 (m, 15H), 7.32–7.28 (m, 3H). ^{13}C NMR (400 MHz, CDCl₃) δ 143.23, 141.48, 140.67, 137.76, 137.20, 136.70, 134.84, 133.30, 132.39, 130.04, 128.17, 127.61, 127.15, 126.99, 126.31, 125.67, 125.64, 124.10, 123.65, 120.51, 120.35, 120.24, 119.08, 119.00, 110.30, 110.21, 110.14. ESI-TOF-MS, m/z : 1060.4 (M⁺). Elemental analysis calcd for C₇₈H₅₃N₃Si: C, 88.35; H, 5.04; N, 3.96; Si, 2.65; found, C, 88.34; H, 5.01; N, 3.98; Si, 2.67.

The DCzBrPSi was synthesized according to the same procedure as used for T(4-Br)PSi. But the crude product was purified by column chromatography on silica gel (petroleum ether: dichloromethane = 3:1, v/v) to afford DCzBrPSi as a white solid (yield = 1.03 g). DCzBrPSi: ^1H NMR (400 MHz, CDCl₃) δ 8.40 (s, 2H), 8.18 (d, 2H, J = 7.64 Hz), 7.77 (d, 4H, J = 7.88 Hz), 7.72–7.66 (m, 8H), 7.63–7.56 (m, 12H), 7.48–7.42 (m, 11H), 7.31–7.30 (m, 2H).

2.2.3. Synthesis of 3,3'-((phenyl(4'-(1-phenyl-1H-benzo[d]imidazole-2-yl)-[1,1'-biphenyl]-4-yl)silanediy)bis(4,1-phenylene))bis(9-phenyl-9H-carbazole) (DCzMzSi)

DCzBrPSi (0.9 g, 1 mmol), (4-(1-Phenyl-1H-benzo[d]imidazole-2-yl)phenyl)boronic acid (0.47 g, 1.2 mmol), *Trans*-Dichlorobis(triphenyl-phosphine)Palladium(II) (0.05 g, 0.07 mmol) and toluene (30 ml) were sequentially added to a 250 ml round-bottom flask. The mixture was stirred 10 min under nitrogen atmosphere until it became clear. Then 2 M Na₂CO₃ (10 ml) was added to the reaction mixture. The mixture was stirred at $105\text{ }^\circ\text{C}$ for 10 h. After cooled down to room temperature, the mixture was extracted with dichloromethane twice. The combined organic layers were washed with water, and dried over anhydrous Na₂SO₄. After filtration the organic layer was stored and evaporated under reduced pressure. Then, the crude product was purified by column chromatography on silica gel (petroleum ether: dichloromethane = 1:1, v/v) to afford DCzMzSi as a white solid (yield = 0.96 g, 88.4%). ^1H NMR (400 MHz, CDCl₃) δ 8.40 (s, 2H), 8.18 (d, 2H, J = 7.48 Hz), 7.97 (d, 1H, J = 8.01 Hz), 7.79–7.74 (m, 10H), 7.70 (t, 6H, J = 8.01 Hz), 7.63–7.57 (m, 12H), 7.54–7.42 (m, 14H), 7.37 (d, 3H, J = 6.94 Hz), 7.32–7.27 (m,

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