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Silafluorene moieties as promising building blocks for constructing wide-energy-gap host materials of blue phosphorescent organic light-emitting devices

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In this article, we reported the synthesis and characterization of a novel silafluorene-based host material, 1,3-bis(5-methyl-5*H*-dibenzo[b,d]silol-5-yl)benzene (Me-DBSiB), for blue phosphorescent organic light-emitting devices (PHOLEDs). The Me-DBSiB was constructed by linking 9-methyl-9-silafluorene units to the phenyl framework through the sp^3-hybridized silica atom to maintain high singlet and triplet energy, as well as to enhance thermal and photo-stability. The calculated result shows that the phenyl core does not contribute to both the highest occupied molecular orbital and lowest unoccupied molecular orbital. Wide optical energy gap of 4.1 eV was achieved. When the Me-DBSiB was used as the host and iridium (III) bis[(4,6-difluorophenyl)pyridinato-N,C2′]picolate (Firpic) as the guest, a maximum current efficiency was 14.8 cd/A, lower than the counterpart of 1,3-bis(9-carbazolyl)benzene (28 cd/A). The unbalanced barrier for electron and hole injection to host layer may be responsible for low efficiency. Even so, our results show that silafluorene moieties are promising building blocks for constructing wide-energy-gap host materials.

silafluorene moiety, wide energy gap, host materials, blue phosphorescence organic light-emitting device

1 Introduction

Blue, especially authentic blue phosphorescent organic light-emitting devices (PHOLEDs) have recently become an intensively concerned area for organic electroluminescent researches because the external quantum efficiencies of the blue PHOLEDs are significantly lower than that of the green and red PHOLEDs, while comparable efficiencies are required for flat panel display applications among the three primary colors. Highly efficient blue PHOLEDs are difficult to be achieved mainly because the blue phosphorescent dopants are required to have a high-lying triplet state (around 2.80–2.90 eV), which would lead to low emission efficiency and short device lifetime. Moreover, the phosphorescent dopant must be dispersed into the matrices of the host materials, in which the energy of the host material would be transferred to dopants such as Ir^{III} or Pt^{II} complexes, which emit phosphorescence via radiation transition. Thus, the host material for blue PHOLEDs is required to have a high triplet energy level (above 2.9 eV), reasonable HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) energy level, and well balanced charge transport properties.

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Elevating triplet energy level of the host material is a primary focus for the development of blue PHOLEDs. The most commonly used host material mCP (*N*,*N*′,-dicarbozalyl-1,3-benzene) has a triplet level of 2.9 eV, but its HOMO level (−5.9 eV) falls near or above that of most blue phosphorescent dopants such as Ir(III)bis(4′,6′-difluorophenylpyridinato)tetrakis(1-pyrazolyl)borate, FIr6 (−6.1) [1], which makes them unsuitable for efficient carrier trapping and subsequent recombining. As for phenylsilane-based ultrawide energy gap hosts (UGHs) [2], the ultrahigh energy gap elevates the barriers of the holes injection to a light-emitting layer and thus resulted in increasing the driving voltage and decreasing power efficiencies. The research for this purpose emphasized the use of the high-triplet-energy building blocks with short π conjugation length to build high triplet-energy host materials. Many successful designs have been achieved by employing carbazole (3.0 eV) [3,4], fluorene (2.89 eV), phenylsilanes [1,2], pyridine [5], benzofuran/dibenzothiophene/pyridoindole moieties [6], or their hybrid combinations [7] as building blocks. Especially, host materials containing fluorene moieties such as 1,3-bis(9-phenyl-9*H*-fluoren-9-yl)benzene (mDPFB, E_T= 2.80 eV) and 1,4-bis(9-phenyl-9*H*-fluoren-9-yl)benzene (E_T=2.83 eV, E_T donating the lowest energy of the triplet excited state) [8], triphenyl-(4-(9-phenyl-9*H*-fluoren-9-yl)-phenyl)silane) (E_T=2.89 eV) [7], show significantly improved efficiencies compared to device based on mCP or UGHs materials. The silafluorene is an analogue of fluorene by substituting carbon atom at 9-position of the fluorene with silica atom and silafluorene-based derivatives that are expected to have higher electron affinity. This expectation is mainly owing to the σ*-π* conjugation and better photostability due to higher oxidation stability of Si at 9-position of silafluorene comparing with counterpart of fluorene derivatives, which usually result in ketone defects [9,10]. Moreover, 9-silafluorene contains the silole structure in the center of the molecular structure and the silole derivatives have been proved to have excellent electrical and optical properties [11–15]. Poly(3,6-silafluorene) was found to be an ultraviolet light- emitting polymer with a wide band gap of 4.0 eV [9,16,17] and many polymers containing silafluorene moieties have been developed as efficient active materials of polymer solar cells [12,18–23]. Therefore, silafluorene derivatives would be promising host material candidates for blue PHOLEDs. However, to our knowledge, there are no reports about silafluorene-based derivatives as host material for blue PHOLEDs to date.

In this paper, we reported the synthesis and characterization of a 9-silafluorene-based wide energy-gap host material, 1,3-bis(5-methyl-5*H*-dibenzo[b,d]silol-5-yl)benzene (Me-DBSiB). The 9-silafluorene is connected to the 1,3-position of the phenyl core like mCP through the sp^3-hybridized silica atom at the Si-9 of the silafluorene, which can perform as a spacer to block extended π-conjugation. Thus the conjugation length and triplet energy level of each building block in the resulting molecule should remain unchanged. As a result, the high triplet energy level and enhanced electrical and optical properties of the resulting material are expected to be achieved. Moreover, the out-of-plane 9-methyl of the silafluorene would suppress undesirable aromatic π-stacking interactions among the silafluorene units, resulting in improved morphological stability.

2 Experimental

2.1 Synthesis of the Me-DBSiB

All the reactions were carried out in an argon atomosphere and reagents were used without further purification. The ^{1}H NMR spectra were recorded on Bruker Avance 400 MHz spectrometers (Bruker, Switzerland) and HRMS experiments were carried out on a EI-TOF (GCT Premier, Waters, USA).

To a rapidly stirred solution of trichloromethylsilane (12 mL, 11.6 mmol) in 100 mL of ether, 100 mL ethereal solution containing 25.64 mmol 2,2′-biphenylenedilithium (prepared by treating 2,2′-dibromobiphenyl (8 g, 25.64 mmol) with BuLi (25 mL, 56 mmol, 2.5 mol/L) under −78 °C) was added over 2.5 h. The mixture was stirred at room temperature for 2 days, after which the ether was distilled and 100 mL of petroleum ether was added and the mixture was filtered under moisture-free nitrogen atmosphere. The lithium salt was washed with several portions of petroleum ether. The solvents, together with *n*-butyl bromide were distilled from the filtrate. The residual material was used for the next reaction immediately.

Under nitrogen atmosphere, 1,3-dibromobenzene (2.5 g, 10.6 mmol) in dry THF was added slowly to a mixture of magnesium (0.56 g, 23.3 mmol) and 9-chloro-9′-methysilafluorene (prepared above) in dry THF (50 mL) at room temperature with rapid stirring. The rate of addition was adjusted to a gentle reflux. The solution was then subsequently heated under reflux for 2 h and allowed to stand at room temperature for one day. After ensuring that the reaction was completed by using TLC, water was added and the organic layer was extracted with diethyl ether and dried over anhydrous magnesium sulfate. Some of the solvent was removed and the precipitation (0.35 g, 0.71 mmol) was formed after several days. The yield was 7.1% (based on the 2,2′-dibromobiphenyl); ^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.89–7.87 (m, 5H), 7.66–7.64 (m, 4H), 7.55 (d, J_1=7.2, J_2=1.6, 2H), 7.51–7.46 (m, 4H), 7.32–7.28 (m, 5H), 0.70 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, δ): 148.35, 140.38, 137.19, 135.87,134.31, 133.39, 130.49, 127.61, 127.59, 120.99, −4.78; HRMS (EI): calc. for $C_{32}H_{26}Si_2$, 466.1573; found: 466.1574 ([M]$^+$).

2.2 Spectroscopy, CV and DSC

The UV absorption and emission spectra in CH_2Cl_2 solution and thin films were measured using Hitachi U-3310 (Japan) spectrophotometers and Edinburgh FS920 fluorometers (UK), respectively. Cyclic voltammetry (CV) was measured on a Princeton Applied Research Model 273 A electrochemical workstation. An Ag/AgCl, platinium disk was used as the working electrode and a Pt-wire as the counter-electrode. The redox measurement was carried out in anhydrous CH_3CN solution with 0.1 mol/L TBAPF6 (*n*-tetrabutylam-monium hexafluorophosphate) as supporting electrolyte under a scan rate of 100 mV/s. The ferroceninium/ferrocence (Fc/Fc^+) was used as an internal standard. The differential scanning calorimetry (DSC) was measured using a Perkin-Elmer diffierential scanning calorimeter (DSC 7, USA) at a heating rate of 10 °C/min.

2.3 The preparation and measurment of OLEDs

The device structure of the blue PHOLEDs was indium tin oxide (ITO, 50 nm), poly(3,4-ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT:PSS, 30 nm), 4,4-cyclohexylidenebis[*N*,*N*-bis(4-methylphenyl)-aniline](TAPC, 20 nm)/mCP(10 nm)/Me-DBSiB:Firpic (20 nm), 1,3,5-tri[(3-pyridyl)-phen-3-yl]benzene (TmPyPB, 35 nm)/LiF (1 nm)/Al (100 nm). All the organic layers were successively deposited by means of vacuum deposition onto the ITO-coated glass substrates, which were previously etched, patterned, and washed with detergent, deionized water, acetone, and ethanol in turn. For the doped layer, blue phosphorescent dopant and host materials were co-evaporated and the doping concentration was controlled by deposition rates. The electroluminescence (EL) spectra and CIE coordinates of the devices were measured by a spectrometer (PR650) and the current-voltage-luminescence characteristics were analyzed by Keithley 2602 source meter (USA).

2.4 Computational details of theoretical calculations

Density functional theory (DFT) calculation was carried out employing B3LYP hybrid function with basis sets 6-31G(d,p). Unrestricted and restricted self-consistent field formalism were used for the triplet state and ground state calculation, respectively. Singlet ground (S_0) and triplet state (^3S) geometries of the Me-DBSiB were fully optimized by using M06 method. All calculations were carried out with the Gaussian 09 program package.

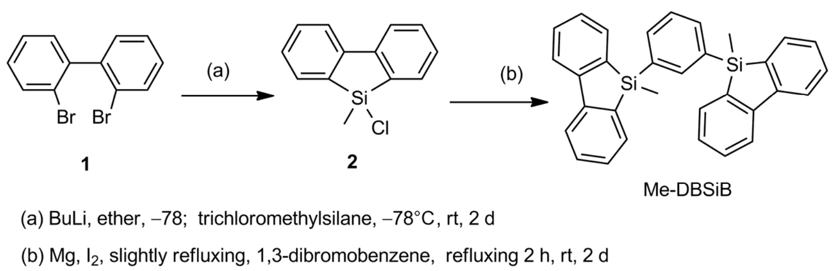
3 Results and discussion

A silafluorene moiety was selected as the building block for host material of blue PHOLEDs due to several advantages of the silafluorene such as (1) high energy gap (above 4.0 eV) [24]; (2) improved thermal and photo-stability besides possessing similar optical properties to the fluorene moieties; (3) sp^3-hybridized silica atom at the Si-9 of the silafluorene, which can act as a junction blocking extended π-conjugation; and (4) ability to graft varieties of substituent on Si-9 of the silafluorene to suppress undesirable aromatic π-stacking interactions and crystallization. Our design is to link both silafluorene units on 1,3-position of phenyl core through sp^3-hybridized silica atom of the silafluorene so as to retain the optical properties of individual silafluorene unit.

Scheme 1 shows the synthetic route to silafluorene-based host material, Me-DBSiB. The 9-chloro-9′-methysilafluorene was first synthesized by treating trichloromethylsilane with 2,2′-biphenylenedilithium at −78 °C, which was prepared by lithium-halo exchange of the 2,2′-dibromobiphenyl with *n*-butyllithium in THF. It should be noted that all dealings for this reaction including filtration should be carefully performed in a moisture-free nitrogen atmosphere because of the moisture sensitivity of the resulting intermediate. The solvent together with *n*-butyl bromide was first distilled under vacuum condition, then dried hexane was added to induce inorganic salt LiCl to be precipitated and removed by filtering. Finally, the solvent hexane was removed by distillation and the produced intermediate was used for the next reaction without further purification. Furthermore, the Grignard reaction of the 9-chloro-9′-methysilafluorene with 1,3-diborombenzene was carried out to produce the target product Me-DBSiB.

DFT calculations of the Me-DBSiB were carried out to get information about the electronic density associated with each energy level, orbital components and the energy gap between the singlet and triplet states. The calculation of orbital components was based on three parts of the Me-DBSiB (two silafluorene units and one central phenyl core). From Figure 1, the HOMO and LUMO were almost completely localized on two different silafluorene units of the Me-DBSiB, respectively, accounting for 95.61% for LUMO and 97.93% for HOMO, while phenyl core segments do not provide any contribution to both orbitals, suggesting that the HOMO and LUMO could be independently modified to tune their energy levels and triplet energy gap. We also noted that the heteroatom Si did not participate in the formation of HOMO and LUMO, showing their limited influence on HOMO and LUMO. This is different from that of the mCP, in which both HOMO and LUMO were mainly delocalized over two carbazole units and central benzene core with comparable contribution (Figure 1). The computed triplet energy gap of the Me-DBSiB (^3E_g) is 3.167 eV.

The experimental HOMO and LUMO levels of the Me-DBSiB were measured by cyclic voltammetry (CV), performed in acetonitrile solution containing 0.1 mol/L *n*-Bu_4NPF_6 as the supporting electrolyte. An Ag/AgCl and platinium disk were used as reference and working electrode, respectively. The onset potential of the irreversible



Scheme 1 The schematic structure and synthetic rout of the Me-DBSiB.

oxidation process (Figure 2) occurs at +1.33 V (Table 1), corresponding to an estimated HOMO level of –6.09 eV according to the empirical formula, $E_{\mathrm{HOMO}}=-(E_{\mathrm{OX}}-E_{\mathrm{Fc^+/Fc}}+4.8)$. Unfortunately, the reduction potential of the Me-DBSiB was not observed in the solvent window of the CH_3CN. A similar phenomenon was also observed in poly(9,9′-dialkyl-3,6-silafluorene) [16]. Thus, the LUMO level was estimated to be about –1.99 eV from the HOMO level and optical energy gap of the Me-DBSiB.

The thermal properties of the Me-DBSiB was inspected by DSC measurement. From the DSC curve shown in Figure 3, the distinct endothermic peak, assigned to melting process, was observed at 180 °C, about 9 °C higher than that of the mCP (171 °C) [25]. Whereas, no glass transition was detected during heating scan of DSC.

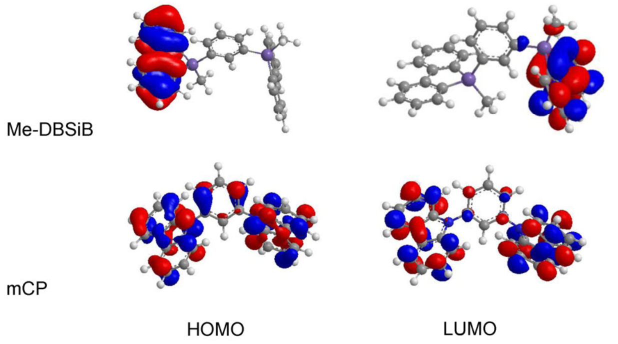


Figure 1 The calculated contours of the HOMO and LUMO orbitals of the Me-DBSiB.

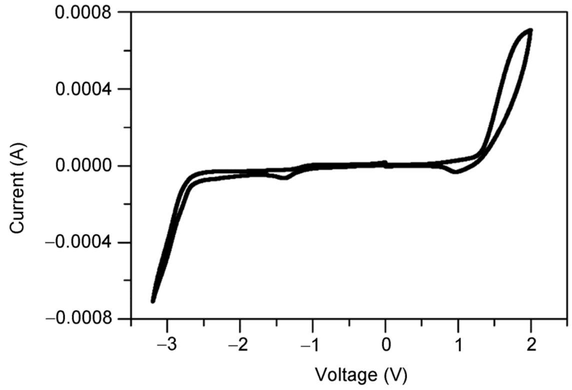


Figure 2 The CV curve of the Me-DBSiB in CH_3CN solution.

The photophysical properties of Me-DBSiB were analyzed by UV-Vis absorption and PL measurements in CH_2Cl_2 solution and thin films (Figure 4). All photophysical datas are summarized in Table 1. In solution, the Me-DBSiB shows two strong absorption bands with a main peak at 288 nm and a secondary peak at 284 nm, which could be assigned as π-π* transition of the silafluorene part. Switching to the solid state, a similar absorption profile was observed, but the peak of the high-energy side became a main peak with a slight hypochromic shift while the low-energy peak became a secondary peak with a slight bathochromic shift. In the PL spectra, the maximum emission wavelength appeared at 333 nm with two shoulder peaks 319 and 344 nm in solution, about 20 nm red shift relative to the fluorene-based countparts mDPFB (313 nm) [8]. While in the solid state, the fine structure of the fluorescent spectra disapppeared due to interactions between the molecules (packing effect) in solid state, and a peak of 356 nm was observed. From the intersection of the absorption and PL spectra of Me-DBSiB in solution, the singlet energy gap could be estimated to be 4.1 eV (302 nm).

The blue PHOLEDs with the Me-DBSiB as host materials and the FIrpic as a blue dopant were fabricated to evaluate the performances of this host. The device structure was ITO (50 nm), PEDOT:PSS (30 nm), TAPC (30 nm), mCP (10 nm), Me-DBSiB:FIrpic (20 nm)/TmPyPB (35 nm), and LiF (1 nm)/Al (100 nm). The doping concentration of the FIrpic was fixed at 5%. Figure 5 shows the characteristic curves of the blue PHOLEDs. The device shows low current density, only up to 10 mA/cm^2 even at 11 V, corresponding to a luminance of 3000 cd/m^2 (Figure 5(a)). A current efficiency of 14.8–10.0 cd/A over a luminance range from 10 to 1000 cd/m^2 (Figure 5(b)) was observed. A typical EL emission at 100 cd/cm^2 from FIrpic (the inset of Figure 5(b)) was observed while there was no emission from the host material. This indicates that the energy transfer from host material to phosphorescent dopant FIrpic is efficient. However, performances of the blue PHOLEDs using Me-DBSiB as the host material were inferior to that of mCP-based device (28 cd/A) at the present state. We speculated that this inferior performance could be attributed to unbalanced electron and hole injection to the host layer. The Me-DBSiB has a HOMO of –6.09 eV, only 0.19 eV barrier for hole injec-

Table 1 The thermal, electrochemical and photophysical characterization of the Me-DBSiB, as well as electroluminescent performances

	λ_{abs} (nm) a)	λ_{em} (nm) a)	T_m (°C)	E^{OX}_{onset} (V)	HOMO	LUMO	$\Delta E_{0\text{-}0}$ b)	Computed triplet level (eV)	Turn on voltage (V)	Luminous efficiency (cd/A Max, at 100, 1000 cd/cm^2)	λ_{EL} (nm) c)
Me-DBSiB	284, 288	333, 319 (sh), 344 (sh)	180	1.33	−6.09	−1.99	4.1	3.167	5.3	14.8, 12.6, 9.8	472

a) The UV absorption emissions were measured in the in CH_2Cl_2 solution, "sh" in the bracket refers to shoulder peak; b) the $\Delta E_{0\text{-}0}$ was obtained from the intersection of the absorption and PL spectra of Me-DBSiB in solution; c) the electroluminescence peak at the luminance of 100 cd/cm^2.

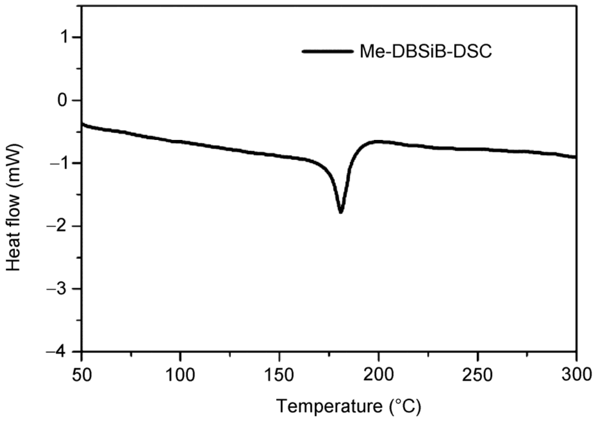


Figure 3 The DSC curve of the Me-DBSiB.

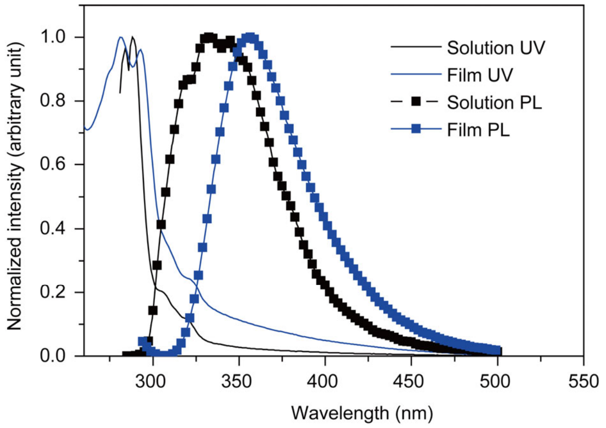


Figure 4 The absorption and photoluminescence spectra of the Me-DBSiB in CH_2Cl_2 solution and thin films.

tion from mCP to Me-DBSiB while it has a LUMO of −1.99 eV, 0.61 eV barrier for electron injection from TmPyPB [26] to the host material. As a result, some of the electrons were blocked at the interface of Me-DBSiB/TmPyPB, resulting in unbalanced electron-hole recombination within the host layer and thus leading to low efficiency. Our consideration could be supported from low current density during device operation. This situation is similar to a UGHs-based device, in which the barrier for hole injection from mCP to UGHs is about 1.2 eV, and thus increasing driving voltage is requested to produce sufficient current [2].

4 Conclusions

A wide-energy-gap host material Me-DBSiB based on silafluorene moieties was designed and successfully synthesized. Two silafluorene units were connected to 1,3-position of the central phenyl core through sp^3 hybridized Si atom, which blocks the extended conjugation between the central phenyl core and silafluorene moiety, and as a result, a high optical energy gap of 4.1 eV and improved thermal properties were achieved. These properties made it suitable to be host of blue PHOLEDs. Although the blue PHOLEDs based on the Me-DBSiB as host and the FIrpic as blue phosphorescent dopant only show a maximum current efficiency of 14.8 cd/A, we are sure that silafluorene moieties would be promising building blocks for constructing wide-energy gap host material. The perfect host materials could be sure to be achieved by combining silafluorene moiety with other building blocks such as carbazol moieties or rationally grafting substituent on silica atom of silafluorene unit,

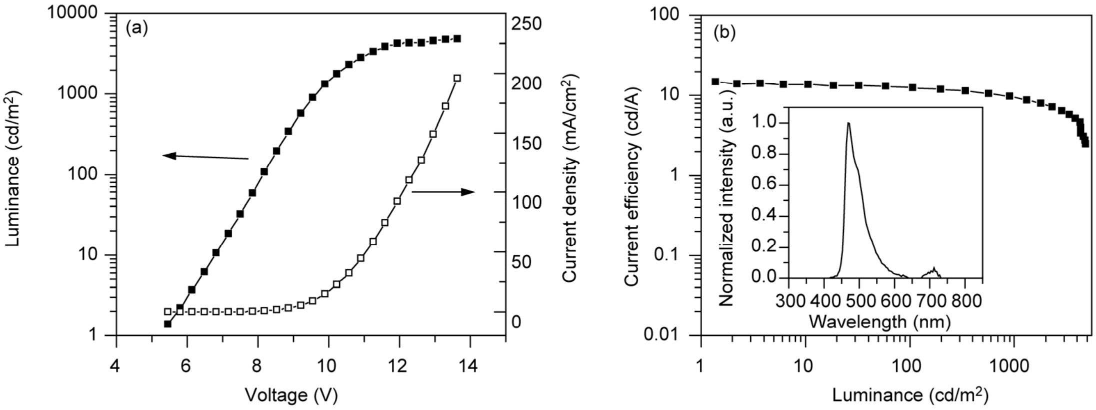


Figure 5 (a) Current density-luminance-voltage; (b) current efficiency-luminance characteristic curve of the device. Inset of (b) is the EL spectra of the device at a luminance of 100 cd/cm^2.

which could tune a triplet energy gap, HOMO and LUMO levels, and molecule packing properties.

Supporting information

The supporting information is available online at chem.scichina.com and link.springer.com/journal/11426. The supporting materials are published as submitted, without typesetting or editing. The responsibility for scientific accuracy and content remains entirely with the authors.

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