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(54) **COMPOUND, EMITTING LAYER OF ORGANIC LIGHT EMITTING DIODE AND ORGANIC LIGHT EMITTING DIODE DEVICE**

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Publication Classification

(51) **Int. Cl.**
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(57) **ABSTRACT**

The present disclosure relates to a compound including a structure of Formula (I), and the use of the compound as a dopant in an emitting layer of an organic light emitting diode. The present disclosure also relates to an emitting layer of an organic light emitting diode and an organic light emitting diode device.

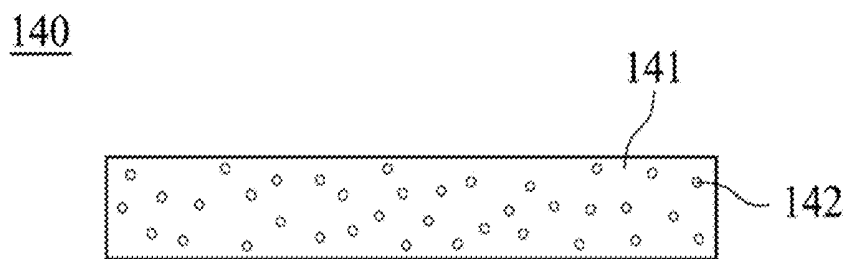


Fig. 1

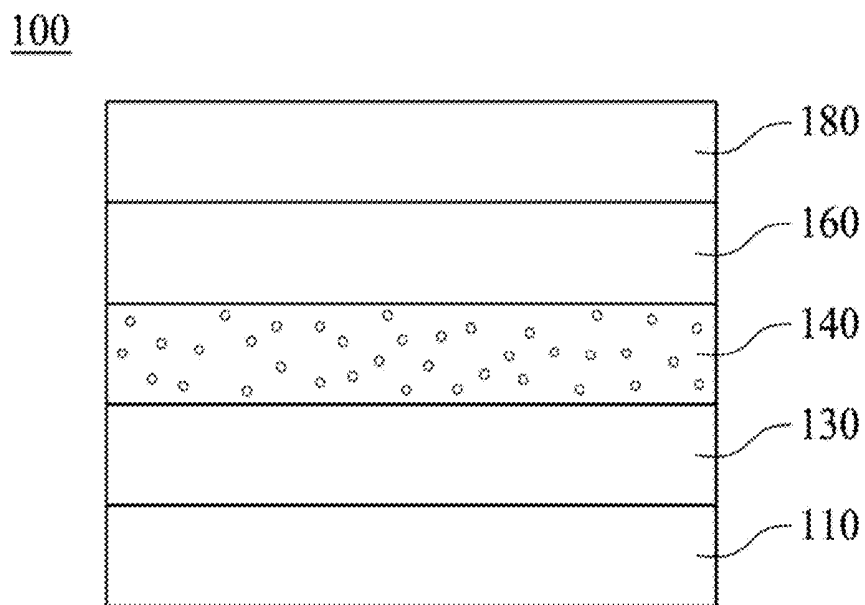


Fig. 2

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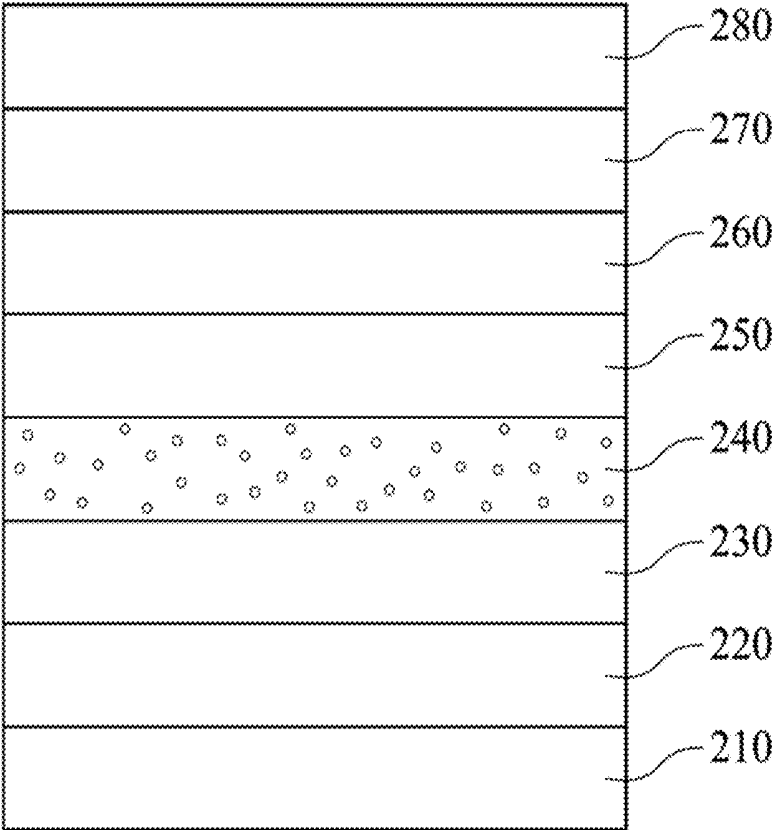


Fig. 3

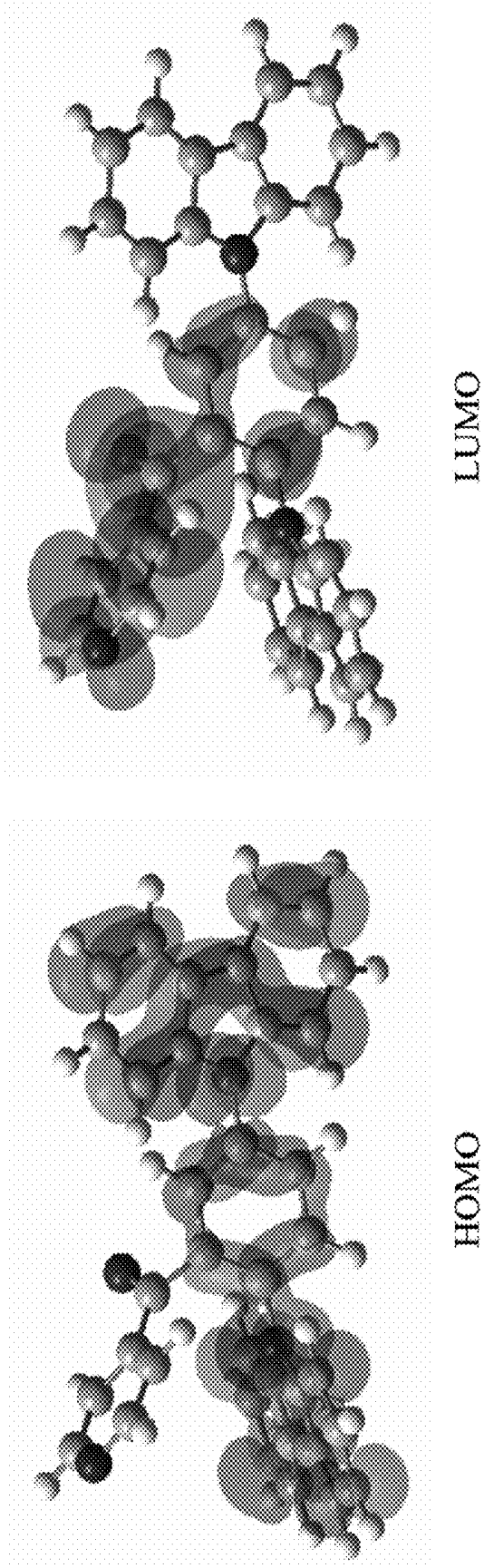


Fig. 4

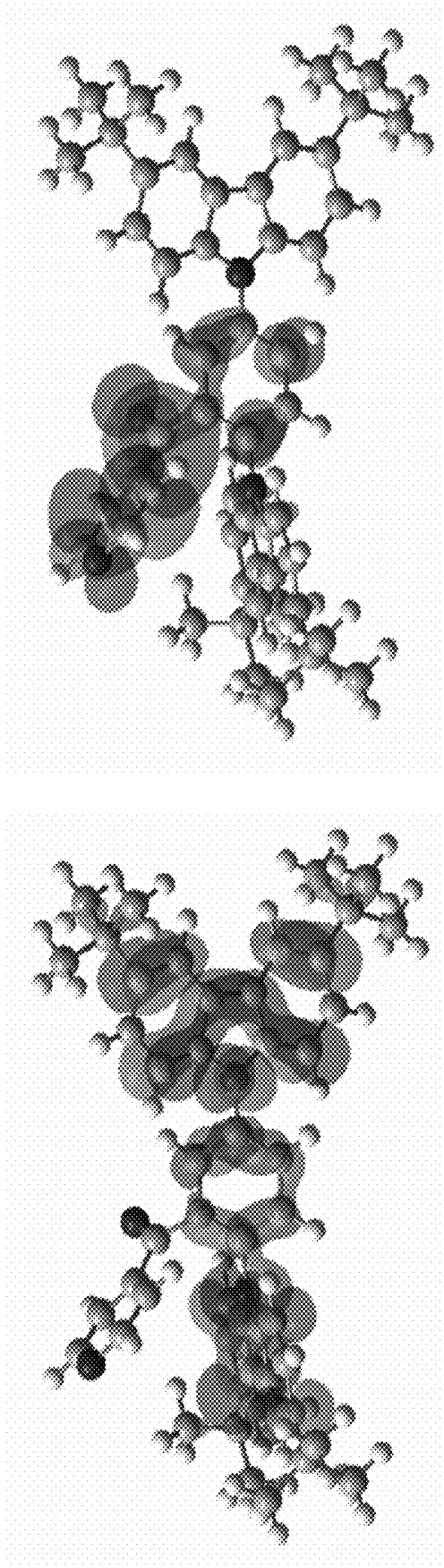


Fig. 5

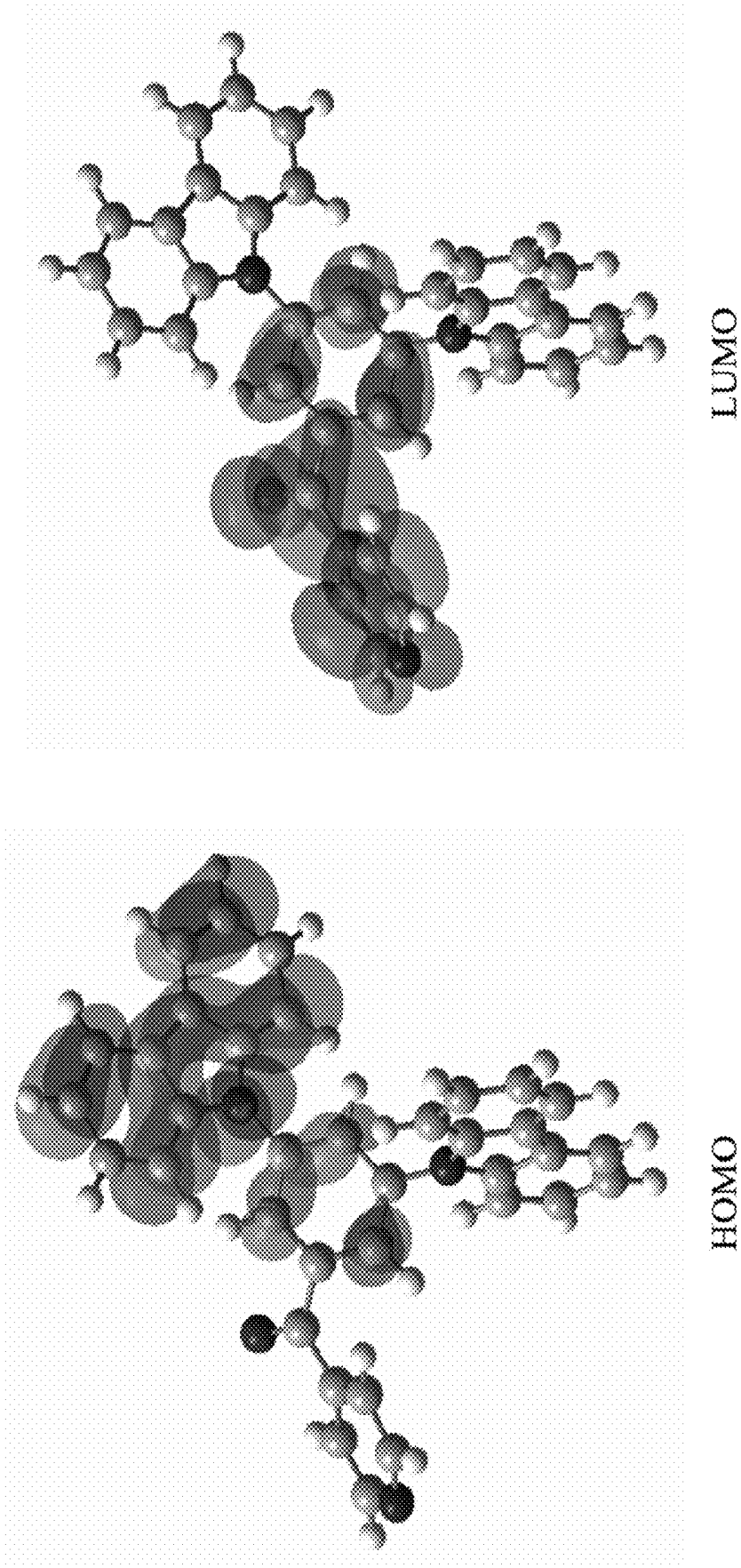
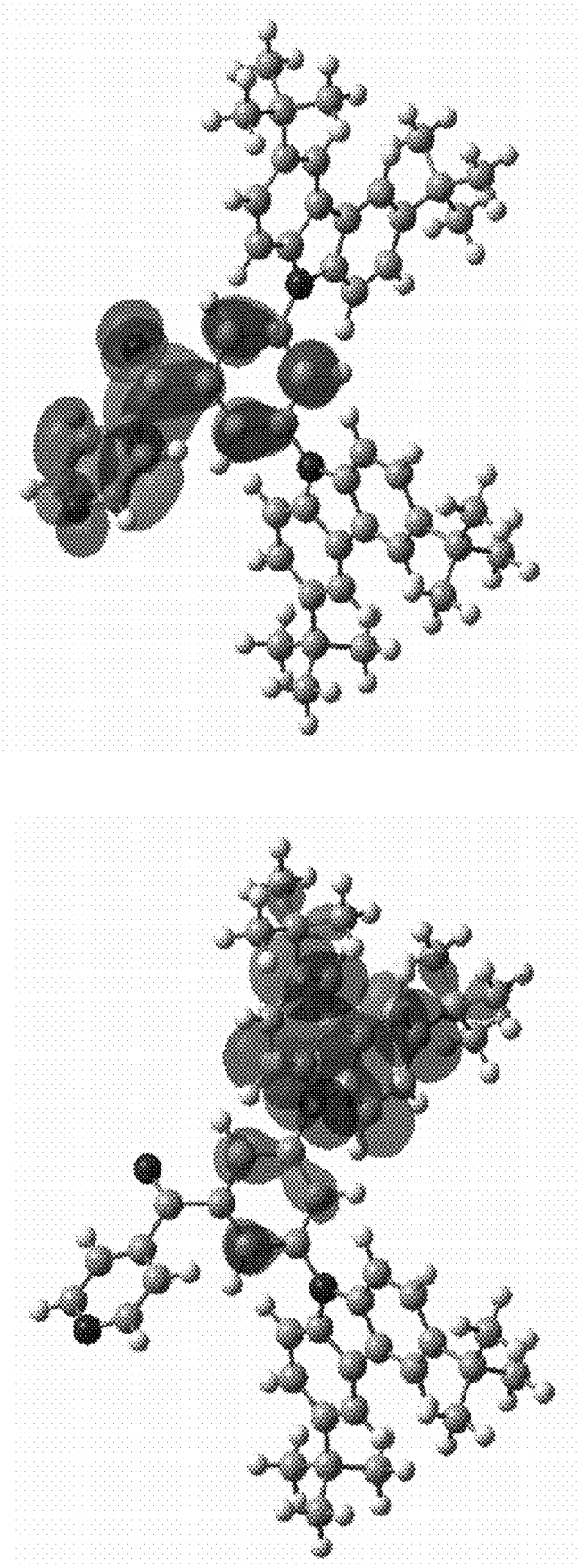


Fig. 6



LUMO

HOMO

Fig. 7

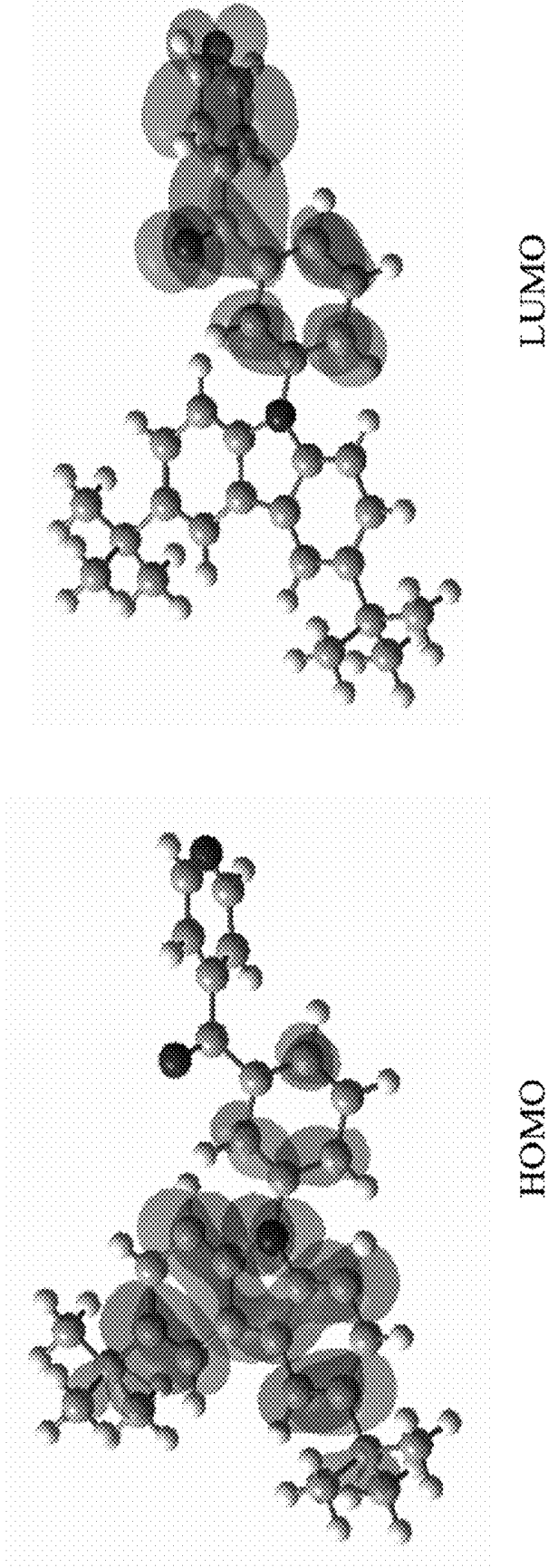
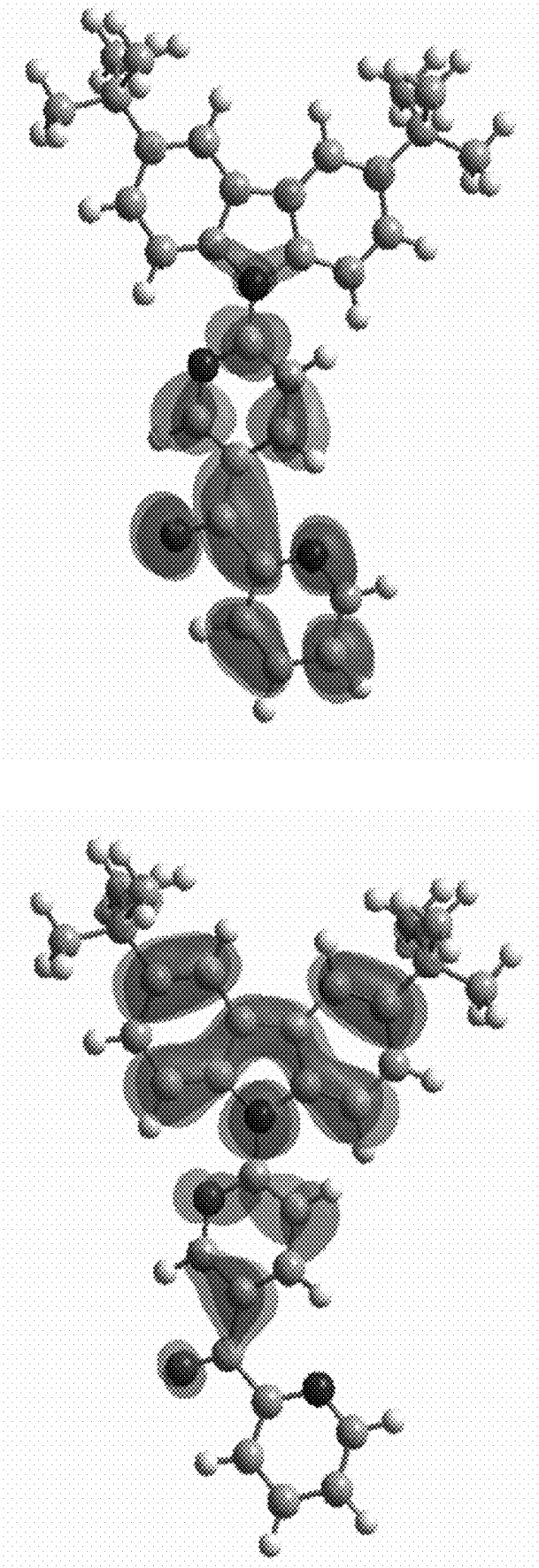


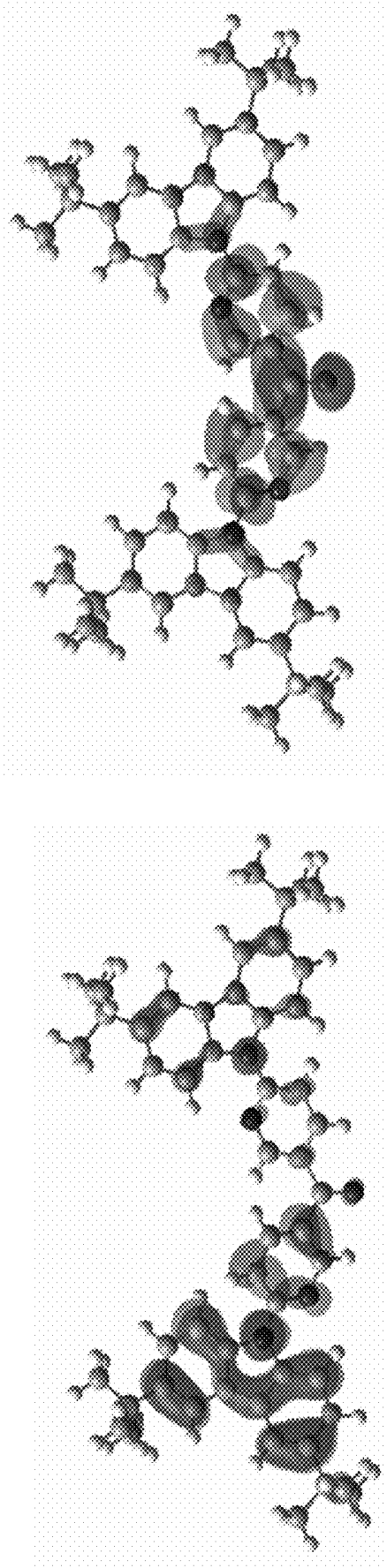
Fig. 8



LUMO

HOMO

Fig. 9



LUMO

HOMO

Fig. 10

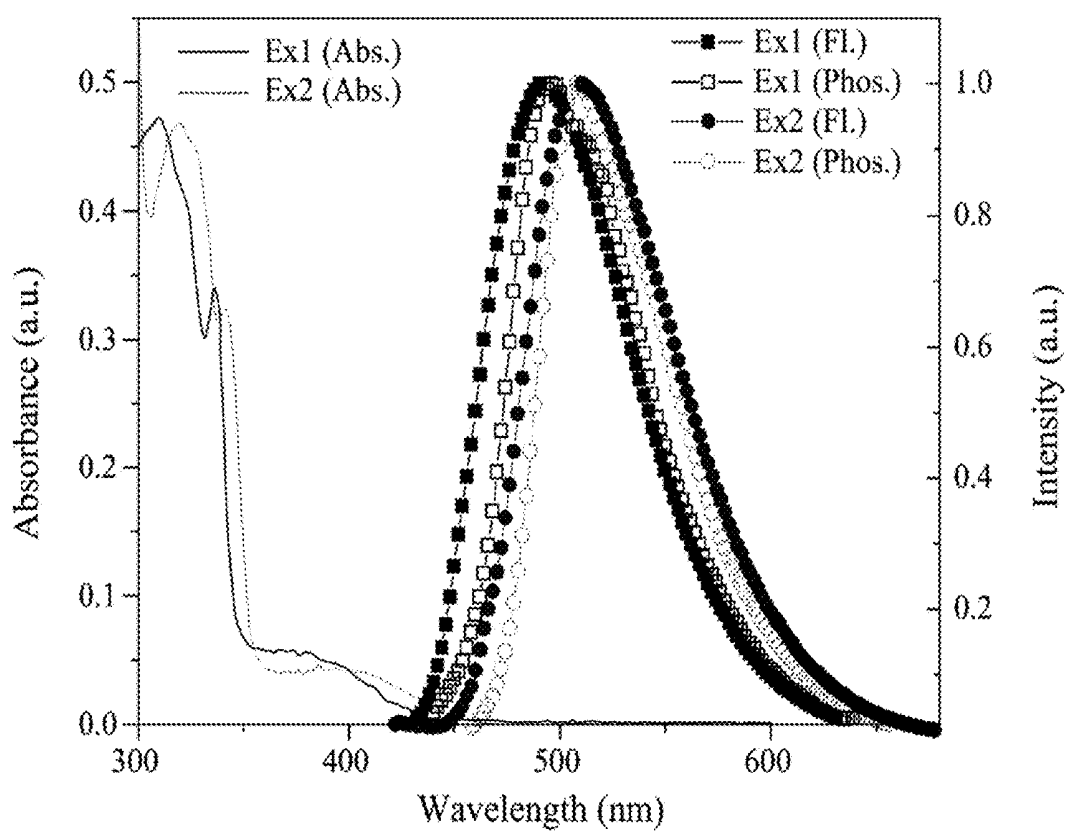


Fig. 11

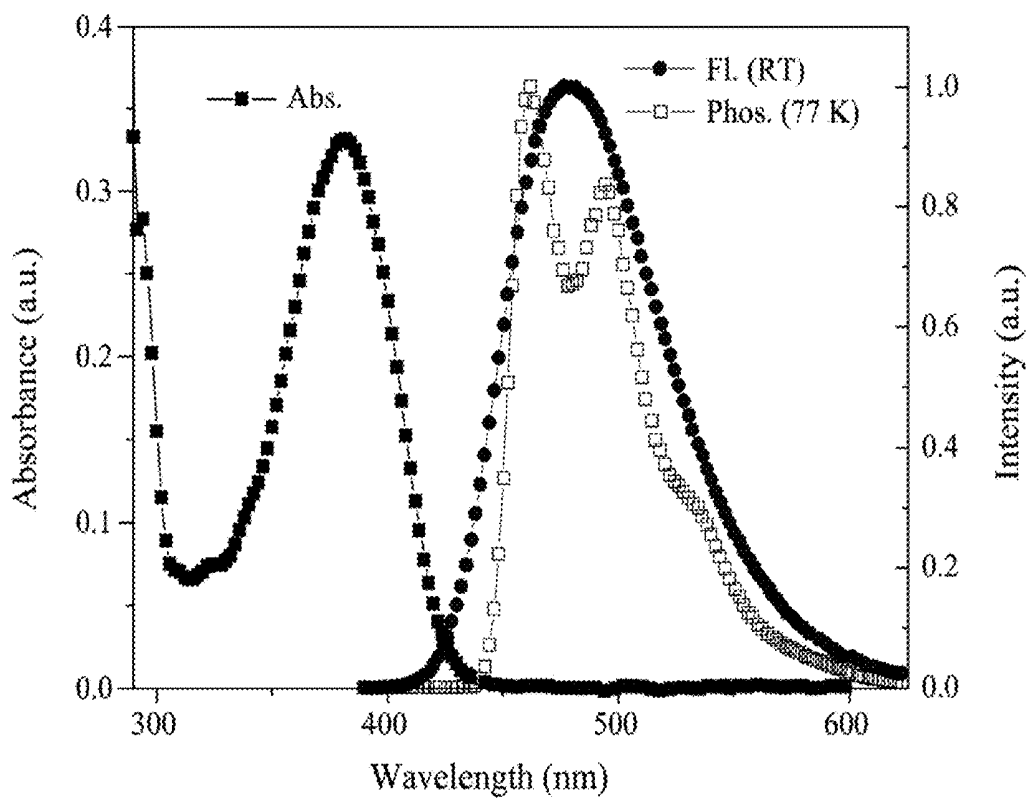


Fig. 12

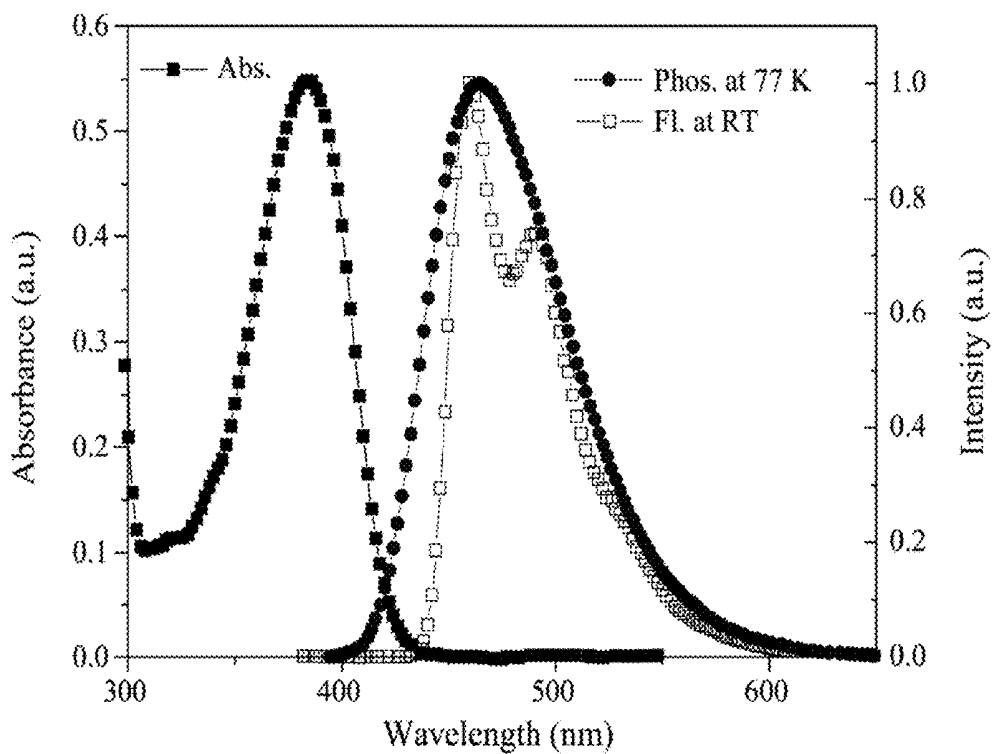


Fig. 13

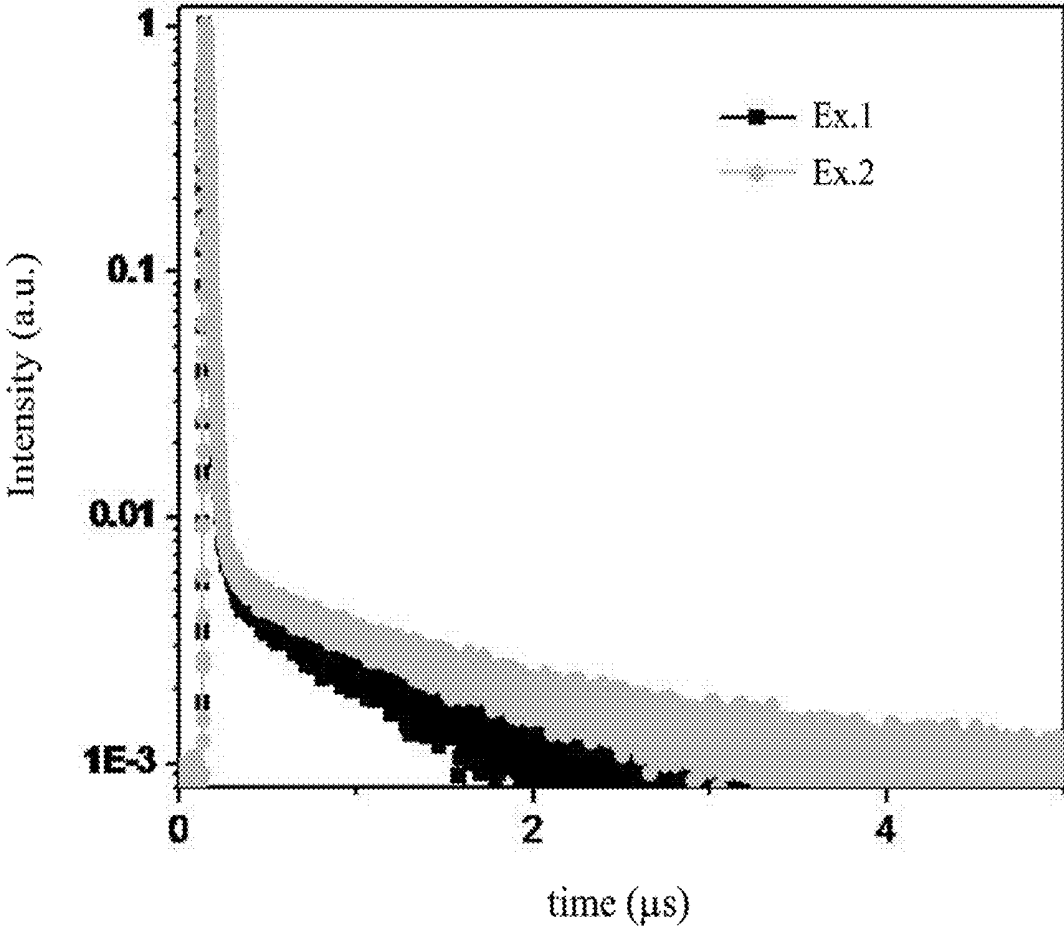


Fig. 14

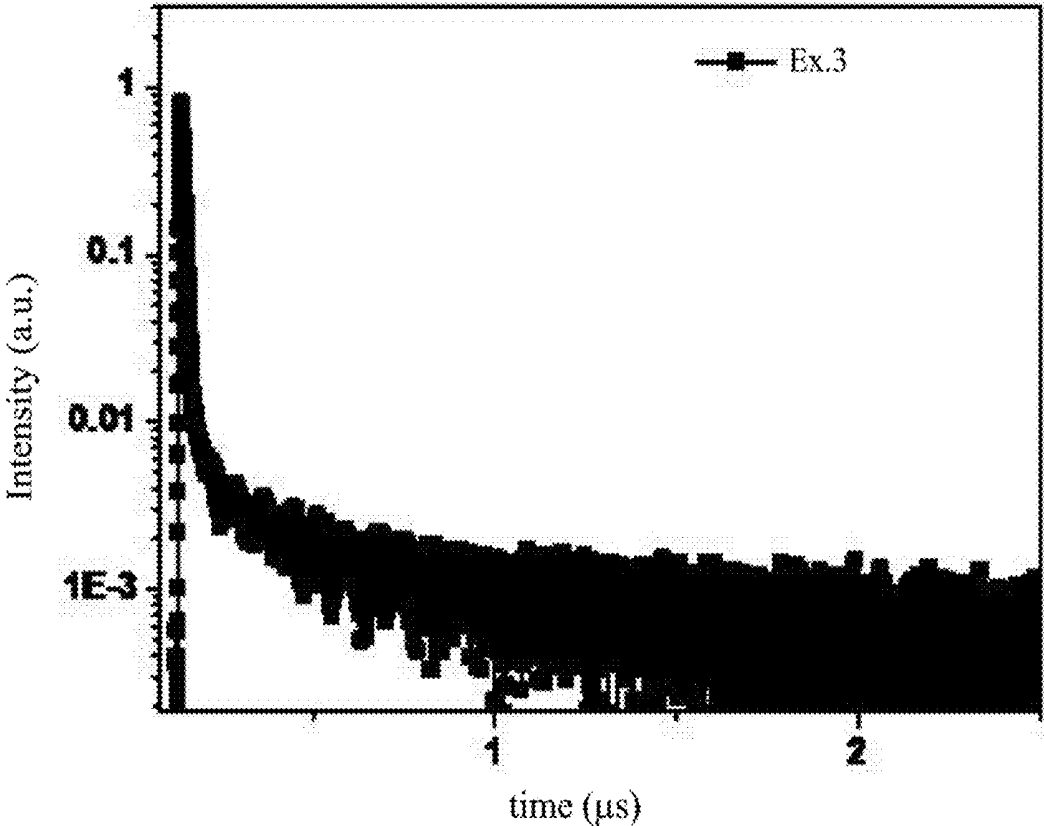


Fig. 15

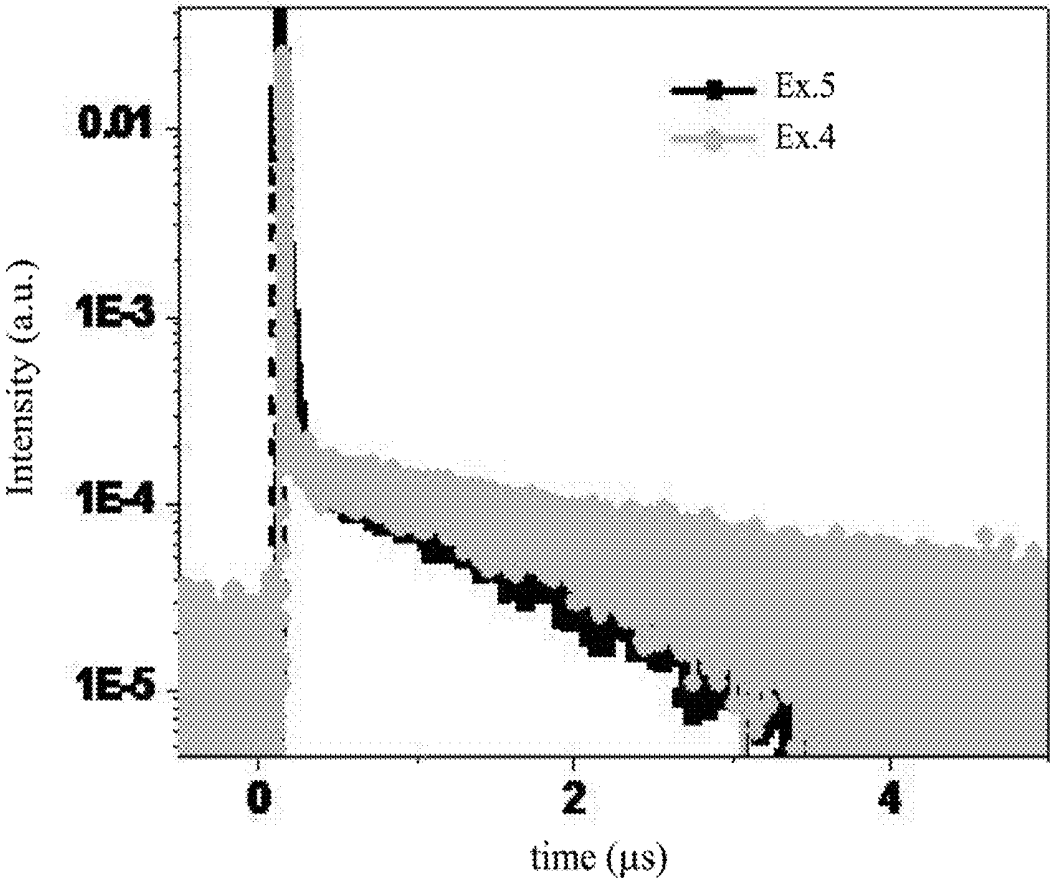


Fig. 16

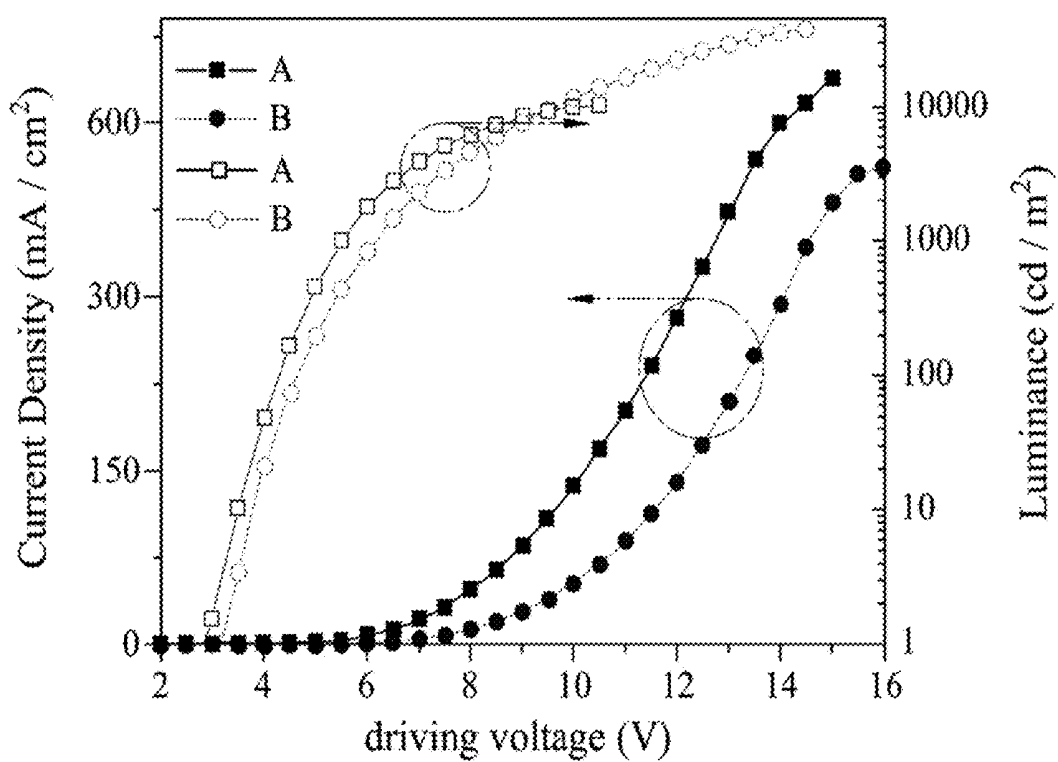


Fig. 17

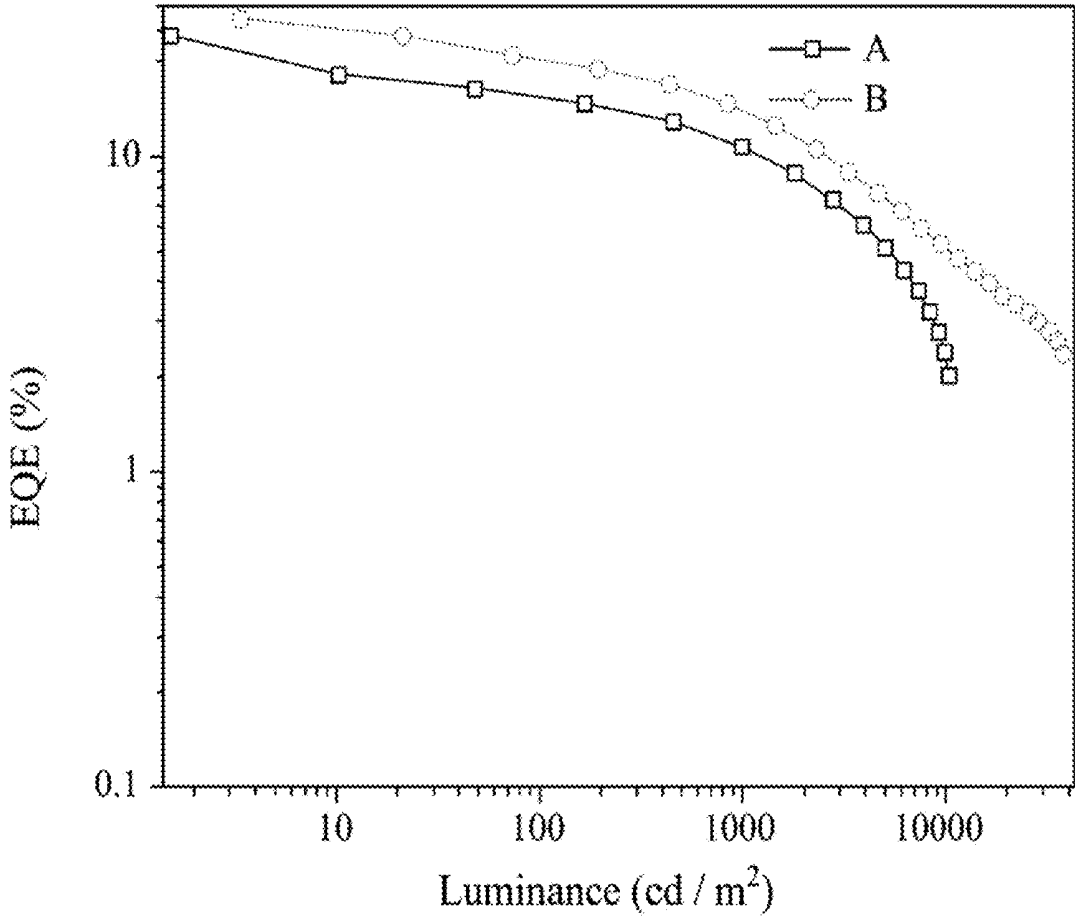


Fig. 18

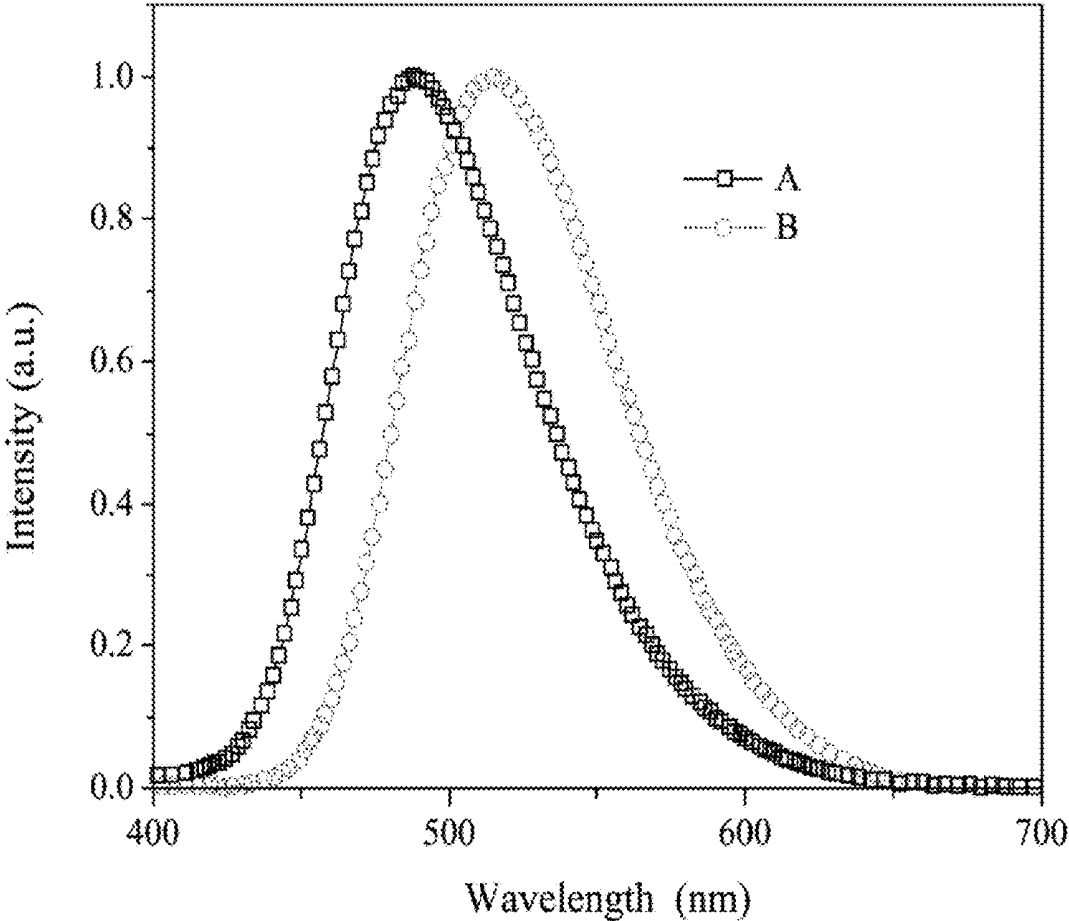


Fig. 19

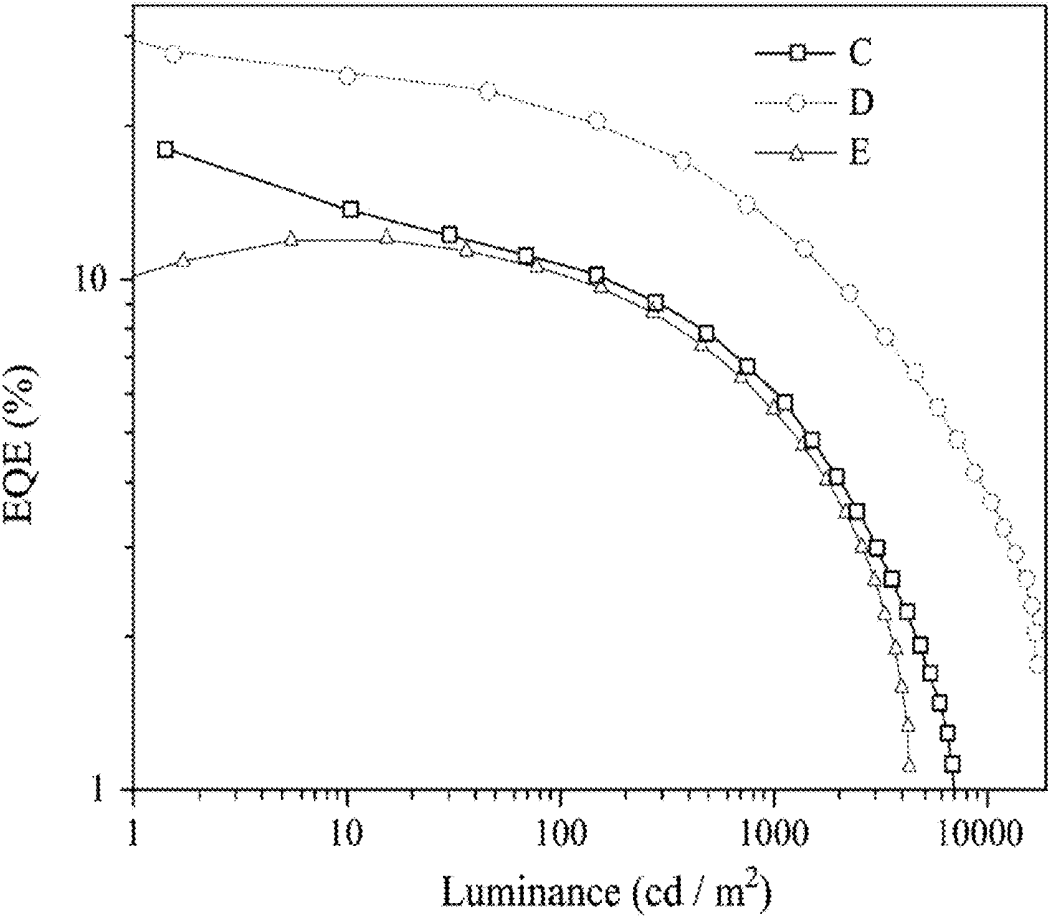


Fig. 20

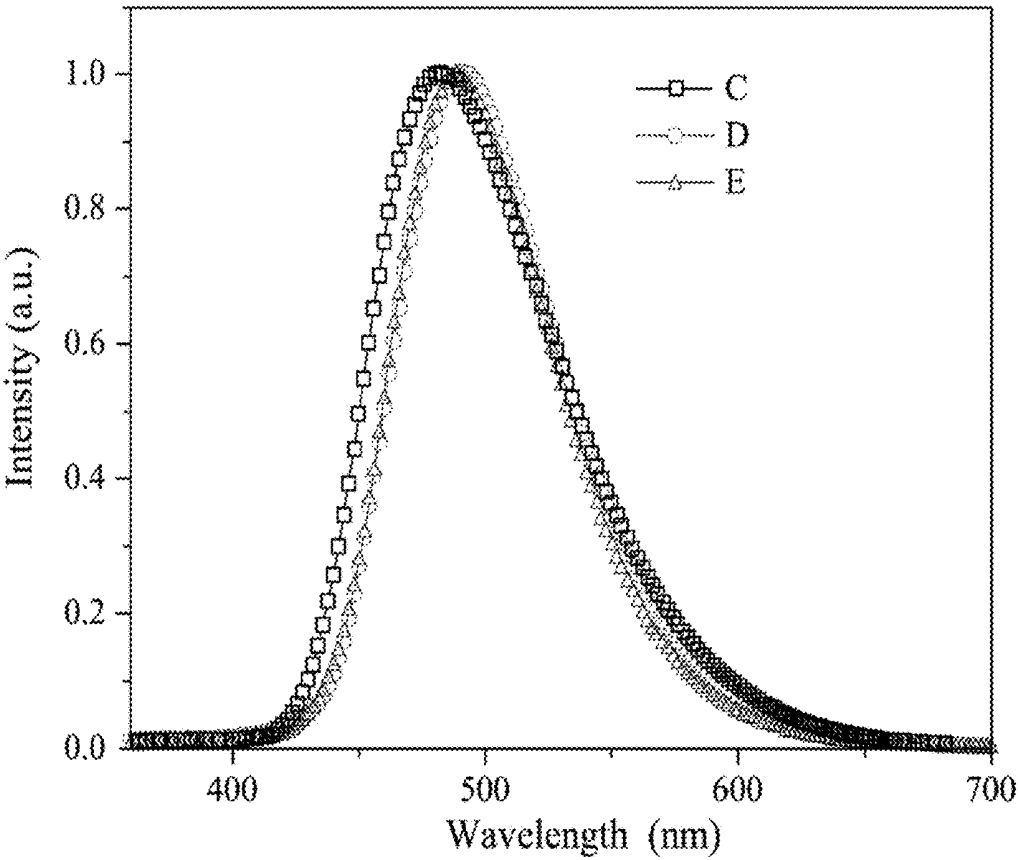


Fig. 21

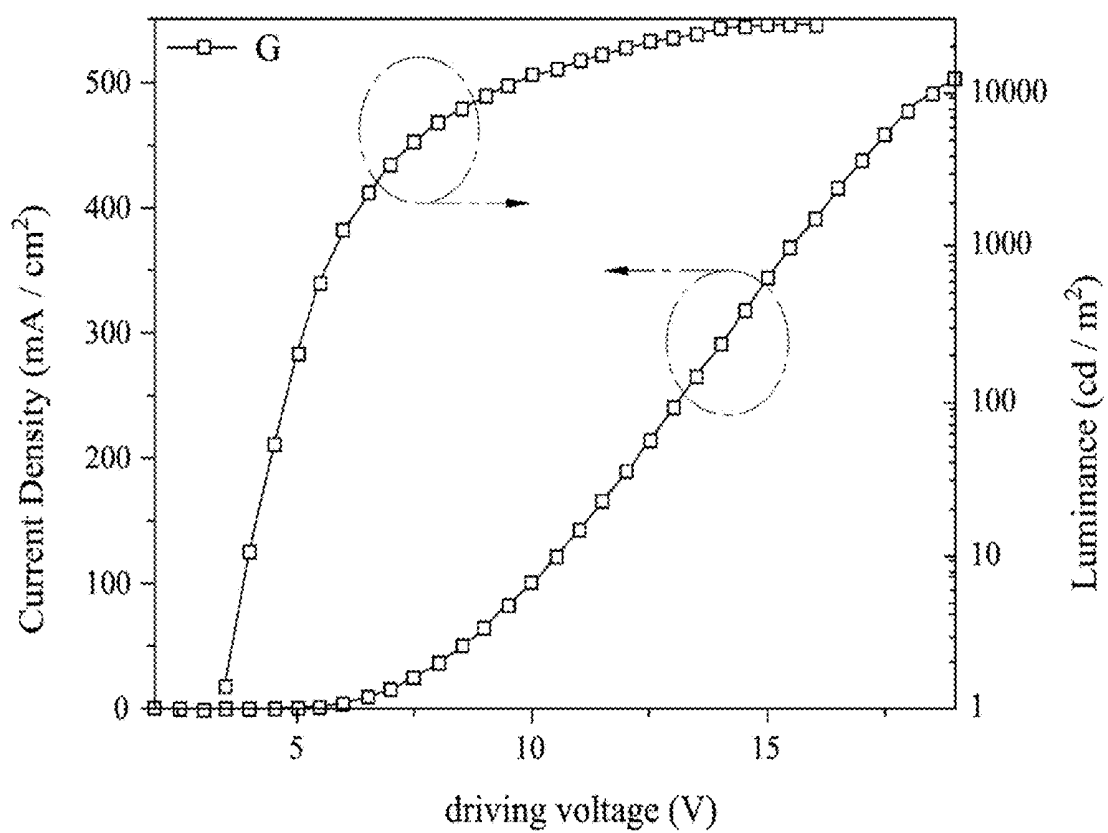


Fig. 22

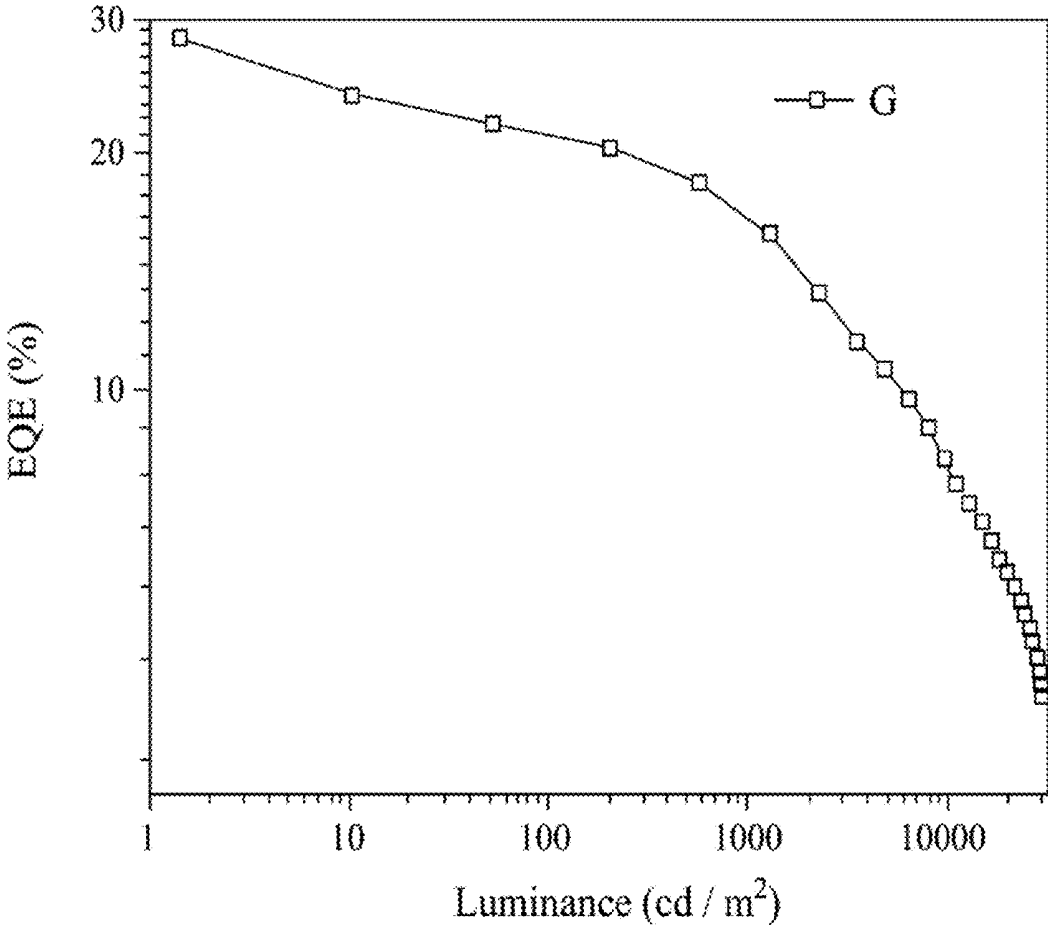


Fig. 23

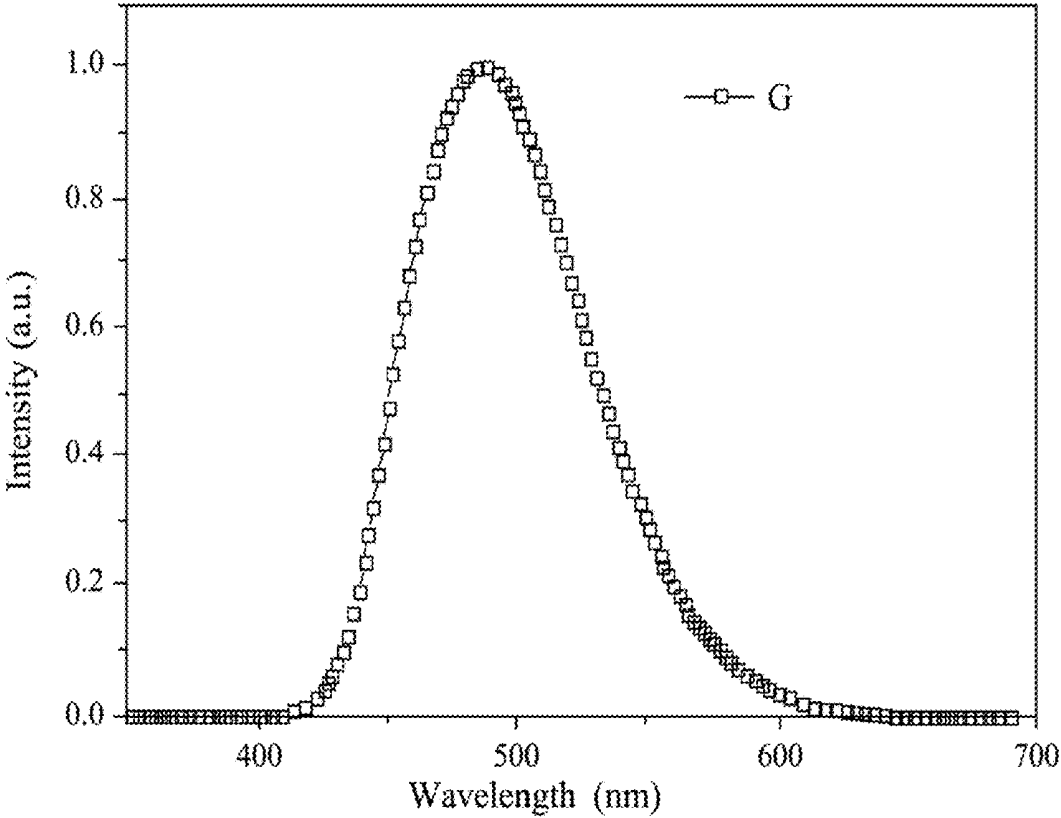


Fig. 24

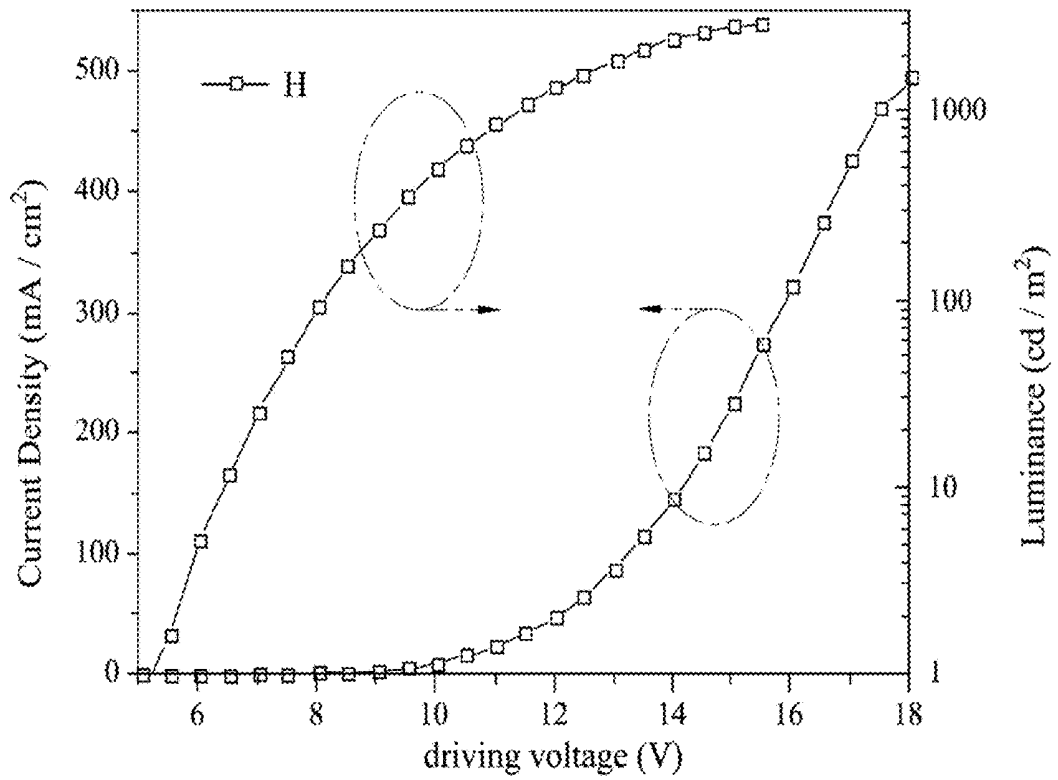


Fig. 25

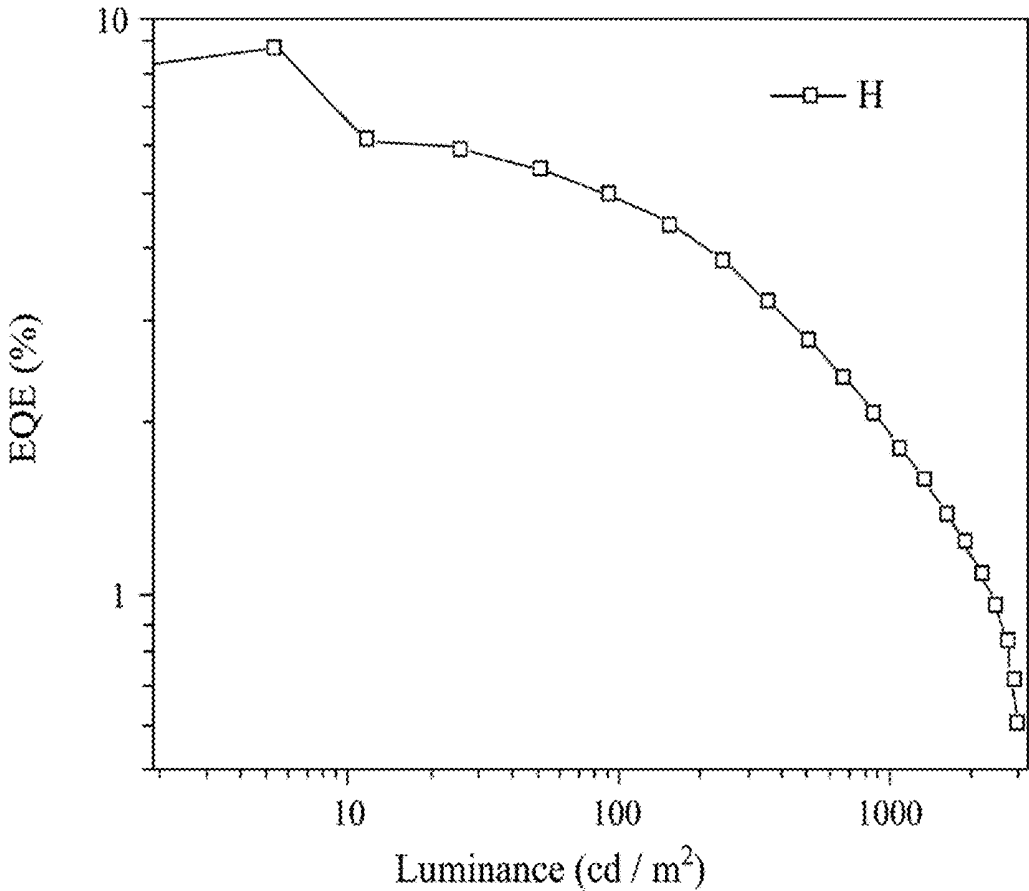


Fig. 26

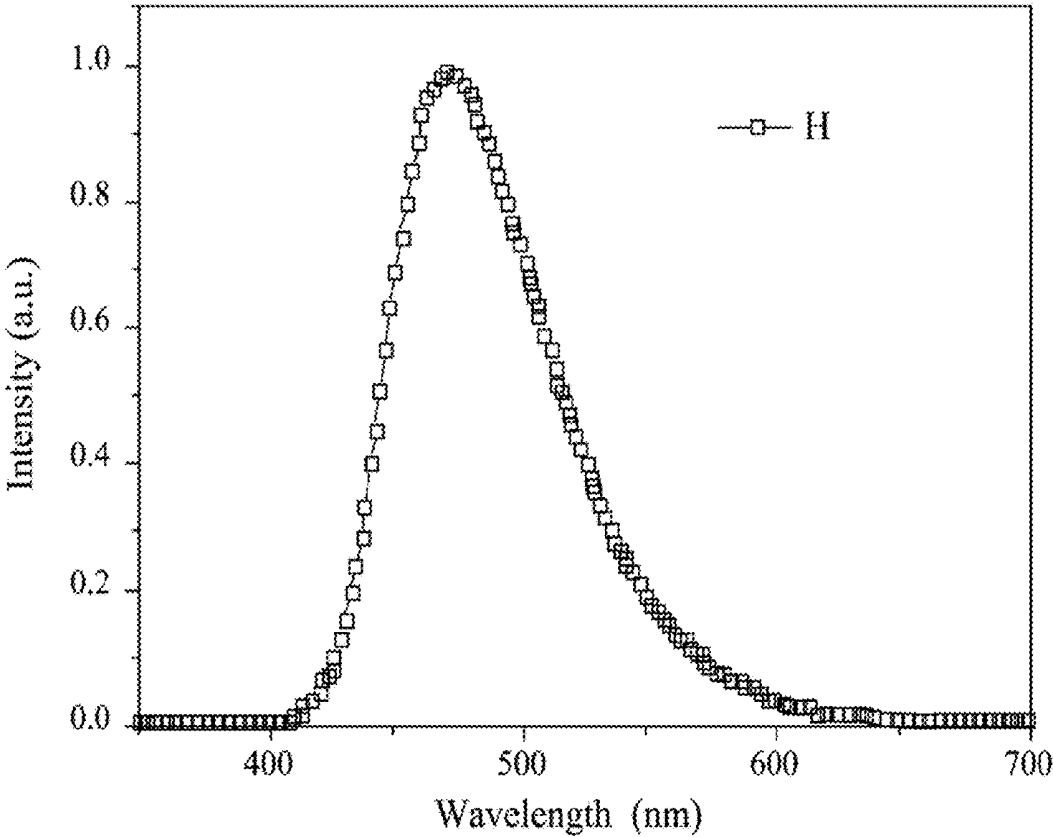


Fig. 27

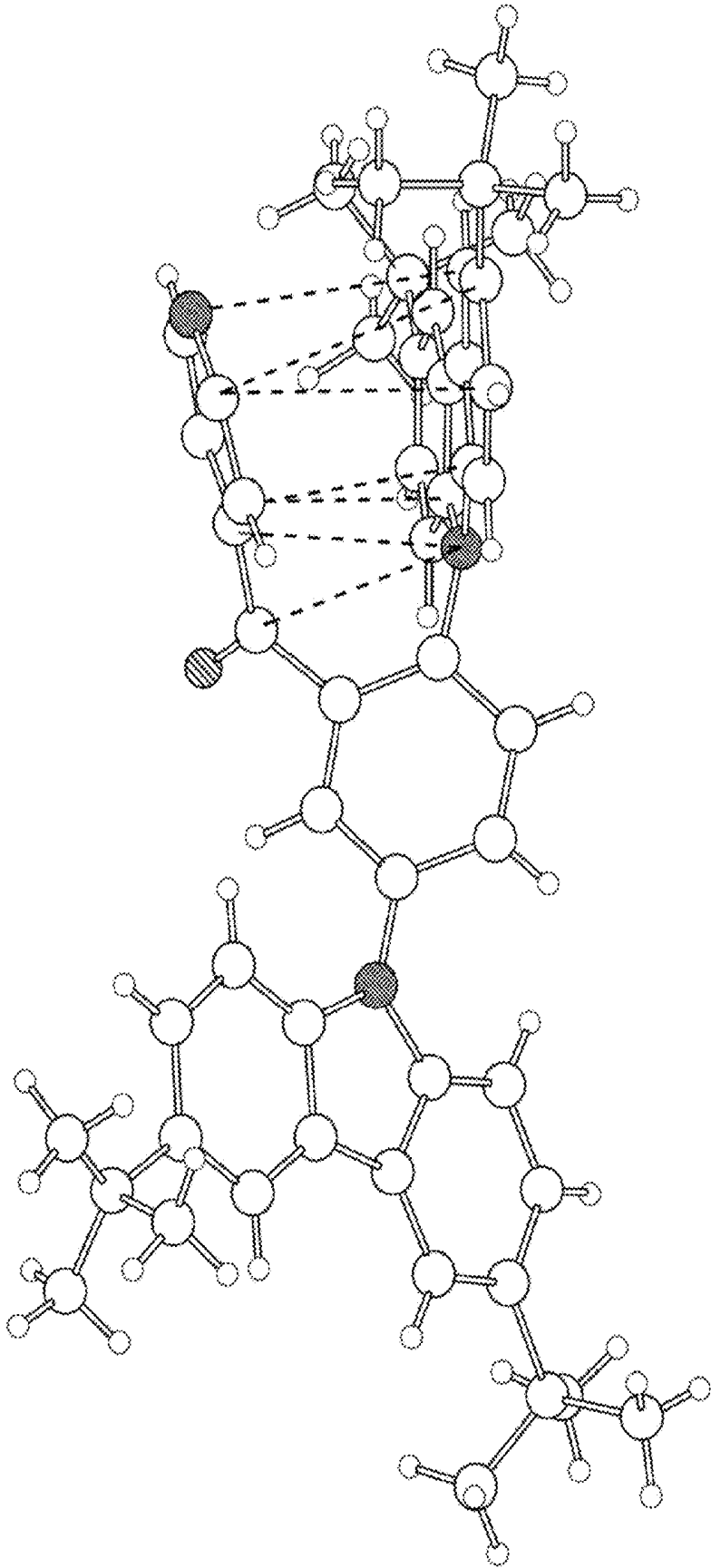


Fig. 28

**COMPOUND, EMITTING LAYER OF
ORGANIC LIGHT EMITTING DIODE AND
ORGANIC LIGHT EMITTING DIODE
DEVICE**

RELATED APPLICATIONS

[0001] This application claims priority to Taiwan Application Serial Number 105113100, filed Apr. 27, 2016, which is herein incorporated by reference.

BACKGROUND

Technical Field

[0002] The present disclosure relates to a compound, an emitting layer of an organic light emitting diode (OLED) and an OLED device. More particularly, the present disclosure relates to a compound can be used as a dopant of an emitting layer of an OLED, and an emitting layer of an OLED and an OLED device having the same.

DESCRIPTION OF RELATED ART

[0003] An OLED refers to a component having an emitting layer made of organic molecules, which can emit light in response to a driving voltage. Comparing to a liquid crystal display, the OLED has advantages of lighter weight, wider view angle, higher contrast ratio, lower power consumption, faster response times, high luminous efficiency, facile color tuning of emitters, access to flexible panels. Accordingly, the OLED draws lots of attention from the relevant industry.

[0004] The earliest OLED adopts fluorescence materials, in which excitons can transition from a singlet excited state to a singlet ground state and release energy in the form of fluorescence. However, the internal quantum efficiency (IQE) of fluorescence materials can only reach to 25%, and the rest of 75% is lost in the non-radiative form of heat. Accordingly, the efficiency of the fluorescence material is poor.

[0005] Then the OLED adopting phosphorescence materials is provided, in which noble metals, such as Ir, Pt, Os and Ru, are introduced into the emitting layer to form complexes with organic molecules so as to generate the effect of spin-orbital coupling. As a result, the fluorescence generated from the transition from the singlet excited state to the singlet ground state and the phosphorescence generated from the transition from a triplet excited state to the singlet ground state can be obtained at the same time, so that the IQE of phosphorescence materials can reach to 100%. Introducing the noble metals into the emitting layer increases the efficiency of the OLED significantly. However, the noble metals are expensive, so that the cost of the phosphorescence materials remains stubbornly high. Furthermore, blue OLEDs still cannot be manufactured with the phosphorescence materials.

[0006] Thermal activated delayed fluorescence (TADF) materials are the third generation organic light emitting materials, which are developed after the fluorescence materials and the phosphorescence materials. The energy gap of the singlet excited state and the triplet excited state (ΔE_{ST}) of the TADF materials is small, which allows excitons to transition from the triplet excited state to the singlet excited state through reverse intersystem crossing (RISC). Therefore, the TADF materials can take advantage of the excitons

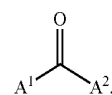
in singlet excited state and triplet excited state releasing energy in radiative form (fluorescence and delayed fluorescence), which enables the IQE of the TADF materials to reach to 100%. The TADF materials are featured with high efficiency, low cost (due to no use of noble metals) and can provide a wide light color tenability (capable of manufacturing blue OLEDs). Accordingly, the TADF materials have received lots of attention.

[0007] However, the OLEDs made of the TADF materials are hardly to provide an external quantum efficiency (EQE) comparable to that of the phosphorescence materials. Researches show that the molecular structure of the TADF material is critical to the performance of the OLEDs. For example, it is realized that in molecules with a small overlap between their highest occupied molecular orbital (HOMO) bearing electron donating groups and lowest unoccupied molecular orbital (LUMO) bearing electron accepting groups can increase the TADF property. Furthermore, by increasing the twist angle between a plane of the electron donating group and a plane of the electron accepting group can lower the ΔE_{ST} , which can increase the probability of RISC. However, an excessive twist angle may inhibit the radiative decay of the transition from the singlet excited state to the singlet ground state, which reduces the luminous efficiency.

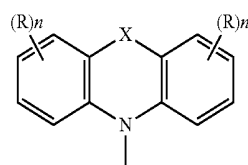
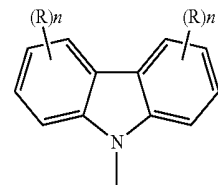
[0008] To sum up, how to improve the molecular structure of the TADF materials, in which the electron donating groups and the electron accepting groups are properly arranged, so as to provide the OLEDs with excellent efficiency is the goal of the relevant industry and academia.

SUMMARY

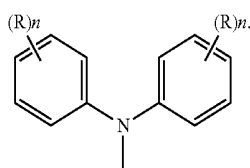
[0009] According to one aspect of the present disclosure, a compound includes a structure of Formula (I):



[0010] In Formula (I), A^1 is a pyridyl group, A^2 is a phenyl group or a pyridyl group, and hydrogens of the A^1 are both unsubstituted or substituted by a structure of Formula (i), Formula (ii) or Formula (iii), and at least one of hydrogens of the A^2 is substituted by the structure of Formula (i), Formula (ii) or Formula (iii):



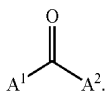
-continued



(iii)

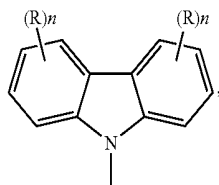
[0011] In Formula (i) to Formula (iii), n is independently an integer of 0 to 4, R is independently a monovalent group having 1 to 60 carbon atoms, X is $-\text{NR}^{14}-$, $-\text{S}-$ or $-\text{CR}^{15}\text{R}^{16}-$, and R^{14} , R^{15} and R^{16} are independently $-\text{H}$, an alkyl group or an aryl group.

[0012] According to another aspect of the present disclosure, an emitting layer of an OLED includes a dopant, the dopant includes a structure of Formula (I):

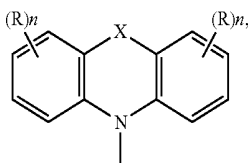


(I)

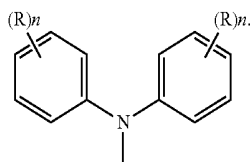
[0013] In Formula (I), A^1 is a pyridyl group, A^2 is a phenyl group or a pyridyl group, and hydrogens of the A^1 are both unsubstituted or substituted by a structure of Formula (i), Formula (ii) or Formula (iii), and at least one of hydrogens of the A^2 is substituted by the structure of Formula (i), Formula (ii) or Formula (iii):



(i)



(ii)



(iii)

[0014] In Formula (i) to Formula (iii), n is independently an integer of 0 to 4, R is independently a monovalent group having 1 to 60 carbon atoms, X is $-\text{NR}^{14}-$, $-\text{S}-$ or $-\text{CR}^{15}\text{R}^{16}-$, and R^{14} , R^{15} and R^{16} are independently $-\text{H}$, an alkyl group or an aryl group.

[0015] According to yet another aspect of the present disclosure, an OLED device includes the aforementioned emitting layer of the OLED.

BRIEF DESCRIPTION OF THE DRAWINGS

[0016] The present disclosure can be more fully understood by reading the following detailed description of the embodiment, with reference made to the accompanying drawings as follows:

[0017] FIG. 1 is a schematic cross-sectional view illustrating an emitting layer of an OLED according to one embodiment of the present disclosure;

[0018] FIG. 2 is a schematic cross-sectional view illustrating an OLED device according to another embodiment of the present disclosure;

[0019] FIG. 3 is a schematic cross-sectional view illustrating an OLED device according to yet another embodiment of the present disclosure;

[0020] FIG. 4 shows molecular orbitals of Example 1 (Ex. 1);

[0021] FIG. 5 shows molecular orbitals of Example 2 (Ex. 2);

[0022] FIG. 6 shows molecular orbitals of Example 3 (Ex. 3);

[0023] FIG. 7 shows molecular orbitals of Example 4 (Ex. 4);

[0024] FIG. 8 shows molecular orbitals of Example 5 (Ex. 5);

[0025] FIG. 9 shows molecular orbitals of Example 6 (Ex. 6);

[0026] FIG. 10 shows molecular orbitals of Example 7 (Ex. 7);

[0027] FIG. 11 shows absorption (Abs.) spectra, fluorescence (Fl.) spectra and phosphorescence (Phos.) spectra of Ex. 1 and Ex. 2;

[0028] FIG. 12 shows an Abs. spectrum, a Fl. spectrum and a Phos. spectrum of Ex. 6;

[0029] FIG. 13 shows an Abs. spectrum, a Fl. spectrum and a Phos. spectrum of Ex. 7;

[0030] FIG. 14 is a diagram showing transient photoluminescence characteristics of Ex. 1 and Ex. 2;

[0031] FIG. 15 is a diagram showing transient photoluminescence characteristics of Ex. 3;

[0032] FIG. 16 is a diagram showing transient photoluminescence characteristics of Ex. 4 and Ex. 5;

[0033] FIG. 17 shows relationships of current density, luminance and driving voltage of an OLED device A and an OLED device B;

[0034] FIG. 18 shows relationships of EQE and luminance of the OLED device A and the OLED device B;

[0035] FIG. 19 shows photoluminescence spectra of the OLED device A and the OLED device B;

[0036] FIG. 20 shows relationships of EQE and luminance of an OLED device C, an OLED device D and an OLED device E;

[0037] FIG. 21 shows photoluminescence spectra of the OLED device C, the OLED device D and the OLED device E;

[0038] FIG. 22 shows relationships of current density, luminance and driving voltage of an OLED device G;

[0039] FIG. 23 shows a relationship of EQE and luminance of the OLED device G;

[0040] FIG. 24 shows photoluminescence spectrum of the OLED device G;

[0041] FIG. 25 shows relationships of current density, luminance and driving voltage of an OLED device H;

[0042] FIG. 26 shows a relationship of EQE and luminance of the OLED device H;

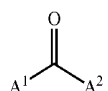
[0043] FIG. 27 shows photoluminescence spectrum of the OLED device H; and

[0044] FIG. 28 shows a single-crystal X-ray diffraction result of Ex. 2.

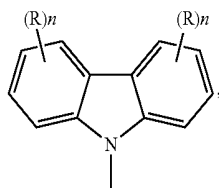
DETAILED DESCRIPTION

Compound

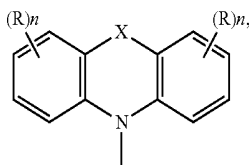
[0045] A compound includes a structure of Formula (I):



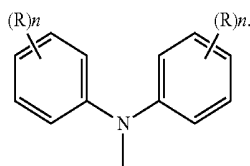
[0046] In Formula (I), A^1 is a pyridyl group, A^2 is a phenyl group or a pyridyl group, and hydrogens of the A^1 are both unsubstituted or substituted by a structure of Formula (i), Formula (ii) or Formula (iii), and at least one of hydrogens of the A^2 is substituted by the structure of Formula (i), Formula (ii) or Formula (iii):



(i)



(ii)



(iii)

[0047] In Formula (i) to Formula (iii), n is independently an integer of 0 to 4, R is independently a monovalent group having 1 to 60 carbon atoms, X is $-\text{NR}^{14}-$, $-\text{S}-$ or $-\text{CR}^{15}\text{R}^{16}-$, and R^{14} , R^{15} and R^{16} are independently $-\text{H}$, an alkyl group or an aryl group.

[0048] For the sake of conciseness, “the compound including the structure of Formula (I)” is also written as “the compound (I)” in the present disclosure.

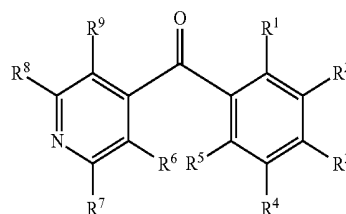
[0049] With the combination of a main body of the pyridyl group of the A^1 , the ketone group and a main body of the phenyl group/pyridyl group of the A^2 being electron accepting group, and the structure of Formula (i), Formula (ii) or Formula (iii) being electron donating group, the compound (I) is featured with TADF property. When the compound (I) is driven by a voltage, the compound (I) can release energy in the form of fluorescence and delayed fluorescence. Therefore, it is favorable to use the compound (I) as a dopant in

an emitting layer of an OLED, which provides the OLED with advantages of high efficiency, low cost and capable of providing a wide light color tenability.

[0050] The aforementioned “main body of the pyridyl group” refers to the cyclic structure encircled by the carbon atoms and the nitrogen atom, but not including the hydrogen atoms or other substituents connecting with the carbon atoms. Similarly, the aforementioned “main body of the phenyl group” refers to the cyclic structure encircled by the carbon atoms, but not including the hydrogen atoms or other substituents connecting with the carbon atoms.

[0051] Specifically, R can be a straight-chain or branched aliphatic group having 1 to 60 carbon atoms, a cyclic aliphatic group having 1 to 60 carbon atoms, an aryl group having 1 to 60 carbon atoms or a heterocyclic group having 1 to 60 carbon atoms. Preferably, R is a group which can enhance the electron donating ability of the structure of Formula (i), Formula (ii) or Formula (iii). More specifically, R can be a methyl group, an ethyl group, a t -butyl group or a carbazole group.

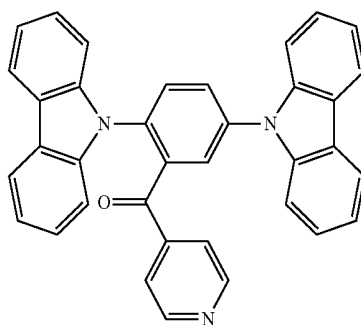
[0052] The compound (I) can include a structure of Formula (I-1):



(I-1)

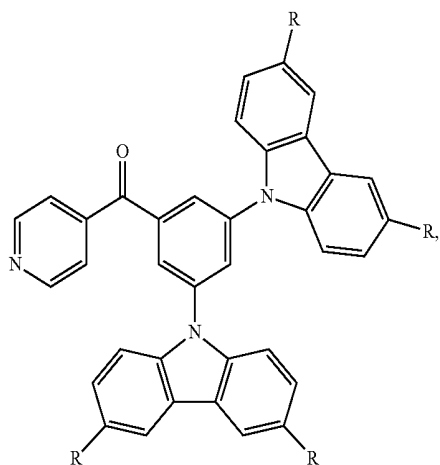
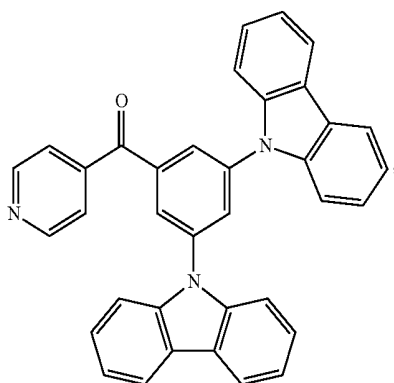
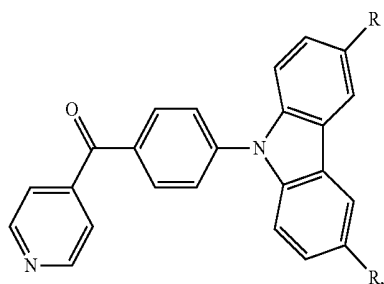
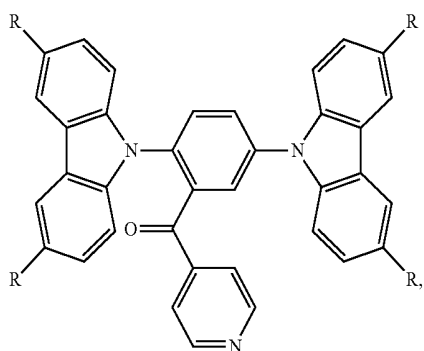
[0053] In Formula (I-1), R^1 , R^2 , R^3 , R^4 and R^5 are independently $-\text{H}$, the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), at least one of the R^1 , R^2 , R^3 , R^4 and R^5 is the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), and R^6 , R^7 , R^8 and R^9 can independently be an electron withdrawing group, an electron donating group or $-\text{H}$. The electron withdrawing group can be but is not limited to $-\text{CN}$ or $-\text{F}$. The electron donating group can be but is not limited to the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii). For example, the electron donating group can be a carbazole group or a diphenyl amine group.

[0054] Examples of the structure of Formula (I-1) can be but are not limited to structures of Formula (I-1-1) to Formula (I-1-7):

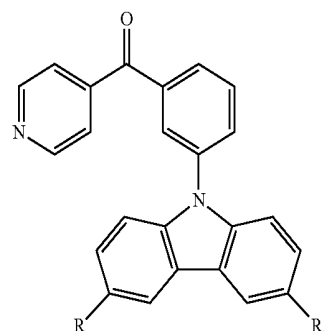
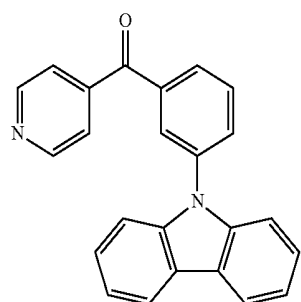


(I-1-1)

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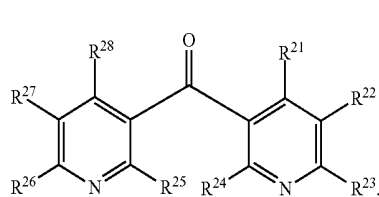


-continued



[0055] In Formula (I-1), when R^2 , R^3 and R^5 are —H, R^1 and R^4 are the structure of Formula (i), $n=0$, and R^6 , R^7 , R^8 and R^9 are —H, the structure of Formula (I-1-1) can be obtained. In Formula (I-1), when R^2 , R^3 and R^5 are —H, R^1 and R^4 are the structure of Formula (i), $n=1$, and R^6 , R^7 , R^8 and R^9 are —H, the structure of Formula (I-1-2) can be obtained. In Formula (I-1), when R^1 , R^2 , R^4 and R^5 are —H, R^3 is the structure of Formula (i), $n=1$, and R^6 , R^7 , R^8 and R^9 are —H, the structure of Formula (I-1-3) can be obtained. In Formula (I-1), when R^1 , R^3 and R^5 are —H, R^2 and R^4 are the structure of Formula (i), $n=0$, and R^6 , R^7 , R^8 and R^9 are —H, the structure of Formula (I-1-4) can be obtained. In Formula (I-1), when R^1 , R^3 and R^5 are —H, R^2 and R^4 are the structure of Formula (i), $n=1$, and R^6 , R^7 , R^8 and R^9 are —H, the structure of Formula (I-1-5) can be obtained. In Formula (I-1), when R^1 , R^2 , R^3 and R^5 are —H, R^4 is the structure of Formula (i), $n=0$, and R^6 , R^7 , R^8 and R^9 are —H, the structure of Formula (I-1-6) can be obtained. In Formula (I-1), when R^1 , R^2 , R^3 and R^5 are —H, R^4 is the structure of Formula (i), $n=1$, and R^6 , R^7 , R^8 and R^9 are —H, the structure of Formula (I-1-7) can be obtained.

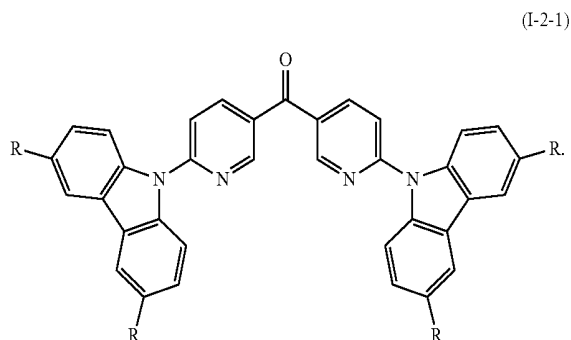
[0056] The compound (I) can include a structure of Formula (I-2):



[0057] In Formula (I-2), R^{21} , R^{22} , R^{23} , R^{24} , R^{25} , R^{26} , R^{27} and R^{28} are independently —H, the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), and at least one of the R^{21} , R^{22} , R^{23} , R^{24} , R^{25} , R^{26} , R^{27} and

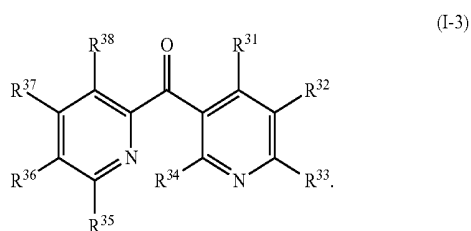
R²⁸ is the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii).

[0058] An example of the structure of Formula (I-2) can be but is not limited to a structure of Formula (I-2-1):



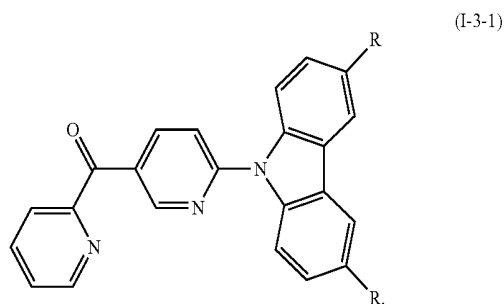
[0059] In Formula (I-2), when R²¹, R²², R²⁴, R²⁵, R²⁷ and R²⁸ are —H, R²³ and R²⁶ are the structure of Formula (i), and n=1, the structure of Formula (I-2-1) can be obtained.

[0060] The compound (I) can include a structure of Formula (I-3):



[0061] In Formula (I-3), R³¹, R³², R³³ and R³⁴ are independently —H, the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), at least one of the R³¹, R³², R³³ and R³⁴ is the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), and R³⁵, R³⁶, R³⁷ and R³⁸ are —H.

[0062] An example of the structure of Formula (I-3) can be but is not limited to a structure of Formula (I-3-1):



[0063] In Formula (I-3), when R³¹, R³² and R³⁴ are —H, R³³ is the structure of Formula (i), and n=1, the structure of Formula (I-3-1) can be obtained.

[0064] Further examples of the structures of Formula (I-1-1) to Formula (I-1-7), Formula (I-2-1) and Formula (I-3-1) can be but are not limited to the compounds listed in Table 1.

TABLE 1

Formula	R	Abbreviation of compound name
(I-1-1)		DCBPy
(I-1-2)	t-butyl group	DTCBPy
(I-1-3)	t-butyl group	pTCBPy
(I-1-3)	carbazole group	p3CzBPy
(I-1-4)		mDCBPy
(I-1-5)	t-butyl group	mDTCBPy
(I-1-6)		mCBPy
(I-1-7)	t-butyl group	mTCBPy
(I-1-7)	carbazole group	m3CzBPy
(I-2-1)	t-butyl group	3BP-pDTC
(I-3-1)	t-butyl group	3BP-pTC
(I-3-1)	carbazole group	3BP-p3C

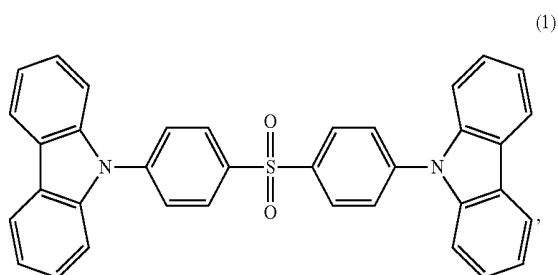
Emitting Layer of OLED

[0065] FIG. 1 is a schematic cross-sectional view illustrating an emitting layer **140** of an OLED according to one embodiment of the present disclosure. In FIG. 1, the emitting layer **140** includes a host material **141** and a dopant **142**, wherein the dopant **142** is the aforementioned compound (I). Thus, the OLED including the emitting layer **140** is featured with advantages of high efficiency, low cost and capable of providing a wide light color tenability. The details of the compound (I) have been recited previously and will not be repeated herein.

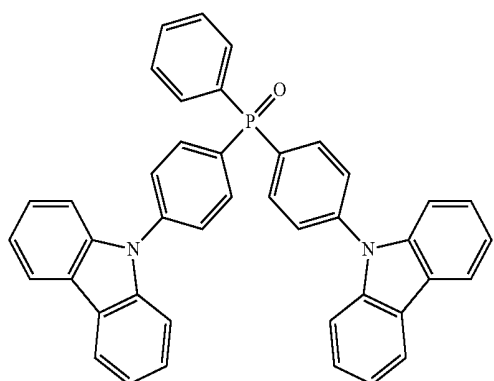
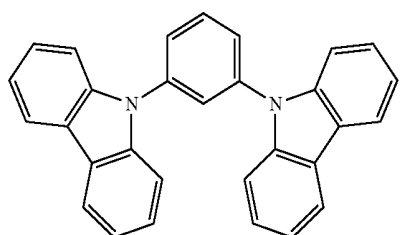
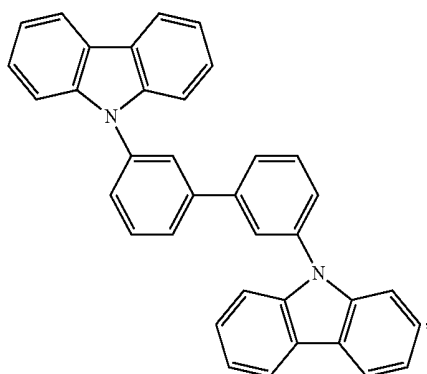
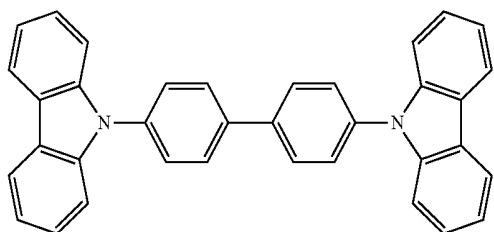
[0066] A doping concentration of the dopant **142** in the emitting layer **140** can be in a range of 5 wt % to 30 wt %.

[0067] By doping the dopant **142** in the emitting layer **140**, the energy of the host material **141** can be transferred to the dopant **142**, so that the light color and the luminous efficiency of the host material **141** can be changed, which can broaden the application of the OLED.

[0068] The host material **141** can be a high triplet energy host material, a hole transport type host material, an electron transport type host material or a bi-polar type host material. Specifically, the proper host material **141** can be decided according to actual demands. For example, the proper host material **141** can be decided according to the desired light color of the OLED. The host material **141** can include any one of structures of Formula (1) to Formula (9):

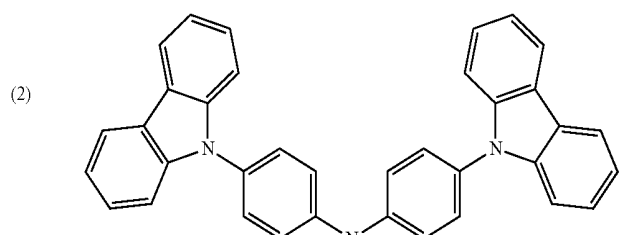


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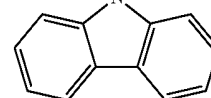
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(6)

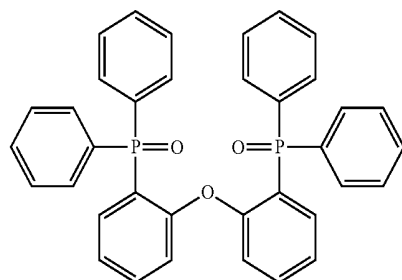


(2)

(3)

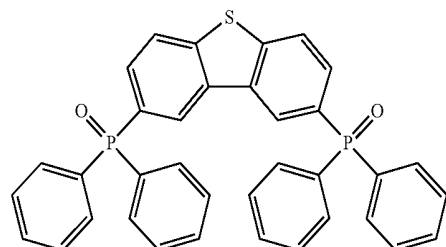


(7)



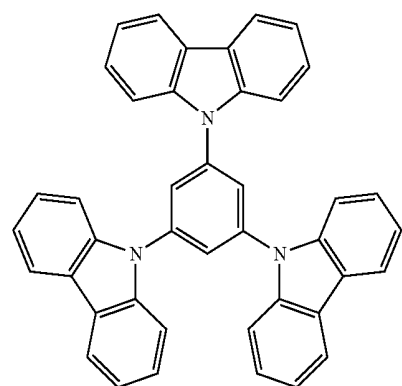
(8)

(4)



(9)

(5)



[0069] The compound name of Formula (1) is 9,9'-(sulfonylbis(4,1-phenylene))bis(9H-carbazole), and the abbreviation thereof is CzPS. The compound name of Formula (2) is 4,4'-di(9H-carbazol-9-yl)-1,1'-biphenyl, and the abbreviation thereof is CBP. The compound name of Formula (3) is 3,3'-di(9H-carbazol-9-yl)-1,1'-biphenyl, and the abbreviation thereof is mCBP. The compound name of Formula (4)

is 1,3-di(9H-carbazol-9-yl)benzene, and the abbreviation thereof is mCP. The compound name of Formula (5) is bis(4-(9H-carbazol-9-yl)phenyl)(phenyl)phosphine oxide, and the abbreviation thereof is BCPO. The compound name of Formula (6) is tris(4-(9H-carbazol-9-yl)phenyl)amine, and the abbreviation thereof is TCTA. The compound name of Formula (7) is oxybis(2,1-phenylene)bis(diphenylphosphine oxide), and the abbreviation thereof is DPEPO. The compound name of Formula (8) is dibenzo[b,d]thiophene-2,8-diylbis(diphenylphosphine oxide), and the abbreviation thereof is PPT. The compound name of Formula (9) is 1,3,5-tri(9H-carbazol-9-yl)benzene, and the abbreviation thereof is TCB. The compounds of Formula (1) and (3)-(9) can be used to manufacture blue, green or red OLEDs. The compound of Formula (2) can be used to manufacture green or red OLEDs.

OLED Device

[0070] An OLED device includes the aforementioned emitting layer of the OLED. Thus, the OLED device including the emitting layer **140** is featured with advantages of high efficiency, low cost and capable of providing a wide light color tenability.

[0071] FIG. 2 is a schematic cross-sectional view illustrating an OLED device **100** according to another embodiment of the present disclosure. In FIG. 2, the OLED device **100** includes an anode **110**, a hole-transporting layer **130**, an emitting layer **140**, an electron-transporting layer **160** and a cathode **180**. The details of the emitting layer **140** have been recited previously and will not be repeated herein.

[0072] Specifically, the anode **110** can be a transparent conductive metal oxide or metal. The transparent conductive metal oxide can be ITO (SnO₂:In₂O₃), ZnO or AZO (Al:ZnO). The metal can be Ni, Au or Pt. When the anode **110** is the metal, a thickness of the anode **110** is preferably less than 15 nm.

[0073] A thickness of the hole-transporting layer **130** can be but is not limited to 200 Å to 600 Å.

[0074] A thickness of the electron-transporting layer **160** can be but is not limited to 300 Å to 700 Å.

[0075] The cathode **180** can be but is not limited to a mixture of Mg and Ag, a mixture of LiF and Al, or Al.

[0076] The OLED device **100** can further include a substrate (not shown). The LED device **100** can be manufactured by sequentially depositing the anode **110**, the hole-transporting layer **130**, the emitting layer **140**, the electron-transporting layer **160** and the cathode **180** on the substrate. The substrate can be a transparent glass substrate or a plastic substrate.

[0077] FIG. 3 is a schematic cross-sectional view illustrating an OLED device **200** according to yet another embodiment of the present disclosure. In FIG. 3, the OLED device **200** includes an anode **210**, a hole injection layer **220**, a hole-transporting layer **230**, an emitting layer **240**, an exciton blocker **250**, an electron-transporting layer **260**, an electron injection layer **270**, and a cathode **280**.

[0078] The hole injection layer **220** is a material with a HOMO energy level which can increase the transport of holes between the anode **210** and the hole-transporting layer **230**. A thickness of the hole injection layer **220** can be but is not limited to 200 Å to 500 Å.

[0079] A thickness of the exciton blocker **250** can be but is not limited to 50 Å to 200 Å.

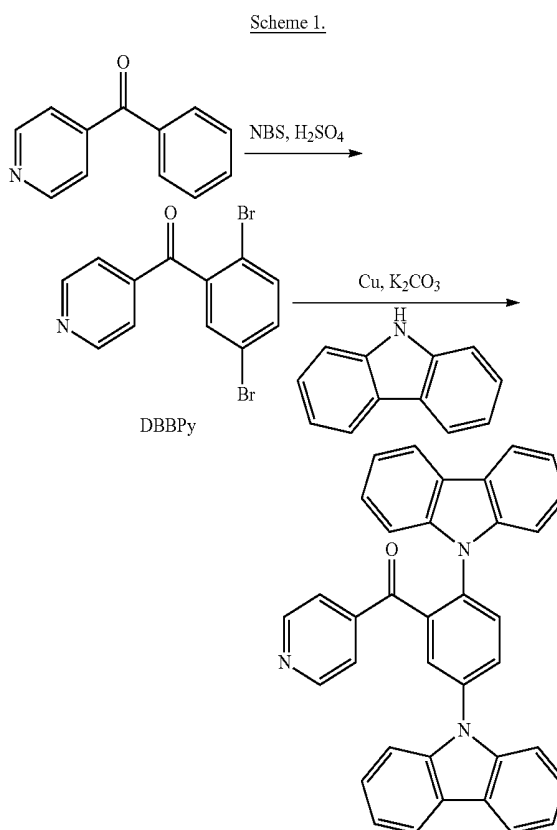
[0080] A thickness of the electron injection layer **270** can be but is not limited to 7 Å to 15 Å.

[0081] The other details of the OLED device **200** can be the same as that of the OLED device **100** in FIG. 2, and will not be repeated herein.

Synthesis of Examples and Comparative Examples

Ex. 1: DCBPy

[0082] The structure of DCBPy can refer to Formula (I-1-1). DCBPy can be synthesized according to Scheme 1:



[0083] In Scheme 1, DCBPy is synthesized by two steps, the first step and the second step.

[0084] In the first step, (2,5-dibromophenyl)(pyridine-4-yl)methanone (DBBPY) is synthesized as follows. To a stirred solution of 4-benzoylpyridine (6.00 g, 32.8 mmol) in conc. H₂SO₄ (20 mL) at 60° C., N-bromosuccinimide (NBS) (14.0 g, 78.7 mmol) was added in four portions with 5 min interval. Then, the reaction was continued for 4 hours at the same temperature and the solution was poured into crushed ice slowly, followed by basification with Na₂CO₃. The solution was extracted with EtOAc twice (2×100 ml) and the combined organic layer was washed with water. The solvent was evaporated under reduced pressure and then purified by a silica gel column (hexane/ethyl acetate (1:5)) to afford the compound DBBPY with 82% yield. From the results of ¹H NMR and High-resolution mass spectrometer (HRMS), it can confirm that the product of the first step is DBBPY. ¹H NMR (400 MHz, CDCl₃): δ 8.83-8.80 (m, 2H), 7.57-7.55

(m, 2H), 7.51-7.50 (m, 2H), 7.47 (d, $J=1.4$ Hz, 1H). HRMS (EI, m/z): $[M^+]$ cal for $C_{12}H_7Br_2NO$ 338.8894, found 338.8891.

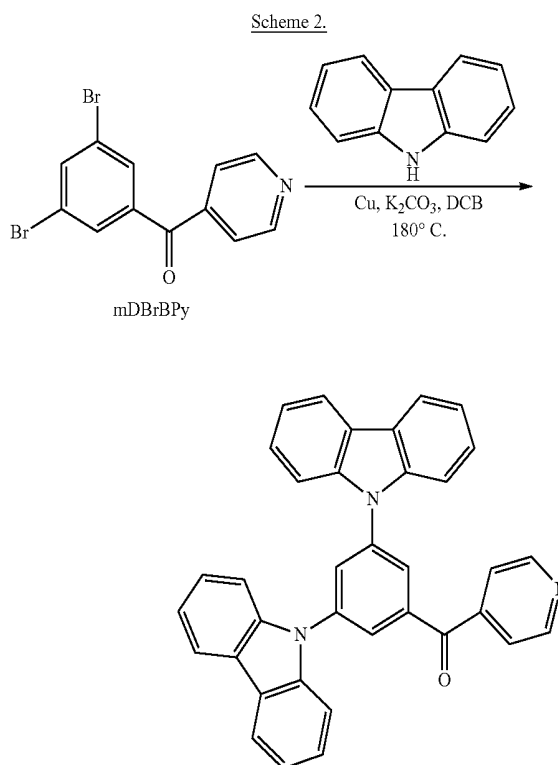
[0085] In the second step, DCBPy is synthesized as follows. To an oven-dried seal tube DBBPY (2.50 g, 7.33 mmol), carbazole (3.06 g, 18.3 mmol), Cu (0.93 g, 14.7 mmol), K_2CO_3 (5.06 g, 36.7 mmol) and 1,2-dichlorobenzene (20 ml) was added. The system was evacuated and purged with nitrogen three times and the mixture was heated and stirred at $180^\circ C$. for 48 hours. The reaction mixture was filtered through Celite and washed with ethyl acetate (30 ml). Solvent was evaporated under reduced pressure and then purified by column chromatography (hexane/ethyl acetate (4:1)) to afford the desired yellow solid in 57% yield. The melting point (m.p.) of the product is $130^\circ C$. From the results of 1H NMR, ^{13}C NMR and HRMS, it can confirm that the product of the second step is DCBPy. 1H NMR (400 MHz, $CDCl_3$): δ 8.21 (sd, $J=2.4$ Hz, 1H), 8.19 (d, $J=7.6$ Hz, 2H), 8.09 (dd, $J=8.4$ Hz, $J=1.6$ Hz, 1H), 7.92-7.90 (m, 3H), 7.83 (d, $J=7.6$ Hz, 2H), 7.65 (d, $J=8.4$ Hz, 2H), 7.53-7.49 (m, 2H), 7.45-7.41 (m, 2H), 7.38 (m, 4H), 7.23 (t, $J=7.6$ Hz, 2H), 6.68 (dd, $J=8.4$ Hz, $J=1.6$ Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.96 (CO), 148.78 (2CH), 142.07 (C), 140.51 (2C), 140.21 (2C), 138.07 (C), 137.21 (C), 134.82 (C), 131.47 (CH), 130.46 (CH), 129.31 (CH), 126.35 (2CH), 126.16 (2CH), 123.84 (2C), 123.19 (2C), 120.81 (2CH), 120.77 (2CH), 120.60 (2CH), 120.38 (2CH), 119.90 (2CH), 109.53 (4 CH); HRMS (EI, m/z): $[M^+]$ cal for $C_{36}H_{23}N_3O$ 513.1841, found 513.1837.

Ex. 2: DTCBPy

[0086] The structure of DTCBPy can refer to Formula (I-1-2), wherein R is a t-butyl group. The synthesis of DTCBPy is similar to that of Ex. 1, but replace the carbazole (3.06 g, 18.3 mmol) in the second step with 3,6-di-t-butyl-9H-carbazole (5.11 g, 18.3 mmol), so that a yellow solid in 61% yield can be obtained. The m.p. of the product is $306^\circ C$. From the results of 1H NMR, ^{13}C NMR and HRMS, it can confirm that the product is DTCBPy. 1H NMR (400 MHz, $CDCl_3$): δ 8.17 (s, 3H), 8.06 (dd, $J=8.4$ Hz, $J=2.4$ Hz, 1H), 7.88 (s, 1H), 7.87-7.85 (m, 2H), 7.81-7.80 (m, 2H), 7.59-7.53 (m, 4H), 7.47 (dd, $J=8.8$ Hz, $J=2.0$ Hz, 2H), 7.25 (d, $J=8.8$ Hz, 2H), 6.65-6.63 (m, 2H), 1.49 (s, 18H), 1.44 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.95 (CO), 148.63 (2CH), 143.84 (2C), 143.79 (2C), 142.03 (C), 139.22 (2C), 138.67 (2C), 138.23 (C), 136.59 (C), 135.01 (C), 130.95 (CH), 130.13 (CH), 128.97 (CH), 123.98 (2CH), 123.89 (2C), 123.76 (2CH), 123.38 (2C), 119.92 (2CH), 116.53 (2CH), 116.36 (2CH), 109.07 (4 CH), 34.79 (2C), 34.73 (2C), 31.97 (6 CH_3), 31.95 (6 CH_3). HRMS (EI, m/z): $[M^+]$ cal for $C_{52}H_{55}N_3O$ 737.4345, found 737.4338.

Ex. 3: mDCBPy

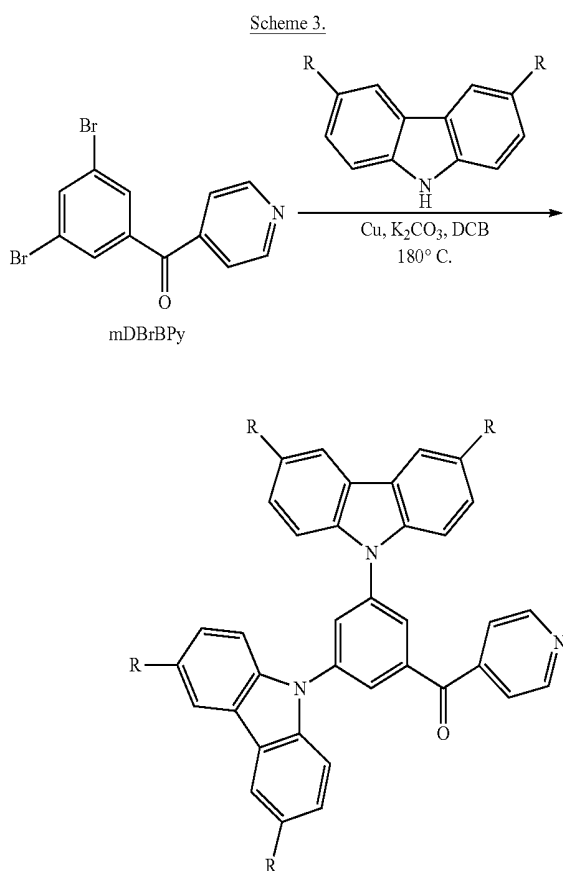
[0087] The structure of mDCBPy can refer to Formula (I-1-4). mDCBPy can be synthesized according to Scheme 2:



[0088] mDCBPy can be synthesized as follows. To a dried seal tube (3,5-dibromophenyl)(pyridin-4-yl)methanone (mDDBrBPY) (2.5 g, 7.33 mmol), carbazole (3.06 g, 18.3 mmol), Cu (0.93 g, 14.7 mmol), K_2CO_3 (5.06 g, 36.7 mmol) and 1,2-dichlorobenzene (20 ml) were added. The reaction tube was evacuated and purged with nitrogen gas three times under stirring followed by heating at $180^\circ C$. for 48 hours. The reaction mixture was filtered through Celite and washed with ethyl acetate (30 ml). The solvent was evaporated under reduced pressure followed by column chromatography purification using EtOAc/n-hexane (1:3) as eluent afforded yellow solid in 57% yield. The m.p. of the product is $219^\circ C$. From the results of 1H NMR, ^{13}C NMR and HRMS, it can confirm that the product is mDCBPy. 1H NMR (400 MHz, $CDCl_3$): δ 8.85-8.83 (m, 2H), 8.14 (d, $J=8.0$ Hz, 4H), 8.13-8.11 (m, 3H), 7.72-7.71 (m, 2H), 7.54 (d, $J=8.0$ Hz, 4H), 7.47-7.43 (m, 4H), 7.35-7.31 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 193.47 (—CO—), 150.67, 143.23, 140.13, 140.05, 139.24, 129.49, 126.51, 126.39, 123.81, 122.66, 120.87, 120.64, 109.29; HRMS (FAB $^+$) cal for $C_{36}H_{23}N_3O$ 513.1841, found 513.1840.

Ex. 4: mDTCBPy

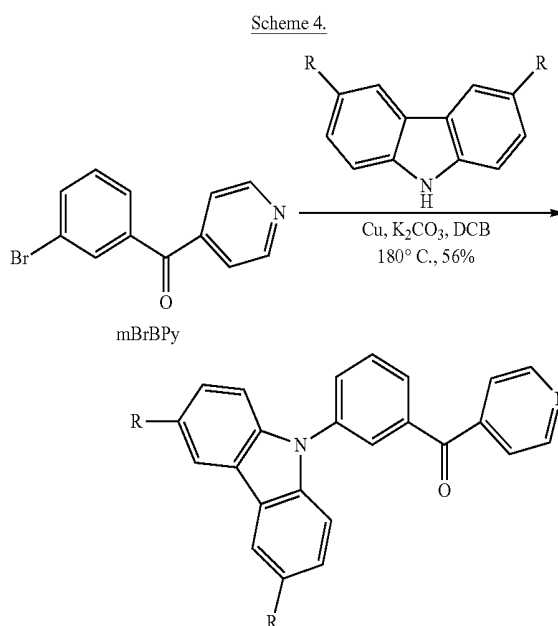
[0089] The structure of mDTCBPy can refer to Formula (I-1-5), wherein R is a t-butyl group. mDTCBPy can be synthesized according to Scheme 3:



[0090] mDTCBPpy can be synthesized as follows. To an oven dried seal tube mDBrBPpy (2.50 g, 7.33 mmol), t-butyl carbazole (5.11 g, 18.3 mmol), Cu (0.93 g, 14.7 mmol), K_2CO_3 (5.06 g, 36.7 mmol) and 1,2-dichlorobenzene (20 ml) was added. The system was evacuated and nitrogen was purged and the mixture was stirred at 180° C. for 48 hours. After completion of reaction, reaction mixture was filtered through Celite and washed with 50 ml of ethyl acetate. Solvent was evaporated under reduced pressure followed by column chromatography purification using n-hexane/EtOAc (3:1) as eluent afforded yellow solid in 78% yield. The m.p. of the product is 355° C. From the results of 1H NMR, ^{13}C NMR and HRMS, it can confirm that the product is mDTCBPpy. 1H NMR (400 MHz, $CDCl_3$): δ 8.84 (d, J=5.2 Hz, 2H), 8.13 (s, 4H), 8.09 (sd, J=1.6 Hz, 1H), 8.04 (sd, J=2.0 Hz, 2H), 7.71 (d, J=5.6 Hz, 2H), 7.49-7.44 (m, 8H), 1.44 (s, 36H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.35 (—CO—), 150.48, 143.85, 143.44, 138.84, 138.75, 137.65, 131.46, 130.22, 128.32, 127.76, 123.80, 123.60, 122.82, 116.43, 108.79, 34.72, 31.94; HRMS (FAB⁺) cal for $C_{52}H_{55}N_3O$ 737.4345, found 737.4335.

Ex. 5: mTCBPpy

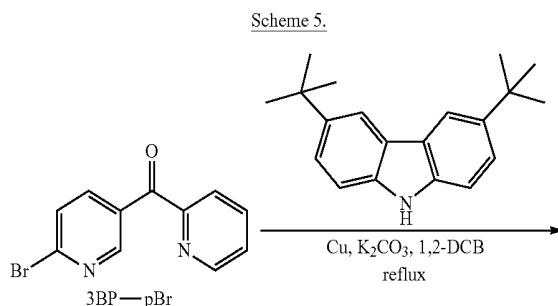
[0091] The structure of mTCBPpy can refer to Formula (I-1-7), wherein R is a t-butyl group. mTCBPpy can be synthesized according to Scheme 4:

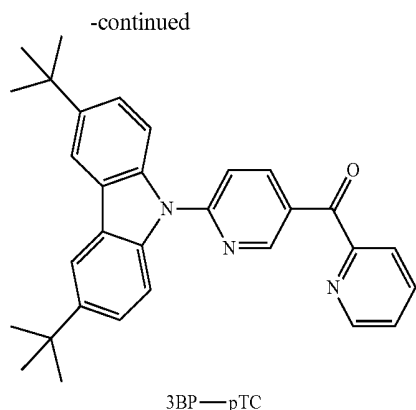


[0092] mTCBPpy can be synthesized as follows. To an oven dried seal tube mBrBPpy (2.5 g, 9.54 mmol), t-butyl carbazole (3.19 g, 11.40 mmol), Cu (0.61 g, 9.54 mmol), K_2CO_3 (3.29 g, 23.80 mmol) and 1,2-dichlorobenzene (20 ml) was added. The system was evacuated and nitrogen was purged and the mixture was stirred at 180° C. for 48 hours. After completion of reaction, reaction mixture was filtered through Celite and washed with 50 ml of ethyl acetate. Solvent was evaporated under reduced pressure followed by column chromatography purification using n-hexane/EtOAc (3:1) as eluent afforded yellow solid in 75% yield. The m.p. of the product is 194° C. From the results of 1H NMR, ^{13}C NMR and HRMS, it can confirm that the product is mTCBPpy. 1H NMR (400 MHz, $CDCl_3$): δ 8.82-8.81 (m, 2H), 8.14 (sd, J=1.6 Hz, 2H), 8.01 (st, J=1.6 Hz, 1H), 7.87-7.84 (m, 2H), 7.73 (d, J=7.8 Hz, 1H), 7.65-7.63 (m, 2H), 7.47 (dd, J=8.8 Hz, J=2.0 Hz, 2H), 7.35 (d, J=8.4 Hz, 2H), 1.46 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.38, 150.50, 143.83, 143.43, 138.82, 138.73, 137.64, 131.46, 130.23, 128.33, 127.75, 123.80, 123.59, 122.79, 116.43, 108.78, 34.73, 31.94; HRMS (FAB⁺) cal for $C_{32}H_{32}N_2O$ 460.2515, found 460.2518.

Ex. 6: 3BP-pTC

[0093] The structure of 3BP-pTC can refer to Formula (I-3-1), wherein R is a t-butyl group. 3BP-pTC can be synthesized according to Scheme 5:

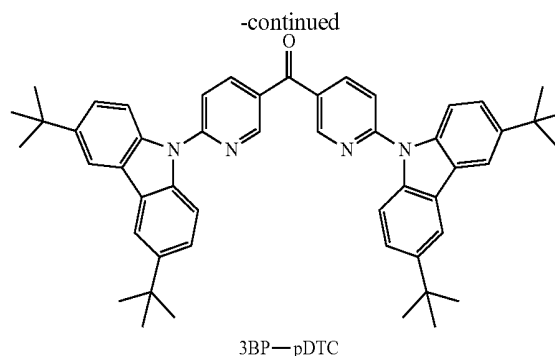
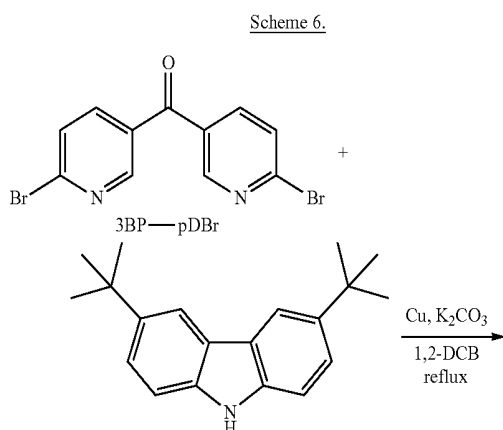




[0094] 3BP-pTC can be synthesized as follows. To an oven dried seal tube was added (6-bromopyridin-3-yl)(pyridin-2-yl)methanone (3BP-pBr) (2.5 g, 9.5 mmol), t-butylcarbazole (3.18 g, 11.40 mmol), Cu (0.60 g, 9.5 mmol), K_2CO_3 (1.31 g, 19.00 mmol) and p-xylene (20 ml). It was evacuated and purged with nitrogen three times under stirring followed by heating at 150° C. for 12 hours. The reaction mixture was filtered through Celite and washed with ethyl acetate (30 ml). Evaporation of solvent under reduced pressure followed by column chromatography purification using n-hexane/EtOAc (3:1) as eluent afforded yellow solid in 82% yield. The m.p. of the product is 217° C. From the results of 1H NMR, ^{13}C NMR and HRMS, it can confirm that the product is 3BP-pTC. 1H NMR (400 MHz, $CDCl_3$): δ 9.48 (sd, $J=2.0$ Hz, 1H), 8.76 (d, $J=4.4$ Hz, 1H), 8.67 (dd, $J=8.4$ Hz, $J=2.0$ Hz, 1H), 8.17 (d, $J=7.6$ Hz, 1H), 8.08 (sd, $J=1.6$ Hz, 2H), 7.98 (d, $J=8.8$ Hz, 2H), 7.95-7.93 (m, 1H), 7.77 (d, $J=8.4$ Hz, 1H), 7.55-7.51 (m, 3H), 1.46 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.83 (—CO—), 154.40, 152.99, 152.98, 148.55, 144.82, 140.71, 137.42, 137.38, 128.08, 126.77, 125.07, 124.65, 124.15, 116.27, 116.14, 111.70, 34.76, 31.85; HRMS (FAB⁺) cal for $C_{31}H_{31}NO_3$ 461.2467, found 461.2462.

Ex. 7: 3BP-pDTC

[0095] The structure of 3BP-pDTC can refer to Formula (I-2-1), wherein R is a t-butyl group. 3BP-pDTC can be synthesized according to Scheme 6:

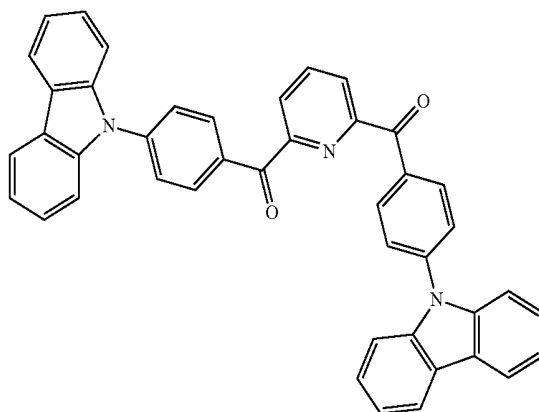


[0096] 3BP-pDTC can be synthesized as follows. To an oven dried seal tube was added bis(6-bromopyridin-3-yl)methanone (3BP-pDBr) (2.0 g, 5.85 mmol), t-butylcarbazole (3.59 g, 11.70 mmol), Cu (0.74 g, 11.69 mmol), K_2CO_3 (3.23 g, 23.40 mmol) and p-xylene (20 ml). It was evacuated and purged with nitrogen three times under stirring followed by heating at 150° C. for 12 hours. The reaction mixture was filtered through Celite and washed with 30 ml of ethyl acetate. Evaporation of solvent under reduced pressure followed by column chromatography purification using n-hexane/EtOAc (3:1) as eluent afforded yellow solid in 84% yield. The m.p. of the product is 400° C. From the results of 1H NMR, ^{13}C NMR and HRMS, it can confirm that the product is 3BP-pDTC. 1H NMR (400 MHz, $CDCl_3$): δ 9.18 (sd, $J=2.0$ Hz, 2H), 8.42 (dd, $J=8.4$ Hz, $J=2.4$ Hz, 2H), 8.10 (sd, $J=1.6$ Hz, 4H), 8.01 (d, $J=8.4$ Hz, 4H), 7.85 (d, $J=8.4$ Hz, 2H), 7.53 (dd, $J=8.8$ Hz, $J=2.0$ Hz, 4H), 1.47 (s, 36H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.04 (—CO—), 155.37, 151.34, 145.15, 139.53, 137.34, 128.67, 125.25, 124.26, 116.67, 116.27, 111.73, 34.80, 31.85; HRMS (FAB⁺) cal for $C_{51}H_{54}N_4O$ 738.4298, found 738.4293.

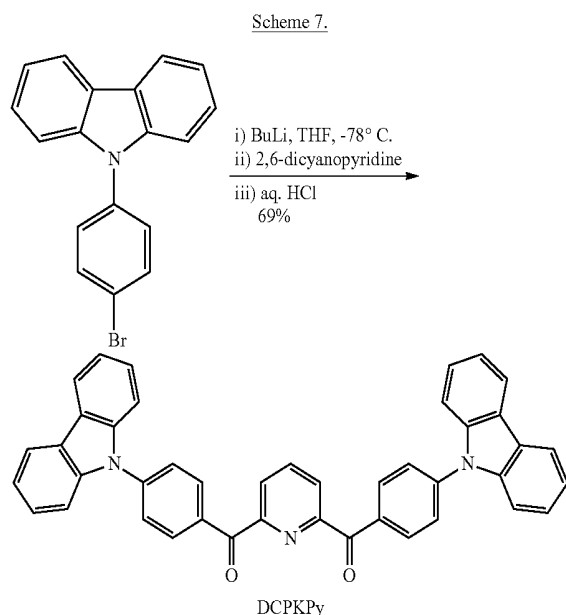
Comparative Ex. 1: DCPKPy

[0097] DCPKPy has a structure of Formula (II):

(II)



[0098] DCPKPy can be synthesized according to Scheme 7:



[0099] DCPKPy can be synthesized as follows. To a stirred solution of 9-(4-bromophenyl)-9H-carbazole (2.87 g, 89.14 mmol) in THF (50 ml) at -78°C . was added n-BuLi (3.41 ml, 8.43 mmol) and stirred for 1 hour at the same temperature. To this solution, 1,3-dicyanopyridine (0.5 g, 3.87 mmol) in THF (20 ml) was added dropwise and the reaction mixture was allowed to stir for another 2 hours at -78°C . It was quenched with aq. HCl at 0°C . and partitioned between water and ethyl acetate. The organic layer was washed with water and dried with Na_2SO_4 . Evaporation of solvent under reduced pressure followed by column chromatography purification afforded yellow solid in 69% yield. From the results of ^1H NMR, ^{13}C NMR and HRMS, it can confirm that the product is DCPKPy. ^1H NMR (400 MHz, CDCl_3): δ 8.48 (d, $J=8.0$ Hz, 4H), 8.38 (d, $J=7.6$ Hz, 2H), 8.19 (t, $J=7.6$ Hz, 1H), 8.07 (d, $J=7.6$ Hz, 4H), 7.68 (d, $J=8.4$ Hz, 4H), 7.40 (d, $J=8.0$ Hz, 4H), 7.20 (t, $J=7.8$ Hz, 4H), 7.12 (t, $J=7.8$ Hz, 4H); ^{13}C NMR (100 MHz, CDCl_3): δ 191.10 (—CO—), 153.78, 142.31, 139.97, 138.62, 134.08, 133.04, 127.27, 126.14, 125.87, 123.79, 120.58, 120.34, 109.57.

[0100] <Property Measurements of Examples and Comparative Examples>

[0101] FIG. 4 shows molecular orbitals of Ex. 1. FIG. 5 shows molecular orbitals of Ex. 2. FIG. 6 shows molecular orbitals of Ex. 3. FIG. 7 shows molecular orbitals of Ex. 4. FIG. 8 shows molecular orbitals of Ex. 5. FIG. 9 shows molecular orbitals of Ex. 6. FIG. 10 shows molecular orbitals of Ex. 7. FIG. 4 to FIG. 10 are obtained from the calculation results of time dependent density functional theory, and show the distribution of HOMOs and LUMOs of Ex. 1 to Ex. 7, respectively. As shown in FIG. 4 to FIG. 10, the HOMOs are mainly distributed over the electron donating group of carbazole group/3,6-di-*t*-butyl-carbazole group,

the LUMOs are mainly distributed over the electron accepting group composed of the main body of the pyridyl group, the ketone group and the main body of the phenyl group/pyridyl group, and there is a small overlap between the HOMOs and the LUMOs, all of which show that Ex. 1 to Ex. 7 have TADF property.

[0102] FIG. 11 shows Abs. spectra, Fl. spectra and Phos. spectra of Ex. 1 and Ex. 2. FIG. 12 shows an Abs. spectrum, a Fl. spectrum and a Phos. spectrum of Ex. 6. FIG. 13 shows an Abs. spectrum, a Fl. spectrum and a Phos. spectrum of Ex. 7. The Abs. spectra and the Fl. spectrum are measured in toluene (10^{-5} M) at room temperature (300 K). The Phos. spectra are measured in toluene (10^{-5} M) at 77 K. The wavelength correspondent to the absorption peak, the wavelength correspondent to the fluorescence peak, and the wavelength correspondent to the phosphorescence peak of Ex. 1, Ex. 2, Ex. 6 and Ex. 7 can be observed from FIG. 11 to FIG. 13, and are recorded in Table 2.

[0103] Table 2 shows the photophysical properties of Ex. 1 to Ex. 7, wherein λ_{abs} represents the wavelength correspondent to the absorption peak, λ_{em1} represents the wavelength correspondent to the fluorescence peak, λ_{em2} represents the wavelength correspondent to the phosphorescence peak, E_S is the energy level of the singlet excited state, E_T is the energy level of the triplet excited state, $\Delta E_{ST}=E_S-E_T$. E_S can be calculated from the Fl. spectrum. E_T can be calculated from the Phos. spectrum.

TABLE 2

Ex.	λ_{abs} (nm)	λ_{em1} (nm)	λ_{em2} (nm)	E_S (eV)	E_T (eV)	ΔE_{ST} (nm)
1	311, 400	490	495	2.87	2.84	0.03
2	320, 418	508	509	2.74	2.70	0.04
3	334, 364	468	467	3.0	2.95	0.05
4	342, 390	496	477	2.87	2.86	0.01
5	343, 374	492	467	2.98	2.93	0.05
6	381	479	462	2.91	2.79	0.12
7	384	464	460	2.96	2.81	0.15

[0104] The thermal decomposition temperatures (Tds) of Ex. 1 to Ex. 7 are measured with thermal gravimetric analysis (TGA), and the voltammograms of Ex. 1 to Ex. 7 are obtained by cyclic voltammetry, from which the HOMO levels and the LUMO levels of Ex. 1 to Ex. 7 can be calculated. The Tds, the HOMO levels and the LUMO levels of Ex. 1 to Ex. 7 are listed in Table 3.

TABLE 3

Ex.	Td ($^{\circ}\text{C}$.)	HOMO (eV)	LUMO (eV)
1	382	-5.75	-2.88
2	412	-5.61	-2.87
3	390	-5.72	-2.72
4	381	-5.67	-2.80
5	327	-5.63	-2.65
6	445	-5.69	-2.78
7	484	-5.72	-2.76

[0105] FIG. 14 is a diagram showing transient photoluminescence characteristics of Ex. 1 and Ex. 2. FIG. 15 is a diagram showing transient photoluminescence characteristics of Ex. 3. FIG. 16 is a diagram showing transient photoluminescence characteristics of Ex. 4 and Ex. 5. FIGS. 14-16 are measured in toluene (10^{-5} M) at room temperature under vacuum. From FIG. 14, it can be calculated that the lifetime of fluorescence (τ_1) of Ex. 1 is 15 ns, the lifetime of delayed fluorescence (τ_2) of Ex. 1 is 0.6 μ s, the τ_1 of Ex. 2 is 18 ns, and the τ_2 of Ex. 2 is 1 μ s. From FIG. 15, it can be calculated that the τ_1 of Ex. 3 is 6.2 ns, and the τ_2 of Ex. 3 is 0.2 μ s. From FIG. 16, it can be calculated that the τ_1 of Ex. 4 is 6.6 ns, the τ_2 of Ex. 4 is 1.9 μ s, the τ_1 of Ex. 5 is 8.9 ns, and the τ_2 of Ex. 5 is 1.3 μ s.

[0106] <OLED Devices Using Examples and Comparative Examples>

[0107] OLED device A: the compound of Ex. 1 is used as a dopant of an emitting layer of the OLED A, and a doping concentration thereof is 5% (in weight percentage). The OLED device A sequentially includes an anode, a hole injection layer, a hole-transporting layer, the emitting layer, an exciton blocker, an electron-transporting layer, an electron injection layer, and a cathode. The structure of the OLED device A can refer to FIG. 3. The material and thickness of each layer of the OLED device A are as follows: ITO/NPB (30 nm)/mCP (20 nm)/CzPS:DCBPpy (5%) (30 nm)/DPEPO (5 nm)/TmPyPb (60 nm)/LiF (1 nm)/Al (100 nm).

[0108] OLED device B: the compound of Ex. 2 is used as a dopant of an emitting layer of the OLED B, and a doping concentration thereof is 5% (in weight percentage). The OLED device B sequentially includes an anode, a hole injection layer, a hole-transporting layer, the emitting layer, an exciton blocker, an electron-transporting layer, an electron injection layer, and a cathode. The structure of the OLED device B can refer to FIG. 3. The material and thickness of each layer of the OLED device B are as follows: ITO/NPB (30 nm)/TAPC (20 nm)/CBP:DTCPpy (5%) (30 nm)/PPT (10 nm)/TmPyPb (55 nm)/LiF (1 nm)/Al (100 nm).

[0109] OLED device C: the compound of Ex. 3 is used as a dopant of an emitting layer of the OLED C, and a doping concentration thereof is 5% (in weight percentage). The OLED device C sequentially includes an anode, a hole injection layer, a hole-transporting layer, the emitting layer, an exciton blocker, an electron-transporting layer, an electron injection layer, and a cathode. The structure of the OLED device C can refer to FIG. 3. The material and thickness of each layer of the OLED device C are as follows: ITO/NPB (30 nm)/mCP (20 nm)/DPEPO:mDCBPpy(5%)(30 nm)/PPT (5 nm)/TmPyPb (60 nm)/LiF(1 nm)/Al (100 nm).

[0110] OLED device D: the compound of Ex. 4 is used as a dopant of an emitting layer of the OLED D, and a doping concentration thereof is 7% (in weight percentage). The OLED device D sequentially includes an anode, a hole injection layer, a hole-transporting layer, the emitting layer, an exciton blocker, an electron-transporting layer, an electron injection layer, and a cathode. The structure of the

OLED device D can refer to FIG. 3. The material and thickness of each layer of the OLED device D are as follows: ITO/NPB (30 nm)/TAPC (20 nm)/mCBP:mDTCPpy (7%) (30 nm)/DPEPO (5 nm)/TmPyPb (60 nm)/LiF (0.8 nm)/Al (100 nm).

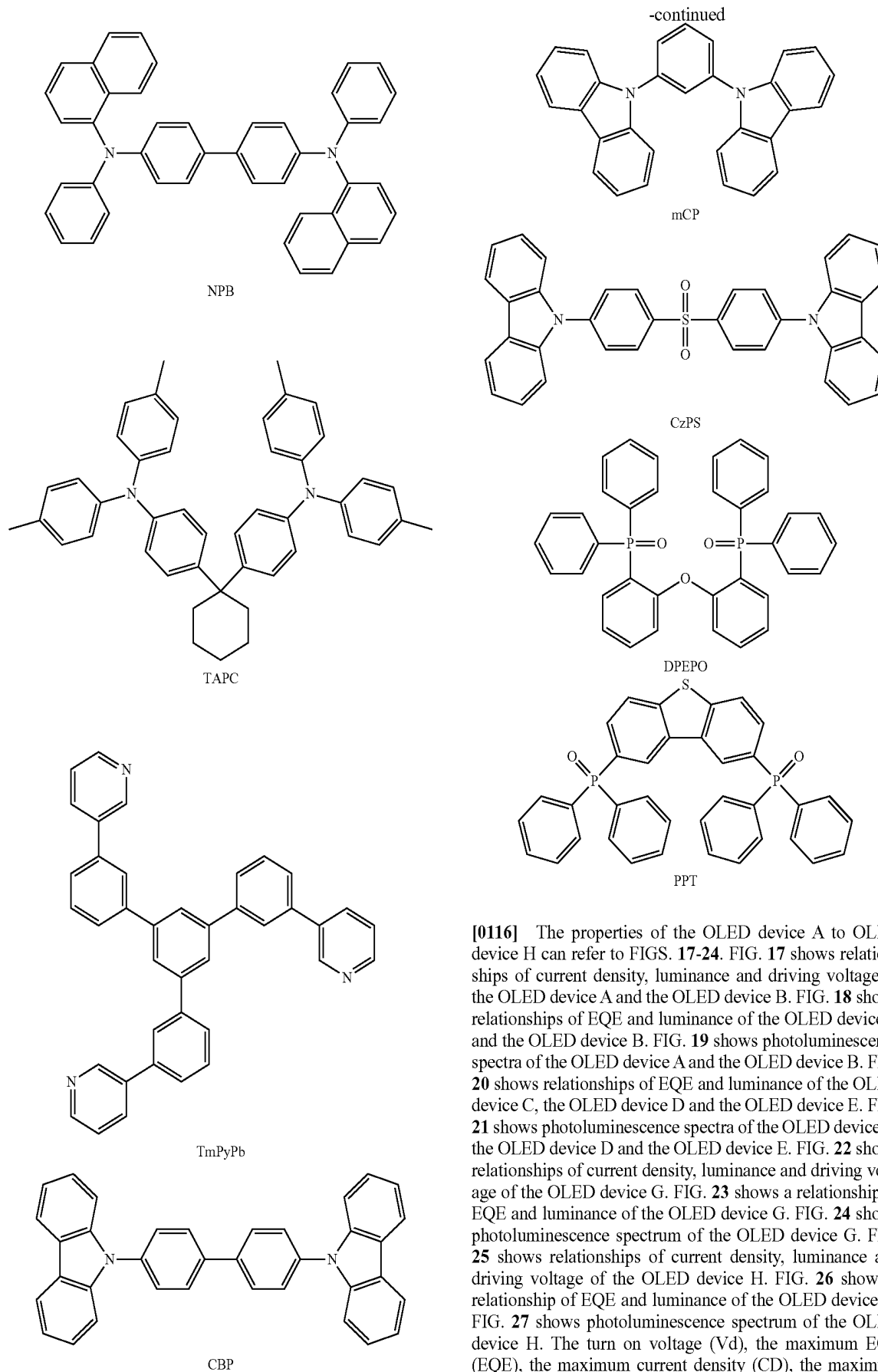
[0111] OLED device E: the compound of Ex. 5 is used as a dopant of an emitting layer of the OLED E, and a doping concentration thereof is 5% (in weight percentage). The OLED device E sequentially includes an anode, a hole injection layer, a hole-transporting layer, the emitting layer, an exciton blocker, an electron-transporting layer, an electron injection layer, and a cathode. The structure of the OLED device E can refer to FIG. 3. The material and thickness of each layer of the OLED device E are as follows: ITO/NPB (30 nm)/mCP (20 nm)/mCBP:mTCBPpy (5%) (30 nm)/DPEPO (5 nm)/TmPyPb (60 nm)/LiF (0.8 nm)/Al (100 nm).

[0112] OLED device F: the compound of Ex. 6 is used as a dopant of an emitting layer of the OLED F, and a doping concentration thereof is 7% (in weight percentage). The OLED device F sequentially includes an anode, a hole injection layer, a hole-transporting layer, the emitting layer, an exciton blocker, an electron-transporting layer, an electron injection layer, and a cathode. The structure of the OLED device F can refer to FIG. 3. The material and thickness of each layer of the OLED device F are as follows: ITO/NPB (30 nm)/TAPC (20 nm)/mCBP:3BP-pTC (7%)(30 nm)/PPT (10 nm)/TmPyPb (55 nm)/LiF (0.8 nm)/Al (100 nm).

[0113] OLED device G: the compound of Ex. 7 is used as a dopant of an emitting layer of the OLED G, and a doping concentration thereof is 7% (in weight percentage). The OLED device G sequentially includes an anode, a hole injection layer, a hole-transporting layer, the emitting layer, an exciton blocker, an electron-transporting layer, an electron injection layer, and a cathode. The structure of the OLED device G can refer to FIG. 3. The material and thickness of each layer of the OLED device G are as follows: ITO/NPB (30 nm)/TAPC (20 nm)/mCBP:3BP-pDTC (7%) (30 nm)/DPEPO (5 nm)/TmPyPb (65 nm)/LiF (0.8 nm)/Al (100 nm).

[0114] OLED device H: the compound of Comparative Ex. 1 is used as a dopant of an emitting layer of the OLED H, and a doping concentration thereof is 7% (in weight percentage). The OLED device H sequentially includes an anode, a hole injection layer, a hole-transporting layer, the emitting layer, an exciton blocker, an electron-transporting layer, an electron injection layer, and a cathode. The structure of the OLED device H can refer to FIG. 3. The material and thickness of each layer of the OLED device H are as follows: ITO/NPB (30 nm)/TAPC (20 nm)/mCBP:DCPKpy (7%) (30 nm)/DPEPO (5 nm)/TmPyPb (60 nm)/LiF (0.8 nm)/Al (100 nm).

[0115] The structures of the compounds used in the OLED device A to the OLED device H are as follows.



[0116] The properties of the OLED device A to OLED device H can refer to FIGS. 17-24. FIG. 17 shows relationships of current density, luminance and driving voltage of the OLED device A and the OLED device B. FIG. 18 shows relationships of EQE and luminance of the OLED device A and the OLED device B. FIG. 19 shows photoluminescence spectra of the OLED device A and the OLED device B. FIG. 20 shows relationships of EQE and luminance of the OLED device C, the OLED device D and the OLED device E. FIG. 21 shows photoluminescence spectra of the OLED device C, the OLED device D and the OLED device E. FIG. 22 shows relationships of current density, luminance and driving voltage of the OLED device G. FIG. 23 shows a relationship of EQE and luminance of the OLED device G. FIG. 24 shows photoluminescence spectrum of the OLED device G. FIG. 25 shows relationships of current density, luminance and driving voltage of the OLED device H. FIG. 26 shows a relationship of EQE and luminance of the OLED device H. FIG. 27 shows photoluminescence spectrum of the OLED device H. The turn on voltage (V_d), the maximum EQE (EQE), the maximum current density (CD), the maximum luminance (L), the maximum current efficiency (CE), the

maximum power efficiency (PE) and the chromaticity coordinate (CIE) of each of the OLED device A to OLED device H are listed in Table 4 and Table 5.

TABLE 4

OLED device	Vd (V)	EQE (%)	CD (mA/cm ²)	L (Cd/m ²)	CE (Cd/A)	PE (lm/W)
A	2.8	24.0	651	10300	54.7	57.2
B	3.1	27.2	519	37700	94.6	84.5
C	2.8	18.0	583	7000	41.3	43.1
D	3.3	28.1	520	17000	67.0	60.1
E	5.2	12.2	464	4332	25.0	14.2
F	3.5	14.9	737	10799	32.3	25.2
G	3.5	27.0	507	12961	58.1	40.7
H	5.1	8.8	492	2900	15.3	8.1

TABLE 5

	OLED device			
	A	B	C	D
CIE (x, y)	(0.17, 0.36)	(0.30, 0.64)	(0.18, 0.32)	(0.17; 0.37)

	OLED device			
	E	F	G	H
CIE (x, y)	(0.16, 0.36)	(0.17, 0.31)	(0.15, 0.31)	(0.15; 0.22)

[0117] As shown in Table 4, when the compounds according to the present disclosure are used as the dopants in the emitting layers of the OLED device A to the OLED device G, the OLED device A to the OLED device G are featured with excellent efficiency. For example, the maximum EQEs of the OLED device A to the OLED device G are all greater than 12.2%. In contrast, the maximum EQE of the OLED device H used the comparative Ex. 1 can only reach to 8.8%. The main difference between the compound of the comparative Ex. 1 and the compounds according to the present disclosure is the electron accepting group. There are one more phenyl group and one more ketone group in the electron accepting group of the compound of the comparative Ex. 1. From the results shown in Table 4, it is known that the structure of the TADF material is critical to the performance of the OLED devices. By improving the molecular structure, the compound according to the present disclosure indeed enhance the efficiency of OLED device.

[0118] Moreover, as shown in Table 5, the blue OLED device can be provided by using the compound according to the present disclosure, which overcomes the disadvantage of the phosphorescence materials and can provide a wide light color tenability.

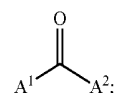
[0119] FIG. 28 shows a single-crystal X-ray diffraction result of Ex. 2. As shown in FIG. 28, the compound of Ex. 2 includes two 3,6-di-t-butyl-carbazole groups, which are located at the ortho position and the meta position in respect to the ketone group, and there is a strong intramolecular space interaction between the ortho 3,6-di-t-butyl-carbazole group and the pyridyl group of the electron accepting group. A distance between the ortho 3,6-di-t-butyl-carbazole group

and the pyridyl group of the electron accepting group is about 2.9 Å to 3.7 Å, the ΔE_{st} can be further reduced thereby, and the probability of RISC can be enhanced. Accordingly, the efficiency of the OLED can be further enhanced.

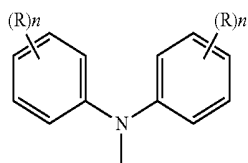
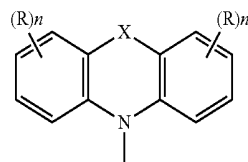
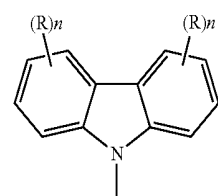
[0120] It will be apparent to those skilled in the art that various modifications and variations can be made to the structure of the present disclosure without departing from the scope or spirit of the disclosure. In view of the foregoing, it is intended that the present disclosure cover modifications and variations of this disclosure provided they fall within the scope of the following claims.

What is claimed is:

1. A compound, comprising a structure of Formula (I):

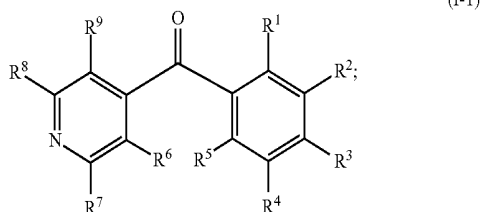


wherein A^1 is a pyridyl group, A^2 is a phenyl group or a pyridyl group, and hydrogens of the A^1 are both unsubstituted or substituted by a structure of Formula (i), Formula (ii) or Formula (iii), and at least one of hydrogens of the A^2 is substituted by the structure of Formula (i), Formula (ii) or Formula (iii):



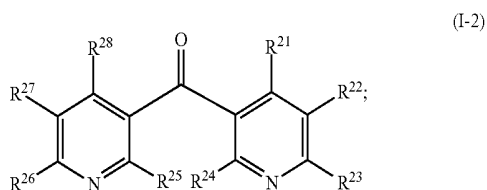
wherein n is independently an integer of 0 to 4, R is independently a monovalent group having 1 to 60 carbon atoms, X is $-\text{NR}^{14}-$, $-\text{S}-$ or $-\text{CR}^{15}\text{R}^{16}-$, and R^{14} , R^{15} and R^{16} are independently $-\text{H}$, an alkyl group or an aryl group.

2. The compound of claim 1, wherein the compound comprises a structure of Formula (I-1):



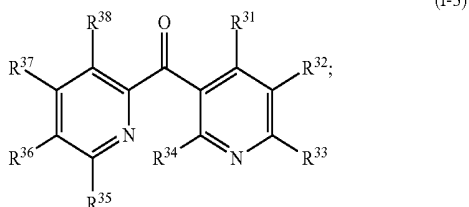
wherein R^1 , R^2 , R^3 , R^4 and R^5 are independently —H, the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), at least one of the R^1 , R^2 , R^3 , R^4 and R^5 is the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), and R^6 , R^7 , R^8 and R^9 are —H.

3. The compound of claim 1, wherein the compound comprises a structure of Formula (I-2):



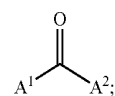
wherein R^{21} , R^{22} , R^{23} , R^{24} , R^{25} , R^{26} , R^{27} and R^{28} are independently —H, the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), and at least one of the R^{21} , R^{22} , R^{23} , R^{24} , R^{25} , R^{26} , R^{27} and R^{28} is the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii).

4. The compound of claim 1, wherein the compound comprises a structure of Formula (I-3):

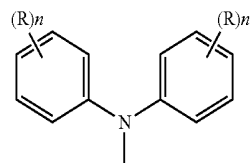
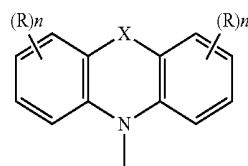
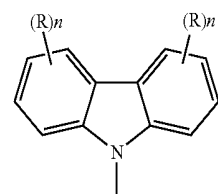


wherein R^{31} , R^{32} , R^{33} and R^{34} are independently —H, the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), at least one of the R^{31} , R^{32} , R^{33} and R^{34} is the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), and R^{35} , R^{36} , R^{37} and R^{38} are —H.

5. An emitting layer of an organic light emitting diode (OLED), comprising a dopant comprising a structure of Formula (I):

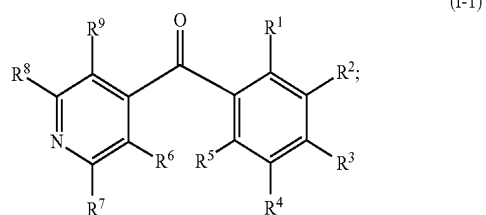


wherein A^1 is a pyridyl group, A^2 is a phenyl group or a pyridyl group, and hydrogens of the A^1 are both unsubstituted or substituted by a structure of Formula (i), Formula (ii) or Formula (iii), and at least one of hydrogens of the A^2 is substituted by the structure of Formula (i), Formula (ii) or Formula (iii):



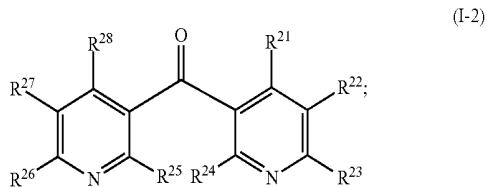
wherein n is independently an integer of 0 to 4, R is independently a monovalent group having 1 to 60 carbon atoms, X is —NR¹⁴—, —S— or —CR¹⁵R¹⁶—, and R^{14} , R^{15} and R^{16} are independently —H, an alkyl group or an aryl group.

6. The emitting layer of the OLED of claim 5, wherein the dopant comprises a structure of Formula (I-1):



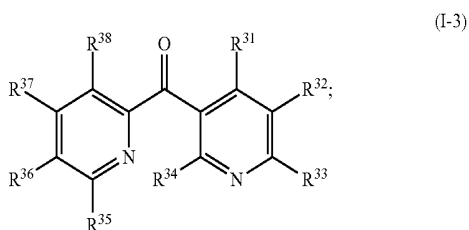
wherein R^1 , R^2 , R^3 , R^4 and R^5 are independently —H, the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), at least one of the R^1 , R^2 , R^3 , R^4 and R^5 is the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), and R^6 , R^7 , R^8 and R^9 are —H.

7. The emitting layer of the OLED of claim 5, wherein the dopant comprises a structure of Formula (I-2):



wherein R^{21} , R^{22} , R^{23} , R^{24} , R^{25} , R^{26} , R^{27} and R^{28} are independently —H, the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), and at least one of the R^{21} , R^{22} , R^{23} , R^{24} , R^{25} , R^{26} , R^{27} and R^{28} is the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii).

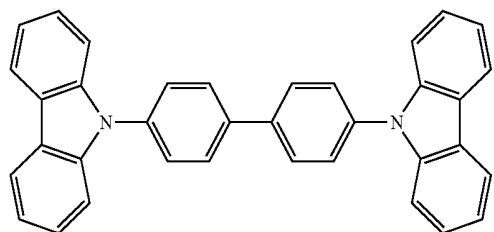
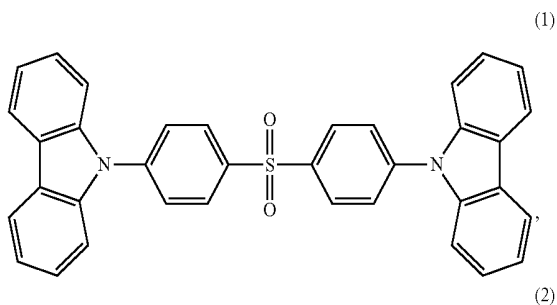
8. The emitting layer of the OLED of claim 5, wherein the dopant comprises a structure of Formula (I-3):



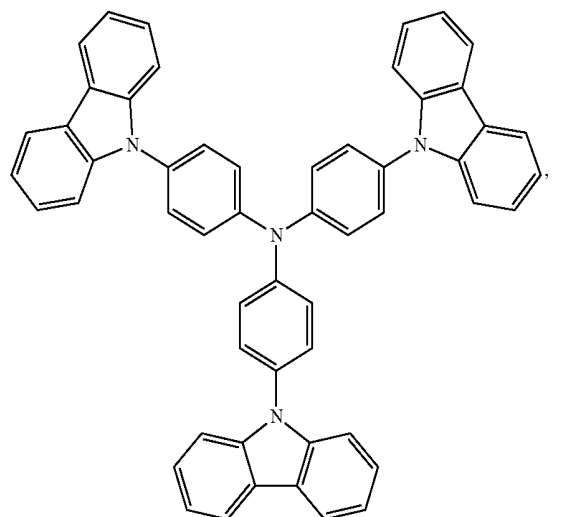
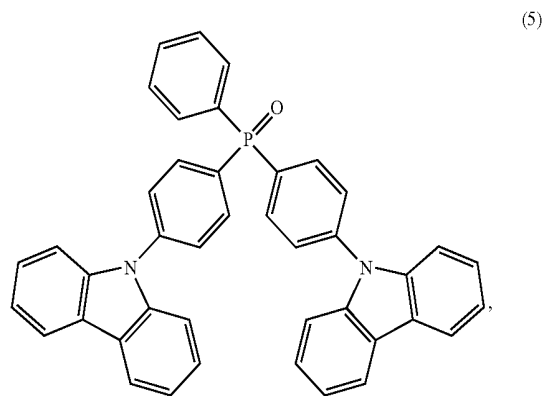
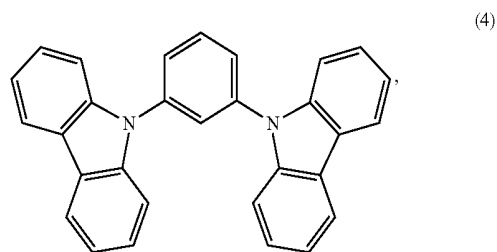
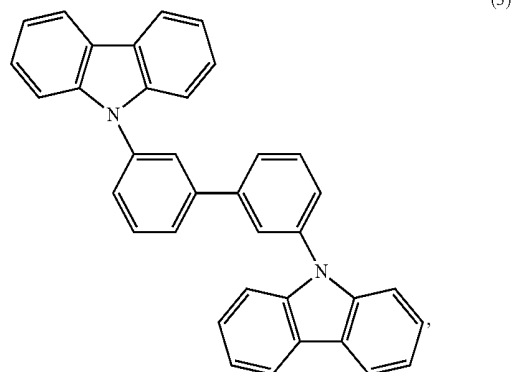
wherein R^{31} , R^{32} , R^{33} and R^{34} are independently —H, the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), at least one of the R^{31} , R^{32} , R^{33} and R^{34} is the structure of Formula (i), the structure of Formula (ii) or the structure of Formula (iii), and R^{35} , R^{36} , R^{37} and R^{38} are —H.

9. The emitting layer of the OLED of claim 5, further comprising:

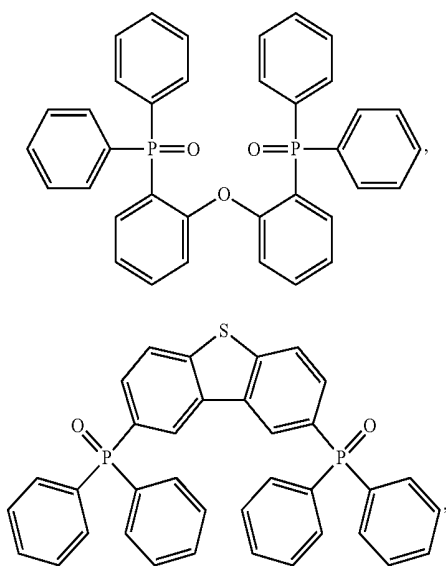
a host material comprising any one of structures of Formula (1) to Formula (9):



-continued



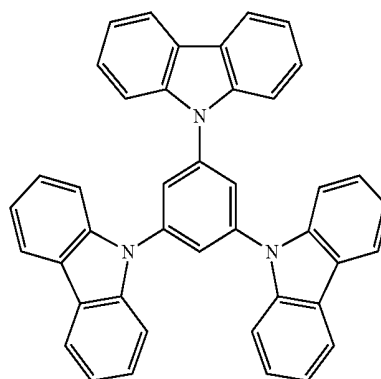
-continued



(7)

(8)

-continued



(9)

10. The emitting layer of the OLED of claim 5, wherein a doping concentration of the dopant in the emitting layer is in a range of 5 wt % to 30 wt %.

11. An OLED device, comprising:
the emitting layer of the OLED of claim 5.

* * * * *

专利名称(译)	化合物，发光层的有机发光二极管和有机发光二极管器件		
公开(公告)号	US20170317292A1	公开(公告)日	2017-11-02
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[标]申请(专利权)人(译)	国立清华大学		
申请(专利权)人(译)	清大		
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优先权	105113100 2016-04-27 TW		
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外部链接	Espacenet USPTO		

摘要(译)

本公开涉及包含式 (1) 的结构的化合物，以及该化合物作为掺杂剂在有机发光二极管的发光层中的用途。本公开还涉及有机发光二极管的发光层和有机发光二极管装置。

(1)

