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(54) ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

(71) Applicant: Universal Display Corporation,

Ewing, NJ (US)

(72) Inventors: Hsiao-Fan CHEN, Lawrence Township, NJ (US); Daniel W. SILVERSTEIN, Ewing, NJ (US); Peter WOLOHAN, Princeton Junction, NJ (US); Tyler FLEETHAM, Newtown, PA (US); Jason BROOKS, Philadelphia, PA (US); Charles J. STANTON, III, Wilmington, DE (US); Olexandr TRETYAK, Newark, DE (US); Raghupathi NEELARAPU,

Newark, DE (US); Katarina ROHLFING, Wilmington, DE (US); Douglas WILLIAMS, Mullica Hill, NJ

(US)

(73) Assignee: Universal Display Corporation,

Ewing, NJ (US)

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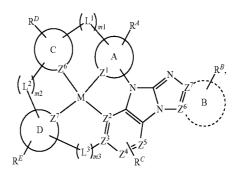
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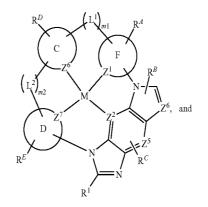
(57)**ABSTRACT**

A novel compound having a benzimidazole based structure is disclosed that is selected from one of the following structures:

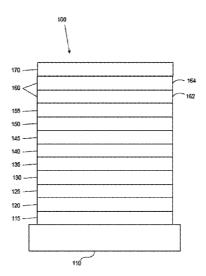
Formula I



Formula II

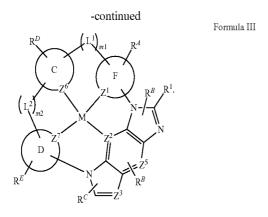


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The compound is useful in improving photophysical performance of OLEDs.

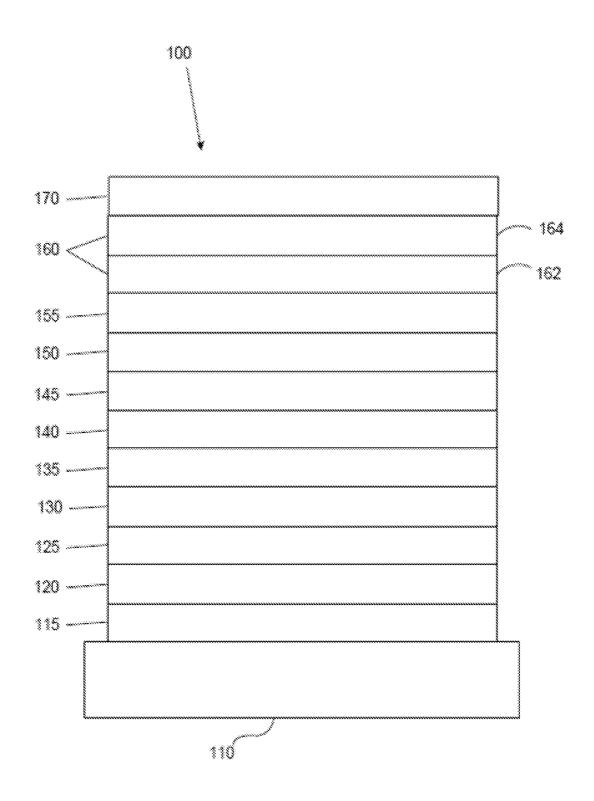


FIG. 1

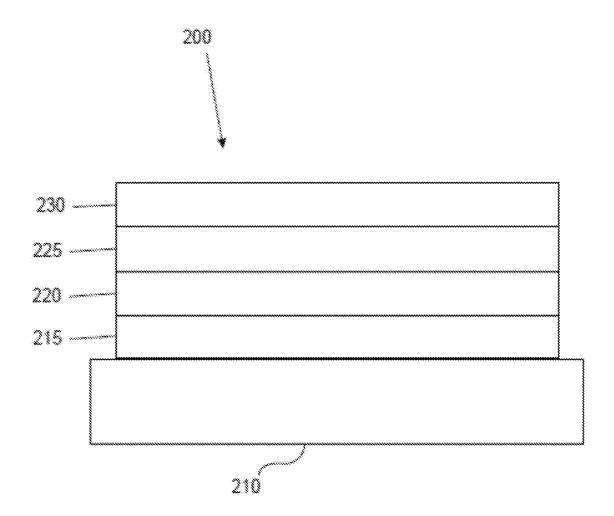


FIG. 2

ORGANIC ELECTROLUMINESCENT MATERIALS AND DEVICES

CROSS-REFERENCE TO RELATED APPLICATIONS

[0001] This application claims priority under 35 U.S.C. § 119(e), to U.S. Provisional Applications No. 62/842,230, filed on May 2, 2019, No. 62/823,922, filed on Mar. 26, 2019, No. 62/859,919, filed on Jun. 11, 2019, and No. 62/898,219, filed on Sep. 10, 2019, the entire contents of which are incorporated herein by reference. This application is also a continuation-in-part of the co-pending U.S. patent application Ser. No. 16/116,439, filed on Aug. 29, 2018, which claims priority under 35 U.S.C. § 119(e) to U.S. Provisional Application No. 62/555,115, filed Sep. 7, 2017, the entire contents of which are incorporated herein by reference.

FIELD

[0002] The present invention relates to compounds for use as emitters, and devices, such as organic light emitting diodes, including the same.

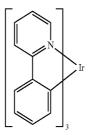
BACKGROUND

[0003] Opto-electronic devices that make use of organic materials are becoming increasingly desirable for a number of reasons. Many of the materials used to make such devices are relatively inexpensive, so organic opto-electronic devices have the potential for cost advantages over inorganic devices. In addition, the inherent properties of organic materials, such as their flexibility, may make them well suited for particular applications such as fabrication on a flexible substrate. Examples of organic opto-electronic devices include organic light emitting diodes/devices (OLEDs), organic phototransistors, organic photovoltaic cells, and organic photodetectors. For OLEDs, the organic materials may have performance advantages over conventional materials. For example, the wavelength at which an organic emissive layer emits light may generally be readily tuned with appropriate dopants.

[0004] OLEDs make use of thin organic films that emit light when voltage is applied across the device. OLEDs are becoming an increasingly interesting technology for use in applications such as flat panel displays, illumination, and backlighting. Several OLED materials and configurations are described in U.S. Pat. Nos. 5,844,363, 6,303,238, and 5,707,745, which are incorporated herein by reference in their entirety.

[0005] One application for phosphorescent emissive molecules is a full color display. Industry standards for such a display call for pixels adapted to emit particular colors, referred to as "saturated" colors. In particular, these standards call for saturated red, green, and blue pixels. Alternatively the OLED can be designed to emit white light. In conventional liquid crystal displays emission from a white backlight is filtered using absorption filters to produce red, green and blue emission. The same technique can also be used with OLEDs. The white OLED can be either a single EML device or a stack structure. Color may be measured using CIE coordinates, which are well known to the art.

[0006] One example of a green emissive molecule is tris(2-phenylpyridine) iridium, denoted Ir(ppy)₃, which has the following structure:



[0007] In this, and later figures herein, we depict the dative bond from nitrogen to metal (here, Ir) as a straight line.

[0008] As used herein, the term "organic" includes polymeric materials as well as small molecule organic materials that may be used to fabricate organic opto-electronic devices. "Small molecule" refers to any organic material that is not a polymer, and "small molecules" may actually be quite large. Small molecules may include repeat units in some circumstances. For example, using a long chain alkyl group as a substituent does not remove a molecule from the "small molecule" class. Small molecules may also be incorporated into polymers, for example as a pendent group on a polymer backbone or as a part of the backbone. Small molecules may also serve as the core moiety of a dendrimer, which consists of a series of chemical shells built on the core moiety. The core moiety of a dendrimer may be a fluorescent or phosphorescent small molecule emitter. A dendrimer may be a "small molecule," and it is believed that all dendrimers currently used in the field of OLEDs are small molecules. [0009] As used herein, "top" means furthest away from the substrate, while "bottom" means closest to the substrate. Where a first layer is described as "disposed over" a second layer, the first layer is disposed further away from substrate. There may be other layers between the first and second layer, unless it is specified that the first layer is "in contact with" the second layer. For example, a cathode may be described as "disposed over" an anode, even though there are various organic layers in between.

[0010] As used herein, "solution processable" means capable of being dissolved, dispersed, or transported in and/or deposited from a liquid medium, either in solution or suspension form.

[0011] A ligand may be referred to as "photoactive" when it is believed that the ligand directly contributes to the photoactive properties of an emissive material. A ligand may be referred to as "ancillary" when it is believed that the ligand does not contribute to the photoactive properties of an emissive material, although an ancillary ligand may alter the properties of a photoactive ligand.

[0012] As used herein, and as would be generally understood by one skilled in the art, a first "Highest Occupied Molecular Orbital" (HOMO) or "Lowest Unoccupied Molecular Orbital" (LUMO) energy level is "greater than" or "higher than" a second HOMO or LUMO energy level if the first energy level is closer to the vacuum energy level. Since ionization potentials (IP) are measured as a negative energy relative to a vacuum level, a higher HOMO energy level corresponds to an IP having a smaller absolute value (an IP that is less negative). Similarly, a higher LUMO energy level corresponds to an electron affinity (EA) having a smaller absolute value (an EA that is less negative). On a conventional energy level diagram, with the vacuum level at the top, the LUMO energy level of a material is higher than

the HOMO energy level of the same material. A "higher" HOMO or LUMO energy level appears closer to the top of such a diagram than a "lower" HOMO or LUMO energy level.

[0013] As used herein, and as would be generally understood by one skilled in the art, a first work function is "greater than" or "higher than" a second work function if the first work function has a higher absolute value. Because work functions are generally measured as negative numbers relative to vacuum level, this means that a "higher" work function is more negative. On a conventional energy level diagram, with the vacuum level at the top, a "higher" work function is illustrated as further away from the vacuum level in the downward direction. Thus, the definitions of HOMO and LUMO energy levels follow a different convention than work functions.

[0014] More details on OLEDs, and the definitions described above, can be found in U.S. Pat. No. 7,279,704, which is incorporated herein by reference in its entirety.

SUMMARY

[0015] A novel compound useful in improving photophysical performance of OLEDs is disclosed. The compound is selected from the group consisting of:

Formula II
$$\mathbb{R}^{D}$$

$$\mathbb{C}$$

Formula III

where; A, B, C, D, and F are each independently a 5-membered or 6-membered aromatic ring; ring B may or may not be present; M is selected from the group consisting of Pt, Pd, Cu, and Au; Z^1 , Z^2 , Z^3 , Z^4 , Z^5 , Z^6 , and Z^7 are each independently selected from the group consisting of C and N; m1, m2 and m3 are each independently an integer of 0 or 1; when m2 is 0, each m1 and m3 is 1; when m2 is 1, each m1 and m3 can be 0 or 1; when m1 is 0, L1 is not present; when m2 is 0, L² is not present; when m3 is 0, L³ is not present; L¹, L², and L³ each independently selected from the group consisting of a direct bond, BR, NR, PR, O, S, Se, C=O, S=O, SO₂, CRR', SiRR', GeRR', alkyl, cycloalkyl, and combinations thereof; each R^A , R^B , R^C , R^D , and R^E represents mono- to maximum possible number of substitutions, or no substitution; each RA, RB, RC, RD, RE, R and R' is a hydrogen or a substituent independently selected from the group consisting of the general substituents defined herein; and any two substituents can be joined or fused into a ring, provided that, in Formula I, if ring C is a 5-membered aromatic ring, L^2 is present and is a direct bond, then at least one pair of R^D , one pair of R^E , or one R^D and one R^E are joined together to form a fused ring.

[0016] An OLED comprising an anode, a cathode, and an organic layer disposed between the anode and the cathode is disclosed, in which, the organic layer comprises the novel compound of the present disclosure.

[0017] A consumer product comprising the OLED is also disclosed.

BRIEF DESCRIPTION OF THE DRAWINGS

[0018] FIG. 1 shows an organic light emitting device. [0019] FIG. 2 shows an inverted organic light emitting device that does not have a separate electron transport layer.

DETAILED DESCRIPTION

[0020] Generally, an OLED comprises at least one organic layer disposed between and electrically connected to an anode and a cathode. When a current is applied, the anode injects holes and the cathode injects electrons into the organic layer(s). The injected holes and electrons each migrate toward the oppositely charged electrode. When an electron and hole localize on the same molecule, an "exciton," which is a localized electron-hole pair having an excited energy state, is formed. Light is emitted when the exciton relaxes via a photoemissive mechanism. In some cases, the exciton may be localized on an excimer or an exciplex. Non-radiative mechanisms, such as thermal relaxation, may also occur, but are generally considered undesirable

[0021] The initial OLEDs used emissive molecules that emitted light from their singlet states ("fluorescence") as disclosed, for example, in U.S. Pat. No. 4,769,292, which is incorporated by reference in its entirety. Fluorescent emission generally occurs in a time frame of less than 10 nanoseconds.

[0022] More recently, OLEDs having emissive materials that emit light from triplet states ("phosphorescence") have been demonstrated. Baldo et al., "Highly Efficient Phosphorescent Emission from Organic Electroluminescent Devices," Nature, vol. 395, 151-154, 1998; ("Baldo-I") and Baldo et al., "Very high-efficiency green organic light-emitting devices based on electrophosphorescence," Appl. Phys. Lett., vol. 75, No. 3, 4-6 (1999) ("Baldo-II"), are

incorporated by reference in their entireties. Phosphorescence is described in more detail in U.S. Pat. No. 7,279,704 at cols. 5-6, which are incorporated by reference.

[0023] FIG. 1 shows an organic light emitting device 100. The figures are not necessarily drawn to scale. Device 100 may include a substrate 110, an anode 115, a hole injection layer 120, a hole transport layer 125, an electron blocking layer 130, an emissive layer 135, a hole blocking layer 140, an electron transport layer 145, an electron injection layer 150, a protective layer 155, a cathode 160, and a barrier layer 170. Cathode 160 is a compound cathode having a first conductive layer 162 and a second conductive layer 164. Device 100 may be fabricated by depositing the layers described, in order. The properties and functions of these various layers, as well as example materials, are described in more detail in U.S. Pat. No. 7,279,704 at cols. 6-10, which are incorporated by reference.

[0024] More examples for each of these layers are available. For example, a flexible and transparent substrate-anode combination is disclosed in U.S. Pat. No. 5,844,363, which is incorporated by reference in its entirety. An example of a p-doped hole transport layer is m-MTDATA doped with F_{4} -TCNQ at a molar ratio of 50:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. Examples of emissive and host materials are disclosed in U.S. Pat. No. 6,303,238 to Thompson et al., which is incorporated by reference in its entirety. An example of an n-doped electron transport layer is BPhen doped with Li at a molar ratio of 1:1, as disclosed in U.S. Patent Application Publication No. 2003/0230980, which is incorporated by reference in its entirety. U.S. Pat. Nos. 5,703,436 and 5,707,745, which are incorporated by reference in their entireties, disclose examples of cathodes including compound cathodes having a thin layer of metal such as Mg:Ag with an overlying transparent, electricallyconductive, sputter-deposited ITO layer. The theory and use of blocking layers is described in more detail in U.S. Pat. No. 6,097,147 and U.S. Patent Application Publication No. 2003/0230980, which are incorporated by reference in their entireties. Examples of injection layers are provided in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety. A description of protective layers may be found in U.S. Patent Application Publication No. 2004/0174116, which is incorporated by reference in its entirety.

[0025] FIG. 2 shows an inverted OLED 200. The device includes a substrate 210, a cathode 215, an emissive layer 220, a hole transport layer 225, and an anode 230. Device 200 may be fabricated by depositing the layers described, in order. Because the most common OLED configuration has a cathode disposed over the anode, and device 200 has cathode 215 disposed under anode 230, device 200 may be referred to as an "inverted" OLED. Materials similar to those described with respect to device 100 may be used in the corresponding layers of device 200. FIG. 2 provides one example of how some layers may be omitted from the structure of device 100.

[0026] The simple layered structure illustrated in FIGS. 1 and 2 is provided by way of non-limiting example, and it is understood that embodiments of the invention may be used in connection with a wide variety of other structures. The specific materials and structures described are exemplary in nature, and other materials and structures may be used. Functional OLEDs may be achieved by combining the

various layers described in different ways, or layers may be omitted entirely, based on design, performance, and cost factors. Other layers not specifically described may also be included. Materials other than those specifically described may be used. Although many of the examples provided herein describe various layers as comprising a single material, it is understood that combinations of materials, such as a mixture of host and dopant, or more generally a mixture, may be used. Also, the layers may have various sublayers. The names given to the various layers herein are not intended to be strictly limiting. For example, in device 200, hole transport layer 225 transports holes and injects holes into emissive layer 220, and may be described as a hole transport layer or a hole injection layer. In one embodiment, an OLED may be described as having an "organic layer" disposed between a cathode and an anode. This organic layer may comprise a single layer, or may further comprise multiple layers of different organic materials as described, for example, with respect to FIGS. 1 and 2.

[0027] Structures and materials not specifically described may also be used, such as OLEDs comprised of polymeric materials (PLEDs) such as disclosed in U.S. Pat. No. 5,247, 190 to Friend et al., which is incorporated by reference in its entirety. By way of further example, OLEDs having a single organic layer may be used. OLEDs may be stacked, for example as described in U.S. Pat. No. 5,707,745 to Forrest et al, which is incorporated by reference in its entirety. The OLED structure may deviate from the simple layered structure illustrated in FIGS. 1 and 2. For example, the substrate may include an angled reflective surface to improve outcoupling, such as a mesa structure as described in U.S. Pat. No. 6,091,195 to Forrest et al., and/or a pit structure as described in U.S. Pat. No. 5,834,893 to Bulovic et al., which are incorporated by reference in their entireties.

[0028] Unless otherwise specified, any of the layers of the various embodiments may be deposited by any suitable method. For the organic layers, preferred methods include thermal evaporation, ink-jet, such as described in U.S. Pat. Nos. 6,013,982 and 6,087,196, which are incorporated by reference in their entireties, organic vapor phase deposition (OVPD), such as described in U.S. Pat. No. 6,337,102 to Forrest et al., which is incorporated by reference in its entirety, and deposition by organic vapor jet printing (OVJP), such as described in U.S. Pat. No. 7,431,968, which is incorporated by reference in its entirety. Other suitable deposition methods include spin coating and other solution based processes. Solution based processes are preferably carried out in nitrogen or an inert atmosphere. For the other layers, preferred methods include thermal evaporation. Preferred patterning methods include deposition through a mask, cold welding such as described in U.S. Pat. Nos. 6,294,398 and 6,468,819, which are incorporated by reference in their entireties, and patterning associated with some of the deposition methods such as ink-jet and organic vapor jet printing (OVJP). Other methods may also be used. The materials to be deposited may be modified to make them compatible with a particular deposition method. For example, substituents such as alkyl and aryl groups, branched or unbranched, and preferably containing at least 3 carbons, may be used in small molecules to enhance their ability to undergo solution processing. Substituents having 20 carbons or more may be used, and 3-20 carbons is a preferred range. Materials with asymmetric structures may have better solution processability than those having symmetric structures, because asymmetric materials may have a lower tendency to recrystallize. Dendrimer substituents may be used to enhance the ability of small molecules to undergo solution processing.

[0029] Devices fabricated in accordance with embodiments of the present invention may further optionally comprise a barrier layer. One purpose of the barrier layer is to protect the electrodes and organic layers from damaging exposure to harmful species in the environment including moisture, vapor and/or gases, etc. The barrier layer may be deposited over, under or next to a substrate, an electrode, or over any other parts of a device including an edge. The barrier layer may comprise a single layer, or multiple layers. The barrier layer may be formed by various known chemical vapor deposition techniques and may include compositions having a single phase as well as compositions having multiple phases. Any suitable material or combination of materials may be used for the barrier layer. The barrier layer may incorporate an inorganic or an organic compound or both. The preferred barrier layer comprises a mixture of a polymeric material and a non-polymeric material as described in U.S. Pat. No. 7,968,146, PCT Pat. Application Nos. PCT/US2007/023098 and PCT/US2009/042829, which are herein incorporated by reference in their entireties. To be considered a "mixture", the aforesaid polymeric and non-polymeric materials comprising the barrier layer should be deposited under the same reaction conditions and/or at the same time. The weight ratio of polymeric to non-polymeric material may be in the range of 95:5 to 5:95. The polymeric material and the non-polymeric material may be created from the same precursor material. In one example, the mixture of a polymeric material and a nonpolymeric material consists essentially of polymeric silicon and inorganic silicon.

[0030] Devices fabricated in accordance with embodiments of the invention can be incorporated into a wide variety of electronic component modules (or units) that can be incorporated into a variety of electronic products or intermediate components. Examples of such electronic products or intermediate components include display screens, lighting devices such as discrete light source devices or lighting panels, etc. that can be utilized by the end-user product manufacturers. Such electronic component modules can optionally include the driving electronics and/or power source(s). Devices fabricated in accordance with embodiments of the invention can be incorporated into a wide variety of consumer products that have one or more of the electronic component modules (or units) incorporated therein. A consumer product comprising an OLED that includes the compound of the present disclosure in the organic layer in the OLED is disclosed. Such consumer products would include any kind of products that include one or more light source(s) and/or one or more of some type of visual displays. Some examples of such consumer products include flat panel displays, curved displays, computer monitors, medical monitors, televisions, billboards, lights for interior or exterior illumination and/or signaling, headsup displays, fully or partially transparent displays, flexible displays, rollable displays, foldable displays, stretchable displays, laser printers, telephones, mobile phones, tablets, phablets, personal digital assistants (PDAs), wearable devices, laptop computers, digital cameras, camcorders, viewfinders, micro-displays (displays that are less than 2 inches diagonal), 3-D displays, virtual reality or augmented

reality displays, vehicles, video walls comprising multiple displays tiled together, theater or stadium screen, and a sign. Various control mechanisms may be used to control devices fabricated in accordance with the present invention, including passive matrix and active matrix. Many of the devices are intended for use in a temperature range comfortable to humans, such as 18 degrees C. to 30 degrees C., and more preferably at room temperature (20-25 degrees C.), but could be used outside this temperature range, for example, from -40 degree C. to +80 degree C.

[0031] The materials and structures described herein may have applications in devices other than OLEDs. For example, other optoelectronic devices such as organic solar cells and organic photodetectors may employ the materials and structures. More generally, organic devices, such as organic transistors, may employ the materials and structures.

[0032] The terms "halo," "halogen," and "halide" are used interchangeably and refer to fluorine, chlorine, bromine, and jodine

[0033] The term "acyl" refers to a substituted carbonyl radical (C(O)— R_s).

[0034] The term "ester" refers to a substituted oxycarbonyl (—O—C(O)—R or —C(O)—O—R $_s$) radical.

[0035] The term "ether" refers to an —OR_s radical.

[0036] The terms "sulfanyl" or "thio-ether" are used interchangeably and refer to a —SR, radical.

[0037] The term "sulfinyl" refers to a —S(O)—R_s radical.

[0038] The term "sulfonyl" refers to a —SO₂—R_s radical.

[0039] The term "phosphino" refers to a — $P(R_s)_3$ radical, wherein each R_s can be same or different.

[0040] The term "silyl" refers to a —Si(R_s)3 radical, wherein each R_s can be same or different.

[0041] The term "boryl" refers to a $-B(R_s)_2$ radical or its Lewis adduct $-B(R_s)_3$ radical, wherein R_s can be same or different.

[0042] In each of the above, R_s can be hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, and combination thereof. Preferred R_s is selected from the group consisting of alkyl, cycloalkyl, aryl, heteroaryl, and combination thereof.

[0043] The term "alkyl" refers to and includes both straight and branched chain alkyl radicals. Preferred alkyl groups are those containing from one to fifteen carbon atoms and includes methyl, ethyl, propyl, 1-methylethyl, butyl, 1-methylpropyl, 2-methylpropyl, pentyl, 1-methylbutyl, 2-methylbutyl, 3-methylbutyl, 1,1-dimethylpropyl, 1,2-dimethylpropyl, 2,2-dimethylpropyl, and the like. Additionally, the alkyl group is optionally substituted.

[0044] The term "cycloalkyl" refers to and includes monocyclic, polycyclic, and spiro alkyl radicals. Preferred cycloalkyl groups are those containing 3 to 12 ring carbon atoms and includes cyclopropyl, cyclopentyl, cyclohexyl, bicyclo[3.1.1]heptyl, spiro[4.5]decyl, spiro[5.5]undecyl, adamantyl, and the like. Additionally, the cycloalkyl group is optionally substituted.

[0045] The terms "heteroalkyl" or "heterocycloalkyl" refer to an alkyl or a cycloalkyl radical, respectively, having at least one carbon atom replaced by a heteroatom. Optionally the at least one heteroatom is selected from O, S, N, P,

B, Si and Se, preferably, O, S or N. Additionally, the heteroalkyl or heterocycloalkyl group is optionally substituted.

[0046] The term "alkenyl" refers to and includes both straight and branched chain alkene radicals. Alkenyl groups are essentially alkyl groups that include at least one carbon-carbon double bond in the alkyl chain. Cycloalkenyl groups are essentially cycloalkyl groups that include at least one carbon-carbon double bond in the cycloalkyl ring. The term "heteroalkenyl" as used herein refers to an alkenyl radical having at least one carbon atom replaced by a heteroatom. Optionally the at least one heteroatom is selected from O, S, N, P, B, Si, and Se, preferably, O, S, or N. Preferred alkenyl, cycloalkenyl, or heteroalkenyl groups are those containing two to fifteen carbon atoms. Additionally, the alkenyl, cycloalkenyl, or heteroalkenyl group is optionally substituted.

[0047] The term "alkynyl" refers to and includes both straight and branched chain alkyne radicals. Preferred alkynyl groups are those containing two to fifteen carbon atoms. Additionally, the alkynyl group is optionally substituted.

[0048] The terms "aralkyl" or "arylalkyl" are used interchangeably and refer to an alkyl group that is substituted with an aryl group. Additionally, the aralkyl group is optionally substituted.

[0049] The term "heterocyclic group" refers to and includes aromatic and non-aromatic cyclic radicals containing at least one heteroatom. Optionally the at least one heteroatom is selected from O, S, N, P, B, Si, and Se, preferably, O, S, or N. Hetero-aromatic cyclic radicals may be used interchangeably with heteroaryl. Preferred heteronon-aromatic cyclic groups are those containing 3 to 7 ring atoms which includes at least one hetero atom, and includes cyclic amines such as morpholino, piperidino, pyrrolidino, and the like, and cyclic ethers/thio-ethers, such as tetrahydrofuran, tetrahydropyran, tetrahydrothiophene, and the like. Additionally, the heterocyclic group may be optionally substituted.

[0050] The term "aryl" refers to and includes both singlering aromatic hydrocarbyl groups and polycyclic aromatic ring systems. The polycyclic rings may have two or more rings in which two carbons are common to two adjoining rings (the rings are "fused") wherein at least one of the rings is an aromatic hydrocarbyl group, e.g., the other rings can be cycloalkyls, cycloalkenyls, aryl, heterocycles, and/or heteroaryls. Preferred aryl groups are those containing six to thirty carbon atoms, preferably six to twenty carbon atoms, more preferably six to twelve carbon atoms. Especially preferred is an aryl group having six carbons, ten carbons or twelve carbons. Suitable aryl groups include phenyl, biphenyl, triphenyl, triphenylene, tetraphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, and azulene, preferably phenyl, biphenyl, triphenyl, triphenylene, fluorene, and naphthalene. Additionally, the aryl group is optionally substituted.

[0051] The term "heteroaryl" refers to and includes both single-ring aromatic groups and polycyclic aromatic ring systems that include at least one heteroatom. The heteroatoms include, but are not limited to O, S, N, P, B, Si, and Se. In many instances, O, S, or N are the preferred heteroatoms. Hetero-single ring aromatic systems are preferably single rings with 5 or 6 ring atoms, and the ring can have from one to six heteroatoms. The hetero-polycyclic ring systems can have two or more rings in which two atoms are common to

two adjoining rings (the rings are "fused") wherein at least one of the rings is a heteroaryl, e.g., the other rings can be cycloalkyls, cycloalkenyls, aryl, heterocycles, and/or heteroaryls. The hetero-polycyclic aromatic ring systems can have from one to six heteroatoms per ring of the polycyclic aromatic ring system. Preferred heteroaryl groups are those containing three to thirty carbon atoms, preferably three to twenty carbon atoms, more preferably three to twelve carbon atoms. Suitable heteroaryl groups include dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine, preferably dibenzothiophene, dibenzofuran, dibenzoselenophene, carbazole, indolocarbazole, imidazole, pyridine, triazine, benzimidazole, 1,2-azaborine, 1,3-azaborine, 1,4-azaborine, borazine, and azaanalogs thereof. Additionally, the heteroaryl group is optionally substituted.

[0052] Of the aryl and heteroaryl groups listed above, the groups of triphenylene, naphthalene, anthracene, dibenzothiophene, dibenzofuran, dibenzoselenophene, carbazole, indolocarbazole, imidazole, pyridine, pyrazine, pyrimidine, triazine, and benzimidazole, and the respective aza-analogs of each thereof are of particular interest.

[0053] The terms alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aralkyl, heterocyclic group, aryl, and heteroaryl, as used herein, are independently unsubstituted, or independently substituted, with one or more general substituents.

[0054] In many instances, the general substituents are selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, boryl, and combinations thereof.

[0055] In some instances, the preferred general substituents are selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, boryl, and combinations thereof.

[0056] In some instances, the more preferred general substituents are selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, alkoxy, aryloxy, amino, silyl, aryl, heteroaryl, sulfanyl, and combinations thereof.

[0057] In yet other instances, the most preferred general substituents are selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof.

[0058] The terms "substituted" and "substitution" refer to a substituent other than H that is bonded to the relevant position, e.g., a carbon. For example, when R^1 represents mono-substitution, then one R^1 must be other than H (i.e., a substitution). Similarly, when R^1 represents di-substitution,

then two of R¹ must be other than H. Similarly, when R¹ represents no substitution, R¹, for example, can be hydrogen for available valencies of ring atoms, as in carbon atoms for benzene and the nitrogen atom in pyrrole, or simply represents nothing for ring atoms with fully filled valencies, e.g., the nitrogen atom in pyridine. The maximum number of substitutions possible in a ring structure will depend on the total number of available valencies in the ring atoms.

[0059] As used herein, "combinations thereof" indicates that one or more members of the applicable list are combined to form a known or chemically stable arrangement that one of ordinary skill in the art can envision from the applicable list. For example, an alkyl and deuterium can be combined to form a partial or fully deuterated alkyl group; a halogen and alkyl can be combined to form a halogenated alkyl substituent; and a halogen, alkyl, and aryl can be combined to form a halogenated arylalkyl. In one instance, the term substitution includes a combination of two to four of the listed groups. In another instance, the term substitution includes a combination of two to three groups. In yet another instance, the term substitution includes a combination of two groups. Preferred combinations of substituent groups are those that contain up to fifty atoms that are not hydrogen or deuterium, or those which include up to forty atoms that are not hydrogen or deuterium, or those that include up to thirty atoms that are not hydrogen or deuterium. In many instances, a preferred combination of substituent groups will include up to twenty atoms that are not hydrogen or deuterium.

[0060] The "aza" designation in the fragments described herein, i.e. aza-dibenzofuran, aza-dibenzothiophene, etc. means that one or more of the C—H groups in the respective fragment can be replaced by a nitrogen atom, for example, and without any limitation, azatriphenylene encompasses both dibenzo[fh]quinoxaline and dibenzo[fh]quinoline. One of ordinary skill in the art can readily envision other nitrogen analogs of the aza-derivatives described above, and all such analogs are intended to be encompassed by the terms as set forth herein.

[0061] As used herein, "deuterium" refers to an isotope of hydrogen. Deuterated compounds can be readily prepared using methods known in the art. For example, U.S. Pat. No. 8,557,400, Patent Pub. No. WO 2006/095951, and U.S. Pat. Application Pub. No. US 2011/0037057, which are hereby incorporated by reference in their entireties, describe the making of deuterium-substituted organometallic complexes. Further reference is made to Ming Yan, et al., *Tetrahedron* 2015, 71, 1425-30 and Atzrodt et al., *Angew. Chem. Int. Ed.* (*Reviews*) 2007, 46, 7744-65, which are incorporated by reference in their entireties, describe the deuteration of the methylene hydrogens in benzyl amines and efficient pathways to replace aromatic ring hydrogens with deuterium, respectively.

[0062] It is to be understood that when a molecular fragment is described as being a substituent or otherwise attached to another moiety, its name may be written as if it were a fragment (e.g. phenyl, phenylene, naphthyl, dibenzofuryl) or as if it were the whole molecule (e.g. benzene,

naphthalene, dibenzofuran). As used herein, these different ways of designating a substituent or attached fragment are considered to be equivalent.

[0063] According to some embodiments of the present disclosure, a novel compound is disclosed that is selected from the group consisting of:

where; A, B, C, D, and F are each independently a 5-membered or 6-membered aromatic ring; ring B may or may not be present; M is selected from the group consisting of Pt, Pd, Cu, and Au; Z^1 , Z^2 , Z^3 , Z^4 , Z^5 , Z^6 , and Z^7 are each independently selected from the group consisting of C and N; m1, m2 and m3 are each independently an integer of 0 or 1; when m2 is 0, each m1 and m3 is 1; when m2 is 1, each m1 and m3 can be 0 or 1; when m1 is 0, L1 is not present; when m2 is 0, L2 is not present; when m3 is 0, L3 is not present; L¹, L², and L³ each independently selected from the group consisting of a direct bond, BR, NR, PR, O, S, Se, C=O, S=O, SO₂, CRR', SiRR', GeRR', alkyl, cycloalkyl, and combinations thereof; each R^A , R^B , R^C , R^D , and R^E represents mono- to maximum possible number of substitutions, or no substitution; each RA, RB, RC, RD, RE, R and R' is independently a hydrogen or a substituent selected from

the group consisting of the general substituents defined herein; and any two substituents can be joined or fused into a ring, provided that, in Formula I, if ring C is a 5-membered aromatic ring, L^2 is present and is a direct bond, then at least one pair of R^D , one pair of R^E , or one R^D and one R^E are joined together to form a fused ring.

[0064] In some embodiments of the compound, each R^A , R^B , R^C , R^D , R^E , R and R' is independently a hydrogen or a substituent selected from the group consisting of the preferred general substituents defined herein.

[0065] In some embodiments of the compound, M is Pt. [0066] In some embodiments of the compound, one of Z^6 and Z^7 is nitrogen, and the other one of Z^6 and Z^7 is carbon. In some embodiments, one of Z^6 and Z^7 is a neutral carbene carbon, and the other one of Z^6 and Z^7 is an anionic carbon. [0067] In some embodiments of the compound, at least one of L^1 , L^2 , and L^3 is present and is not a direct bond. In some embodiments, L^2 is present and is a direct bond. In some embodiments, L^3 and Z^4 are fused to form a 5-membered or 6-membered carbocyclic or heterocyclic ring. In some embodiments, L^3 is present and is selected from the group consisting of O, S, and CRR'.

[0068] In some embodiments of the compound, m1 is 0, m2 is 1, and m3 is 1.

[0069] In some embodiments of the compound, rings A, B, C, D, and E are each independently selected from the group consisting of phenyl, pyridine, pyrimidine, triazine, pyrazole, triazole, imidazole, and imidazole derived carbene. In some embodiments, ring D is a 6-membered aromatic ring. In some embodiments, ring B is present and is a 6-membered aromatic ring. In some embodiments, ring C is a 5-membered aromatic ring.

[0070] In some embodiments of the compound, the compound is Formula I and ring A is pyridine with N coordinating to M.

[0071] In some embodiments of the compound, the compound is selected from the group consisting of:

$$\begin{array}{c} R^{D} \\ C \\ Z^{12} \\ D \\ Z^{13} \\ R^{E} \\ \end{array} \begin{array}{c} Z^{13} \\ Z^{12} \\ Z^{13} \\ R^{C} \\ \end{array} \begin{array}{c} Z^{13} \\ Z^{2} \\ R^{F} \\ \end{array} \begin{array}{c} Z^{13} \\ R^{C} \\ \end{array} \begin{array}{c} Z^{13} \\ \end{array} \begin{array}{c} Z^{13} \\ \end{array} \begin{array}{c} Z^{13} \\ \end{array} \begin{array}{c} Z^{14} \\ \end{array} \begin{array}{c} Z^{13} \\ \end{array} \begin{array}{c} Z^{13} \\ \end{array} \begin{array}{c} Z^{14} \\ \end{array} \begin{array}{c} Z^{1$$

$$\begin{array}{c}
\mathbb{R}^{D} \\
\mathbb{R}^{D} \\
\mathbb{C} \\
\mathbb{C}^{14} \\
\mathbb{R}^{E}
\end{array}$$

$$\begin{array}{c}
\mathbb{C} \\
\mathbb{C}^{14} \\
\mathbb{C}^{13} \\
\mathbb{C}^{14} \\
\mathbb{C}^{13} \\
\mathbb{C}^{15} \\
\mathbb{C}^{15} \\
\mathbb{C}^{15} \\
\mathbb{C}^{15} \\
\mathbb{C}^{10} \\
\mathbb{$$

where:

 $Z^1, Z^2, Z^3, Z^4, Z^5, Z^6, Z^7, Z^8, Z^9, Z^{10}, Z^{11}, Z^{12}, Z^{13}, Z^{14}$, and Z^{15} are each independently C or N; R^A , R^B , R^C , R^D , R^E , L^1 , L^2 , L^3 , m1, m2, and m3 are as defined above in connection with Formulas I, II, and III; R^F represents mono- to maximum possible number of substitutions, or no substitution; each R^F is independently a hydrogen or a substituent selected from the group consisting of the general substituents defined herein; and any two substituents can be joined or fused into a ring. In some embodiments of the compound each R^A , R^B , R^C , R^D , R^E , and R^F is independently a hydrogen or a substituent selected from the group consisting of the preferred general substituents defined herein.

[0072] In some embodiments of the compound, wherein the compound has the structure according to Formula X

$$\mathbb{R}^{F}$$

$$\mathbb{R}^{E}$$

$$\mathbb{R}^{E}$$

$$\mathbb{R}^{E}$$

$$\mathbb{R}^{B}$$

$$\mathbb{R}^{B}$$

where; R^Y represents mono- to tetra-substitutions, or no substitution; any two substituents can be joined or fused into a ring; R^Y is a hydrogen or a substituent selected from the group consisting of the general substituents defined herein; and where R^Z is selected from the group consisting of alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, silyl, aryl, heteroaryl, boryl, partially or fully deturated variants thereof, partially or fully fluorinated variants thereof, and combinations thereof.

[0073] In some embodiments of the compound, at least one of R^A , R^B , R^C , R^D , R^E , R^F , R^B , and R' comprises a chemical group containing at least three 6-membered aromatic rings that are not fused next to each other. In some embodiments of the compound, at least one of R^A , R^B , R^C , R^D , R^E , R^F , R and R' comprises a chemical group containing at least four 6-membered aromatic rings that are not fused next to each other. In some embodiments of the compound, at least one of R^A , R^B , R^C , R^D , R^E , R^F , R and R' comprises a chemical group containing at least five 6-membered aromatic rings that are not fused next to each other. In some embodiments of the compound, at least one of R^A , R^B , R^C , R^D , R^E , R^F , R and R' comprises a chemical group containing at least six 6-membered aromatic rings that are not fused next to each other.

[0074] In some embodiments of the compound having the structure according to Formula X, at least one of R^{Y} and R^{Z} comprises a chemical group containing at least three 6-membered aromatic rings that are not fused next to each other. In some embodiments, at least one of R^{Y} and R^{Z} comprises a chemical group containing at least four 6-membered aromatic rings that are not fused next to each other. In some embodiments, at least one of R^{Y} and R^{Z} comprises a chemical group containing at least three 6-membered aromatic rings that are not fused next to each other. In some embodiments, at least one of R^{Y} and R^{Z} comprises a chemical group containing at least four 6-membered aromatic rings that are not fused next to each other. In some embodiments, at least one of R^{Y} and R^{Z} comprises at least five 6-membered aromatic rings that are not fused next to each other. In some embodiments, at least one of R^{Y} and R^{Z} comprises at least six 6-membered aromatic rings that are not fused next to each other.

[0075] In some embodiments of the compound, the compound is the compound x having the formula $(L_{Xi})Pt(L_{Yj})$ (L_{Zk}) ;

[0076] where,

[0077] L_{Xi} is a bidentate ligand;

[0078] L_{y_i} is a monodentate ligand;

[0079] L_{Zk} is a monodentate ligand;

[0080] L_{Xi} is linked to L_{Zk} by a linking group L^3 ;

[0081] L_{Zk} is linked to L_{Yj} by a direct bond;

[0082] x=30(k-1)+j+1200(i-1), i is an integer from 1 to 212258,j is an integer from 1 to 30, and k is an integer from 1 to 40; when k=41, 42, or 43, x=25(k-41)+j+75(i-1)+254709600, i is an integer from 1 to 212258,j is an integer from 1 to 25;

[0083] L_{Xi} is selected from the group consisting of L_{X1} to $L_{X212258}$ whose structures are defined as follows:

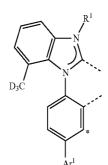
L_{Xi}	Structure of L_{Xi}	Ar ¹ , R ¹	i
wherein L_{X1} to L_{X9900} have the structure	R ¹	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m - 1) + n
wherein $L_{\chi_{9901}}$ - $L_{\chi_{19800}}$ have the structure	Ar ¹	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 9900
wherein L_{X19801} - L_{X29700} have the structure	Ar ¹ *	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 19800
wherein L_{X29701} - L_{X39600} have the structure	Ar ¹ *	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 29700
wherein L_{X39601} - L_{X49500} have the structure	* Ar ¹ N N	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 39600

	-cor	ntinued	
\mathcal{L}_{Xi}	Structure of L_{Xi}	Ar^1 , R^1	i
wherein L_{X49501} - L_{X59400} have the structure	N. N.	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m - 1) + n + 49500
	* Ar¹		
wherein L_{X59401} - L_{X69300} have the structure	R ¹	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m - 1) + n + 59400
wherein L_{X69301} - L_{X79200} have the structure	Ar ¹ *	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 69300
wherein L_{X79201} to L_{X79530} have the structure	* Ar' N	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 79200
wherein	N ***	wherein $R^1 = Rn$,	y = n + 79530
L _{X79531} -L _{X79860} have the structure	N N N N N N N N N N N N N N N N N N N	wherein <i>n</i> is an integer from 1 to 330, and	

-continued			
\mathbb{L}_{Xi}	Structure of L_{Xi}	Ar^1 , R^1	i
wherein L_{X79861} - L_{X80190} have the structure	N N N *	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 79860
wherein L_{X80191} - L_{X80520} have the structure	N N N N N N N N N N N N N N N N N N N	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 80190
wherein L_{X80521} to L_{X90420} have the structure	CD ₃ R Ar *	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 80520
wherein L_{X90421} to $L_{X100320}$ have the structure	D_3C N $*$	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 90420
wherein $L_{X100321}$ to $L_{X110220}$ have the structure	CD_3 R^1 D_3C N $*$	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 100320

	-cont	inued	
L_{Xi}	Structure of L_{Xi}	Ar^1 , R^1	i
wherein $L_{X110221}$ to $L_{X120120}$ have the structure	D ₃ C R ¹ N N Ar ¹	wherein $Ar^1 = Am$ and $R^1 = y = 3$ Rn, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	330(m-1) + n + 110220
wherein ${ m L}_{X120121}$ to ${ m L}_{X130020}$ have the structure	R ¹ N N *	wherein $Ar^1 = Am$ and $R^1 = y = 3$ Rn , wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	330(m - 1) + n + 120120
wherein $L_{X130021}$ to $L_{X139920}$ have the structure	CD ₃	wherein $Ar^1 = Am$ and $R^1 = y = 3$ Rn , wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	330(<i>m</i> – 1) + <i>n</i> + 130020

wherein $L_{X139921}$ to $L_{X149820}$ have the structure



wherein $Ar^1 = Am$ and $R^1 = y = 330(m-1) + n + Rn$, 139920 wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and

-continued

L_{Xi}	Structure of L_{Xi}	Ar ¹ , R ¹	i
wherein $L_{X149821}$ to $L_{X159720}$ have the structure	D_3C N N Ar^1	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 149820
wherein $L_{X159721}$ to $L_{X169620}$ have the structure	Ar R ¹	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 159720
wherein $L_{X169621}$ to $L_{X169950}$ have the structure	CD ₃ R ¹	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 169620
wherein $L_{X169951}$ to $L_{X170280}$ have the structure	PI N N N N N N N N N N N N N N N N N N N	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 169950
wherein $L_{X170281}$ to $L_{X170610}$ have the structure	D ₃ C R ¹	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 170280

-continued

\mathbb{L}_{Xi}	Structure of L_{Xi}	Ar^1 , R^1	i
wherein ${\cal L}_{X170610}$ to ${\cal L}_{X170940}$ have the structure	R ¹	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 170610
wherein $L_{X170941}$ to $L_{X171270}$ have the structure	* N N *	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 170940
wherein $L_{X171271}$ to $L_{X171600}$ have the structure	D R ¹	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 171270
wherein $L_{X171601}$ to $L_{X181500}$ have the structure	D R ¹	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 171600
wherein $L_{X181501}$ to $L_{X191400}$ have the structure	Ar ¹ * D R ¹ N *	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 181500

-continued

-continued				
\mathbb{L}_{Xi}	Structure of L_{Xi}	Ar^1 , R^1	i	
wherein $L_{X191401}$ to $L_{X191430}$ to $L_{X191730}$ have the structure	D R ¹ N *	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 191400	
wherein ${\rm L}_{X191731}$ to ${\rm L}_{X192060}$ have the structure	D ₃ C R ¹	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 191730	
wherein ${ m L}_{X192061}$ to ${ m L}_{X201960}$ have the structure	D_3C R^1 D_3C N	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 192060	
wherein ${\rm L}_{\rm X201961}$ to ${\rm L}_{\rm X211860}$ have the structure	Ar ¹ * D ₃ C N N N N N N N N N N N N N	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 201960	
wherein ${\rm L}_{X211861}$ to ${\rm L}_{X212190}$ have the structure	Ar^{1} $D_{3}C$ N N $*$	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 211860	

 $L_{X212191}$

 $L_{X212196}$

 $L_{X212206}$

 $L_{X212208}$

-continued

$$L_{\lambda212203}$$

$$L_{X212207}$$

 $\mathcal{L}_{X212212}$

 $L_{X212215}$

-continued

L_{X212211}

L_{X212221}

 $\mathcal{L}_{X212234}$

 $L_{X212235}$

 $L_{X212236}$

-continued

L_{X212232}

L_{X212233}

-continued

 $L_{X212237}$ N * $L_{X212238}$

 $L_{X212241}$

 $L_{X212240}$

L_{X212242}

 $\mathcal{L}_{X212245}$

-continued

L_{X212246}

 $L_{\rm X212253}$

 $L_{X212254}$

 $L_{X212255}$

-continued

-continued

$$\begin{array}{c} L_{X212257} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array}$$

[0084] wherein A1 to A30 have the following structures:

A3

-continued

A12

tBu,

iPr,

A13

A6

A8

A22

A24

-continued

[0085] and R1 to R330 have the following structures:

$$D \longrightarrow D$$

A30

$$\begin{array}{c} \\ D \\ D \\ D \\ D \\ D \end{array} \begin{array}{c} D, \\ D \\ D \end{array}$$

$$i P r, $$ t B u, $$$$

$$\mathbb{R}^{14}$$

$$\begin{array}{c} & & \\ & & \\ D \\ D \\ D \\ D \end{array}$$

$$D_3C$$
 CD_3 ,

$$CF_3$$
 D
 D
 D
 D
 D

$$F_3C$$

R77

R85

R93

R112

R113

R114

-continued

R126

R160

R172

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

R196

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

$$\begin{array}{c} D \\ D \\ D \\ D \end{array}$$

-continued

R238

R244

R248

R249

R250

R259

R254

R255

R262

-continued

R266

R268

-continued

R269

R272

-continued

R282

R283

R284

R285

R289

R287

R288

-continued

R296

R300

R306

R307

R308

R309

R313

R322

-continued

-continued

[0086] L_{yj} is selected from the group consisting of:

$$L_{y_7}$$

$$L_{Y|4}$$

$$L_{120}$$

$$N \underset{**}{ \searrow} S,$$

$$L_{1/24}$$

$$L_{129}$$

[0087] L_{Zk} is selected from the group consisting of:

$$\mathbb{L}_{Z1}$$

 L_{Z18}

 L_{Z20}

$$L_{Z30}$$

 \mathbb{L}_{Z33}

 L_{Z36}

-continued

$$\begin{array}{c} L_{Z39} \\ \\ ** \\ N \\ N \\ \end{array}$$

L_{Z41}

[0088] and the * of L_{Zk} attaches to the * of L_{Xi} , and the ** of L_{Zk} attaches to the ** of L_{Yj} .

[0089] In some embodiments, the compound is compound x having the formula $(L_{Xi})Pt(L_{Yj})(L_{Zk})$; where x=5(k-41)+(j-25)+15(i-1)+270628950, i is an integer from 1 to 212258, j is an integer from 26 to 30, and k is an integer from 41 to 43.

[0090] In some embodiments, the compound is selected from the group consisting of:

[0091] An organic light emitting device (OLED) is disclosed, where the OLED comprises: an anode; a cathode; and an organic layer, disposed between the anode and the cathode, comprising a compound selected from the group consisting of:

Formula I

Formula I

-continued Fort

wherein; A, B, C, D, and F are each independently a 5-membered or 6-membered aromatic ring; ring B may or may not be present; M is selected from the group consisting of Pt, Pd, Cu, and Au; Z^1 , Z^2 , Z^3 , Z^4 , Z^5 , Z^6 , and Z^7 are each independently selected from the group consisting of C and N; m1, m2 and m3 are each independently an integer of 0 or 1; when m2 is 0, each m1 and m3 is 1; when m2 is 1, each m1 and m3 can be 0 or 1; when m1 is 0, L^1 is not present; when m2 is 0, L^2 is not present; when m3 is 0, L^3 is not present; L¹, L², and L³ each independently selected from the group consisting of a direct bond, BR, NR, PR, O, S, Se, C=O, S=O, SO₂, CRR', SiRR', GeRR', alkyl, cycloalkyl, and combinations thereof; each R^A , R^B , R^C , R^D , and R^E represents mono- to maximum possible number of substitutions, or no substitution; each R^A , R^B , R^C , R^D , R^E , R and R' is a hydrogen or a substituent independently selected from the group consisting of the general substituents as defined herein; any two substituents can be joined or fused into a ring, provided that, in Formula I, if ring C is a 5-membered aromatic ring, L² is present and is a direct bond, then at least one pair of R^D , one pair of R^E , or one R^D and one R^E are joined together to form a fused ring.

[0092] In some embodiments of the OLED, the compound is a sensitizer; wherein the device further comprises an acceptor; and wherein the acceptor is selected from the group consisting of fluorescent emitter, delayed fluorescence emitter, and combination thereof.

[0093] A consumer product comprising the OLED is also disclosed, where the OLED comprises: an anode; a cathode; and an organic layer, disposed between the anode and the cathode, comprising a compound selected from the group consisting of:

where; A, B, C, D, and F are each independently a 5-membered or 6-membered aromatic ring; ring B may or may not be present; M is selected from the group consisting of Pt, Pd, Cu, and Au; Z^1 , Z^2 , Z^3 , Z^4 , Z^5 , Z^6 , and Z^7 are each independently selected from the group consisting of C and N; m1, m2 and m3 are each independently an integer of 0 or 1; when m2 is 0, each m1 and m3 is 1; when m2 is 1, each m1 and m3 can be 0 or 1; when m1 is 0, L1 is not present; when m2 is 0, L^2 is not present; when m3 is 0, L^3 is not present; L¹, L², and L³ each independently selected from the group consisting of a direct bond, BR, NR, PR, O, S, Se, C=O, S=O, SO₂, CRR', SiRR', GeRR', alkyl, cycloalkyl, and combinations thereof; each R^A , R^B , R^C , R^D , and R^E represents mono- to maximum possible number of substitutions, or no substitution; each $\mathbf{\hat{R}}^A$, \mathbf{R}^B , \mathbf{R}^C , \mathbf{R}^D , \mathbf{R}^E , \mathbf{R} and R' is a hydrogen or a substituent independently selected from the group consisting of the general substituents defined herein; and any two substituents can be joined or fused into a ring, provided that, in Formula I, if ring C is a 5-membered aromatic ring, L² is present and is a direct bond, then at least

one pair of R^D , one pair of R^E , or one R^D and one R^E are joined together to form a fused ring.

[0094] In some embodiments, the OLED has one or more characteristics selected from the group consisting of being flexible, being rollable, being foldable, being stretchable, and being curved. In some embodiments, the OLED is transparent or semi-transparent. In some embodiments, the OLED further comprises a layer comprising carbon nanotubes.

[0095] In some embodiments, the OLED further comprises a layer comprising a delayed fluorescent emitter. In some embodiments, the OLED comprises a RGB pixel arrangement or white plus color filter pixel arrangement. In some embodiments, the OLED is a mobile device, a hand held device, or a wearable device. In some embodiments, the OLED is a display panel having less than 10 inch diagonal or 50 square inch area. In some embodiments, the OLED is a display panel having at least 10 inch diagonal or 50 square inch area. In some embodiments, the OLED is a lighting panel.

[0096] In some embodiments, the compound can be an emissive dopant. In some embodiments, the compound can produce emissions via phosphorescence, fluorescence, thermally activated delayed fluorescence, i.e., TADF (also referred to as E-type delayed fluorescence; see, e.g., U.S. application Ser. No. 15/700,352, which is hereby incorporated by reference in its entirety), triplet-triplet annihilation, or combinations of these processes. In some embodiments, the emissive dopant can be a racemic mixture, or can be enriched in one enantiomer. In some embodiments, the compound can be homoleptic (each ligand is the same). In some embodiments, the compound can be heteroleptic (at least one ligand is different from others).

[0097] When there are more than one ligand coordinated to a metal, the ligands can all be the same in some embodiments. In some other embodiments, at least one ligand is different from the other ligand(s). In some embodiments, every ligand can be different from each other. This is also true in embodiments where a ligand being coordinated to a metal can be linked with other ligands being coordinated to that metal to form a tridentate, tetradentate, pentadentate, or hexadentate ligands. Thus, where the coordinating ligands are being linked together, all of the ligands can be the same in some embodiments, and at least one of the ligands being linked can be different from the other ligand(s) in some other embodiments.

[0098] In some embodiments, the compound can be used as a phosphorescent sensitizer in an OLED where one or multiple layers in the OLED contains an acceptor in the form of one or more fluorescent and/or delayed fluorescence emitters. In some embodiments, the compound can be used as one component of an exciplex to be used as a sensitizer. As a phosphorescent sensitizer, the compound must be capable of energy transfer to the acceptor and the acceptor will emit the energy or further transfer energy to a final emitter. The acceptor concentrations can range from 0.001% to 100%. The acceptor could be in either the same layer as the phosphorescent sensitizer or in one or more different layers. In some embodiments, the acceptor is a TADF emitter. In some embodiments, the acceptor is a fluorescent emitter. In some embodiments, the emission can arise from any or all of the sensitizer, acceptor, and final emitter.

[0099] In some embodiments, the compound of the present disclosure is neutrally charged.

[0100] According to another aspect, a formulation comprising the compound described herein is also disclosed. The formulation can include one or more components selected from the group consisting of a solvent, a host, a hole injection material, hole transport material, electron blocking material, hole blocking material, and an electron transport material, disclosed herein.

[0101] The OLED disclosed herein can be incorporated into one or more of a consumer product, an electronic component module, and a lighting panel. The organic layer can be an emissive layer and the compound can be an emissive dopant in some embodiments, while the compound can be a non-emissive dopant in other embodiments.

[0102] The organic layer can also include a host. In some embodiments, two or more hosts are preferred. In some embodiments, the hosts used may be a) bipolar, b) electron transporting, c) hole transporting or d) wide band gap materials that play little role in charge transport. In some embodiments, the host can include a metal complex. The host can be a triphenylene containing benzo-fused thiophene or benzo-fused furan. Any substituent in the host can be an unfused substituent independently selected from the group consisting of C_nH_{2n+1} , OC_nH_{2n+1} , OAr_1 , $N(C_nH_{2n+1})_2$, $N(Ar_1)(Ar_2)$, $CH = CH - C_nH_{2n+1}$, $C = C - C_nH_{2n+1}$, Ar_1 , Ar_1 — Ar_2 , and C_nH_{2n} — Ar_1 , or the host has no substitutions. In the preceding substituents n can range from 1 to 10; and Ar and Ar₂ can be independently selected from the group consisting of benzene, biphenyl, naphthalene, triphenylene, carbazole, and heteroaromatic analogs thereof. The host can be an inorganic compound. For example a Zn containing inorganic material e.g. ZnS.

[0103] The host can be a compound comprising at least one chemical group selected from the group consisting of triphenylene, carbazole, dibenzothiophene, dibenzofuran, dibenzoselenophene, azatriphenylene, azacarbazole, azadibenzothiophene, aza-dibenzofuran, and aza-dibenzoselenophene. The host can include a metal complex. The host can be, but is not limited to, a specific compound selected from the Host Group consisting of:

and combinations thereof.

Additional information on possible hosts is provided below. [0104] An emissive region in an OLED is also disclosed, the emissive region comprises a compound selected from the group consisting of:

Formula II

$$\begin{pmatrix}
L^2 \\
D Z^7
\end{pmatrix}$$

$$\begin{pmatrix}
L^2 \\
M
\end{pmatrix}$$

$$\begin{pmatrix}
L$$

-continued

Formula III

$$\begin{array}{c}
\mathbb{R}^{D} \\
\mathbb{C} \\
\mathbb{C} \\
\mathbb{C} \\
\mathbb{C}^{6}
\end{array}$$

Formula III

 $\begin{array}{c}
\mathbb{R}^{2} \\
\mathbb{R}^{2}
\end{array}$
 $\begin{array}{c}
\mathbb{R}^{2} \\
\mathbb{R}^{2}
\end{array}$
 $\begin{array}{c}
\mathbb{R}^{2} \\
\mathbb{R}^{B}
\end{array}$

where; A, B, C, D, and F are each independently a 5-membered or 6-membered aromatic ring; ring B may or may not be present; M is selected from the group consisting of Pt, Pd, Cu, and Au; Z^1 , Z^2 , Z^3 , Z^4 , Z^5 , Z^6 , and Z^7 are each independently selected from the group consisting of C and N; m1, m2 and m3 are each independently an integer of 0 or 1; when m2 is 0, each m1 and m3 is 1; when m2 is 1, each m1 and m3 can be 0 or 1; when m1 is 0, L¹ is not present; when m2 is 0, L^2 is not present; when m3 is 0, L^3 is not present; L^1 , L^2 , and L^3 each independently selected from the group consisting of a direct bond, BR, NR, PR, O, S, Se, C=O, S=O, SO₂, CRR', SiRR', GeRR', alkyl, cycloalkyl, and combinations thereof; each R^A , R^B , R^C , R^D , and R^E represents mono- to maximum possible number of substitutions, or no substitution; each R^A , R^B , R^C , R^D , R^E , R and R' is a hydrogen or a substituent independently selected from the group consisting of the general substituents defined herein; and any two substituents can be joined or fused into a ring, provided that, in Formula I, if ring C is a 5-membered aromatic ring, L^2 is present and is a direct bond, then at least one pair of R^D , one pair of R^E , or one R^D and one R^E are joined together to form a fused ring.

[0105] In some embodiments of the emissive region, the compound is an emissive dopant or a non-emissive dopant. In some embodiments, the emissive region further comprises a host, wherein the host comprises at least one selected from the group consisting of metal complex, triphenylene, carbazole, dibenzothiophene, dibenzofuran, dibenzothiophene, aza-triphenylene, aza-carbazole, aza-dibenzothiophene, aza-dibenzofuran, and aza-dibenzoselenophene.

[0106] In some embodiments, the emissive region further comprises a host, wherein the host is selected from the Host Group defined herein.

[0107] In yet another aspect of the present disclosure, a formulation that comprises the novel compound disclosed herein is described. The formulation can include one or more components selected from the group consisting of a solvent, a host, a hole injection material, hole transport material, electron blocking material, hole blocking material, and an electron transport material, disclosed herein.

[0108] The present disclosure encompasses any chemical structure comprising the novel compound of the present disclosure, or a monovalent or polyvalent variant thereof. In other words, the inventive compound, or a monovalent or polyvalent variant thereof, can be a part of a larger chemical structure. Such chemical structure can be selected from the group consisting of a monomer, a polymer, a macromolecule, and a supramolecule (also known as supermolecule). As used herein, a "monovalent variant of a compound"

refers to a moiety that is identical to the compound except that one hydrogen has been removed and replaced with a bond to the rest of the chemical structure. As used herein, a "polyvalent variant of a compound" refers to a moiety that is identical to the compound except that more than one hydrogen has been removed and replaced with a bond or bonds to the rest of the chemical structure. In the instance of a supramolecule, the inventive compound is can also be incorporated into the supramolecule complex without covalent bonds.

Combination with Other Materials

[0109] The materials described herein as useful for a particular layer in an organic light emitting device may be used in combination with a wide variety of other materials present in the device. For example, emissive dopants disclosed herein may be used in conjunction with a wide variety of hosts, transport layers, blocking layers, injection layers, electrodes and other layers that may be present. The materials described or referred to below are non-limiting examples of materials that may be useful in combination with the compounds disclosed herein, and one of skill in the art can readily consult the literature to identify other materials that may be useful in combination.

Conductivity Dopants:

[0110] A charge transport layer can be doped with conductivity dopants to substantially alter its density of charge carriers, which will in turn alter its conductivity. The conductivity is increased by generating charge carriers in the matrix material, and depending on the type of dopant, a change in the Fermi level of the semiconductor may also be achieved. Hole-transporting layer can be doped by p-type conductivity dopants and n-type conductivity dopants are used in the electron-transporting layer.

[0111] Non-limiting examples of the conductivity dopants that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: EP01617493, EP01968131, EP2020694, EP2684932, US20050139810, US20070160905, US20090167167, US2010288362, WO006081780, WO2009003455, WO2009008277, WO2009011327, WO2014009310, US2007252140, US2015060804, US20150123047, and US2012146012.

$$NCC_6F_4$$
 F
 C_6F_4CN ,

$$N$$
 F
 F
 F
 F
 N
 N

HIL/HTL:

[0112] A hole injecting/transporting material to be used in the present invention is not particularly limited, and any compound may be used as long as the compound is typically used as a hole injecting/transporting material. Examples of the material include, but are not limited to: a phthalocyanine or porphyrin derivative; an aromatic amine derivative; an indolocarbazole derivative; a polymer containing fluorohydrocarbon; a polymer with conductivity dopants; a conducting polymer, such as PEDOT/PSS; a self-assembly mono-

mer derived from compounds such as phosphonic acid and silane derivatives; a metal oxide derivative, such as MoO_x ; a p-type semiconducting organic compound, such as 1,4,5, 8,9,12-Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

[0113] Examples of aromatic amine derivatives used in HIL or HTL include, but not limit to the following general structures:

$$Ar^{2}$$
 Ar^{3}
 Ar^{3}
 Ar^{3}
 Ar^{4}
 Ar^{4}
 Ar^{4}
 Ar^{4}
 Ar^{5}
 Ar^{5}
 Ar^{5}
 Ar^{5}
 Ar^{6}
 Ar^{7}
 Ar^{8}
 Ar^{9}
 Ar^{7}
 Ar^{8}
 Ar^{8}
 Ar^{9}
 Ar^{9}
 Ar^{9}
 Ar^{9}
 Ar^{9}
 Ar^{9}
 Ar^{9}
 Ar^{9}
 Ar^{9}
 Ar^{9}

Each of Ar¹ to Ar⁹ is selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, and azulene; the group consisting of aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benbenzoxazole, zimidazole, indazole, indoxazine, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and the group consisting of 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Each Ar may be unsubstituted or may be substituted by a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acids, ether, ester, nitrile, isonitrile, sulfanyl, sulfanyl, sulfonyl, phosphino, and combinations thereof.

[0114] In one aspect, Ar¹ to Ar⁹ is independently selected from the group consisting of:

wherein k is an integer from 1 to 20; X^{101} to X^{108} is C (including CH) or N; Z^{101} is NAr¹, O, or S; Ar¹ has the same group defined above.

[0115] Examples of metal complexes used in HIL or HTL include, but are not limited to the following general formula:

$$\begin{bmatrix} \begin{pmatrix} Y^{101} \\ Y^{102} \end{pmatrix}_{l'} \text{Met} & --(L^{101})_{k'} \end{bmatrix}$$

wherein Met is a metal, which can have an atomic weight greater than 40; $(Y^{101}\text{-}Y^{102})$ is a bidentate ligand, Y^{101} and Y^{102} are independently selected from C, N, O, P, and S; L^{01} is an ancillary ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal; and k'+k" is the maximum number of ligands that may be attached to the metal.

[0116] In one aspect, $(Y^{101}-Y^{102})$ is a 2-phenylpyridine derivative. In another aspect, $(Y^{101}-Y^{102})$ is a carbene ligand. In another aspect, Met is selected from Ir, Pt, Os, and Zn. In a further aspect, the metal complex has a smallest oxidation potential in solution vs. Fc⁺/Fc couple less than about 0.6 V.

[0117] Non-limiting examples of the HIL and HTL materials that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: CN102702075, EP01624500, DE102012005215, EP01698613, EP01806334, EP01930964, EP01972613, EP01997799, EP02011790, EP02055700, EP02055701, EP1725079, EP2085382, EP2660300, EP650955, JP07-073529, JP2005112765, JP2007091719, JP2008021687, JP2014-009196. KR20110088898, KR20130077473. TW201139402, U.S. Ser. No. 06/517,957, US20020158242, US20050123751, US20030162053, US20060182993, US20060240279, US20070145888, US20070181874, US20070278938, US20080014464, US20080091025, US20080106190, US20080124572, US20080145707, US20080233434, US20080303417, US20080220265, US2008107919, US20090115320, US20090167161, US2009066235, US2011007385, US20110163302, US2011240968, US2011278551, US2012205642, US2013241401, US20140117329, US2014183517, U.S. Pat. Nos. 5,061,569, 5,639,914, WO05075451, WO07125714, WO08023550, WO08023759, WO2009145016, WO2010061824, WO2011075644, WO2012177006, WO2013018530, WO2013039073. WO2013087142, WO2013118812, WO2013120577, WO2013157367, WO2013175747, WO2014002873, WO2014015935, WO2014015937, WO2014030872, WO2014030921, WO2014034791, WO2014104514, WO2014157018.

EBL:

[0118] An electron blocking layer (EBL) may be used to reduce the number of electrons and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies, and/or longer lifetime, as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED. In some embodiments, the EBL material has a higher LUMO (closer to the vacuum level) and/or higher triplet energy than the emitter closest to the EBL interface. In some embodiments, the EBL material has a higher LUMO (closer to the vacuum level) and/or higher triplet energy than one or more of the hosts closest to the EBL interface. In one aspect, the compound used in EBL contains the same molecule or the same functional groups used as one of the hosts described below.

Host:

[0119] The light emitting layer of the organic EL device of the present invention preferably contains at least a metal complex as light emitting material, and may contain a host material using the metal complex as a dopant material. Examples of the host material are not particularly limited, and any metal complexes or organic compounds may be used as long as the triplet energy of the host is larger than that of the dopant. Any host material may be used with any dopant so long as the triplet criteria is satisfied.

[0120] Examples of metal complexes used as host are preferred to have the following general formula:

$$\begin{bmatrix} Y^{103} \\ Y^{104} \end{bmatrix}_{k'} \text{Met} \longrightarrow (L^{101})_{k'}$$

wherein Met is a metal; $(Y^{103}-Y^{104})$ is a bidentate ligand, Y^{103} and Y^{104} are independently selected from C, N, O, P, and S; L^{101} is an another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached

to the metal; and k'+k" is the maximum number of ligands that may be attached to the metal.

[0121] In one aspect, the metal complexes are:

$$\begin{bmatrix} O \\ N \end{bmatrix}_{\nu} Al \longrightarrow (L^{101})_{3-k'} \quad \begin{bmatrix} O \\ N \end{bmatrix}_{\nu} Zn \longrightarrow (L^{101})_{2-k'}$$

wherein (O—N) is a bidentate ligand, having metal coordinated to atoms O and N.

[0122] In another aspect, Met is selected from Ir and Pt. In a further aspect, $(Y^{103} - Y^{104})$ is a carbene ligand.

[0123] Examples of other organic compounds used as host are selected from the group consisting of aromatic hydrocarbon cyclic compounds such as benzene, biphenyl, triphenyl, triphenylene, tetraphenylene, naphthalene, anthracene, phenalene, phenanthrene, fluorene, pyrene, chrysene, perylene, and azulene; the group consisting of aromatic heterocyclic compounds such as dibenzothiophene, dibenzofuran, dibenzoselenophene, furan, thiophene, benzofuran, benzothiophene, benzoselenophene, carbazole, indolocarbazole, pyridylindole, pyrrolodipyridine, pyrazole, imidazole, triazole, oxazole, thiazole, oxadiazole, oxatriazole, dioxazole, thiadiazole, pyridine, pyridazine, pyrimidine, pyrazine, triazine, oxazine, oxathiazine, oxadiazine, indole, benzimidazole, indazole, indoxazine, benzoxazole, benzisoxazole, benzothiazole, quinoline, isoquinoline, cinnoline, quinazoline, quinoxaline, naphthyridine, phthalazine, pteridine, xanthene, acridine, phenazine, phenothiazine, phenoxazine, benzofuropyridine, furodipyridine, benzothienopyridine, thienodipyridine, benzoselenophenopyridine, and selenophenodipyridine; and the group consisting of 2 to 10 cyclic structural units which are groups of the same type or different types selected from the aromatic hydrocarbon cyclic group and the aromatic heterocyclic group and are bonded to each other directly or via at least one of oxygen atom, nitrogen atom, sulfur atom, silicon atom, phosphorus atom, boron atom, chain structural unit and the aliphatic cyclic group. Each option within each

group may be unsubstituted or may be substituted by a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acids, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof.

[0124] In one aspect, the host compound contains at least one of the following groups in the molecule:

-continued Z¹⁰¹

$$X^{102}$$
 X^{103}
 X^{104}
 X^{105}
 X^{108}
 X^{106}
 X^{107}
 X^{108}
 X^{108}
 X^{108}
 X^{108}
 X^{108}
 X^{108}
 X^{108}
 X^{108}
 X^{109}
 X^{109

wherein R^{101} is selected from the group consisting of hydrogen, deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acids, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, and when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above. k is an integer from 0 to 20 or 1 to 20. X^{101} to X^{108} are independently selected from C (including CH) or N. Z^{101} and Z^{102} are independently selected from NR¹⁰¹, O, or S.

[0125] Non-limiting examples of the host materials that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: EP2034538, EP2034538A, EP2757608, JP2007254297, KR20100079458, KR20120088644, KR20120129733, KR20130115564, TW201329200, US20030175553. US20050238919, US20060280965, US20090017330, US20090030202, US20090167162, US20090302743. US20090309488, US20100012931, US20100084966, US20100187984, US2010187984, US2012075273, US2012126221, US2013009543, US2013105787, US2013175519, US2014001446. US20140183503, US20140225088, US2014034914, U.S. Pat. No. 7,154,114, WO2001039234, WO2005014551, WO2004093207. WO2005089025. WO2006072002. WO2006114966. WO2007063754, WO2008056746, WO2009003898, WO2009021126, WO2009063833, WO2009066778, WO2009066779. WO2009086028, WO2010056066, WO2010107244, WO2011081423, WO2011081431, WO2011086863, WO2012128298, WO2012133644, WO2012133649, WO2013024872, WO2013035275,

WO2013081315, WO2013191404, WO2014142472, US20170263869, US20160163995, U.S. Pat. No. 9,466, 803,

Additional Emitters:

[0126] One or more additional emitter dopants may be used in conjunction with the compound of the present disclosure. Examples of the additional emitter dopants are not particularly limited, and any compounds may be used as long as the compounds are typically used as emitter materials. Examples of suitable emitter materials include, but are not limited to, compounds which can produce emissions via phosphorescence, fluorescence, thermally activated delayed fluorescence, i.e., TADF (also referred to as E-type delayed fluorescence), triplet-triplet annihilation, or combinations of these processes.

[0127] Non-limiting examples of the emitter materials that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: CN103694277, CN1696137, EB01238981, EP01239526, EP01961743, EP1239526. EP1244155. EP1642951. EP1647554. EP1841834, EP1841834B, EP2062907, EP2730583, JP2012074444, JP2013110263. JP4478555, KR1020090133652, KR20120032054, KR20130043460, TW201332980, U.S. Ser. No. 06/699,599, U.S. Ser. No. 06/916,554, US20010019782, US20020034656, US20030068526, US20030072964, US20030138657. US20050123788, US20050244673. US2005123791. US2005260449, US20060008670, US20060065890, US20060127696, US20060134459, US20060134462, US20060202194, US20060251923, US20070034863, US20070087321, US20070103060, US20070111026, US20070190359, US20070231600, US2007034863, US2007104979, US2007104980, US2007138437, US2007224450, US2007278936, US20080020237, US20080233410, US20080261076, US20080297033, US200805851, US2008161567, US2008210930, US20090115322, US20090039776, US20090108737, US20090179555, US2009085476, US2009104472, US20100090591. US20100148663, US20100244004, US20100295032, US2010102716, US2010105902. US2010244004. US2010270916. US20110057559, US20110108822. US20110204333, US2011215710, US2011227049, US2011285275, US2012292601, US20130146848. US2013033172 US2013165653, US2013181190, US2013334521, US20140246656, US2014103305, U.S. Pat. Nos. 6,303,238, 6,413,656, 6,653, 654, 6,670,645, 6,687,266, 6,835,469, 6,921,915, 7,279,704, 7,332,232, 7,378,162, 7,534,505, 7,675,228, 7,728,137, 7,740,957, 7,759,489, 7,951,947, 8,067,099, 8,592,586, 8,871,361, WO06081973, WO06121811, WO07018067, WO07108362, WO07115970, WO07115981. WO08035571, WO2002015645, WO2003040257, WO2005019373. WO2006056418, WO2008054584. WO2008078800, WO2008096609, WO2008101842, WO2009000673, WO2009050281. WO2009100991. WO2010028151. WO2010054731. WO2010086089. WO2010118029, WO2011044988. WO2011051404, WO2011107491, WO2012020327. WO2012163471, WO2013094620, WO2013107487, WO2013174471, WO2014007565, WO2014008982, WO2014023377, WO2014024131, WO2014031977, WO2014038456, WO2014112450.

Re(CO)₄

$$\begin{bmatrix} \\ \\ \\ \\ \\ \\ \end{bmatrix}_3$$
 Ir,
$$\begin{bmatrix} \\ \\ \\ \\ \\ \end{bmatrix}_2$$
 Ir,

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-continued

HBL:

[0128] A hole blocking layer (HBL) may be used to reduce the number of holes and/or excitons that leave the emissive layer. The presence of such a blocking layer in a device may result in substantially higher efficiencies and/or longer lifetime as compared to a similar device lacking a blocking layer. Also, a blocking layer may be used to confine emission to a desired region of an OLED. In some embodiments, the HBL material has a lower HOMO (further from the vacuum level) and/or higher triplet energy than the emitter closest to the HBL interface. In some embodiments, the HBL material has a lower HOMO (further from the vacuum level) and/or higher triplet energy than one or more of the hosts closest to the HBL interface.

[0129] In one aspect, compound used in HBL contains the same molecule or the same functional groups used as host described above.

[0130] In another aspect, compound used in HBL contains at least one of the following groups in the molecule:

wherein k is an integer from 1 to 20; L^{101} is an another ligand, k' is an integer from 1 to 3.

ETL:

[0131] Electron transport layer (ETL) may include a material capable of transporting electrons. Electron transport layer may be intrinsic (undoped), or doped. Doping may be used to enhance conductivity. Examples of the ETL material

are not particularly limited, and any metal complexes or organic compounds may be used as long as they are typically used to transport electrons.

[0132] In one aspect, compound used in ETL contains at least one of the following groups in the molecule:

wherein R^{101} is selected from the group consisting of hydrogen, deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acids, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof, when it is aryl or heteroaryl, it has the similar definition as Ar's mentioned above. Ar 1 to Ar 3 has the similar definition as Ar's mentioned above. k is an integer from 1 to 20. X^{101} to X^{108} is selected from C (including CH) or N.

[0133] In another aspect, the metal complexes used in ETL contains, but not limit to the following general formula:

$$\left[\left(\begin{array}{c} O \\ N \end{array} \right)_{k'} Al \longrightarrow (L^{101})_{3-k'} \quad \left[\left(\begin{array}{c} O \\ N \end{array} \right)_{k'} Be \longrightarrow (L^{101})_{2-k'} \right]$$

-continued

$$\left[\left(\begin{array}{c} O \\ N \end{array} \right)_{k'} Zn - (L^{101})_{2-k'} \right] \left[\left(\begin{array}{c} N \\ N \end{array} \right)_{k'} Zn - (L^{101})_{2-k'} \right]$$

wherein (O - N) or (N - N) is a bidentate ligand, having metal coordinated to atoms O, N or N, N; L^{101} is another ligand; k' is an integer value from 1 to the maximum number of ligands that may be attached to the metal.

[0134] Non-limiting examples of the ETL materials that may be used in an OLED in combination with materials disclosed herein are exemplified below together with references that disclose those materials: CN103508940, EP01602648, EP01734038, EP01956007, JP2004-022334, JP2005149918, JP2005-268199, KR0117693, KR20130108183. US20040036077, US20070104977. US2007018155, US20090101870, US20090115316, US20090140637. US20090179554. US2009218940. US2010108990, US2011156017, US2011210320, US2012193612, US2012214993, US2014014925, US2014014927, US20140284580, U.S. Pat. Nos. 6,656,612, WO2007111263, 8,415,031, WO2003060956, WO2009148269, WO2010067894, WO2010072300, WO2013079217, WO2011074770, WO2011105373, WO2013145667, WO2013180376, WO2014104499, WO2014104535,

Charge Generation Layer (CGL)

[0135] In tandem or stacked OLEDs, the CGL plays an essential role in the performance, which is composed of an n-doped layer and a p-doped layer for injection of electrons and holes, respectively. Electrons and holes are supplied from the CGL and electrodes. The consumed electrons and holes in the CGL are refilled by the electrons and holes injected from the cathode and anode, respectively; then, the bipolar currents reach a steady state gradually. Typical CGL materials include n and p conductivity dopants used in the transport layers.

[0136] In any above-mentioned compounds used in each layer of the OLED device, the hydrogen atoms can be partially or fully deuterated. Thus, any specifically listed substituent, such as, without limitation, methyl, phenyl, pyridyl, etc. may be undeuterated, partially deuterated, and fully deuterated versions thereof. Similarly, classes of substituents such as, without limitation, alkyl, aryl, cycloalkyl, heteroaryl, etc. also may be undeuterated, partially deuterated, and fully deuterated versions thereof.

EXPERIMENTAL

[0137] Examples of the inventive compounds (Compound 254629586 and Compound 254678878) can be synthesized by the procedure shown in the following schemes.

[0138] Compound 254629586 and Compound 254678878 may be synthesized by the same synthetic strategy. Intermediate-1 and Intermediate-4 may be prepared by S_NAr reaction between starting material and 2-aminopyridine in the presence of base followed by reduction of the nitro group by SnCl₂ and a previously reported procedure (Bioorg. Med Chem. Lett. 2008, 18, 6067-6070) to form dihydrobenzimidazole-2-one ring. Intermediate-2 and Intermediate-5 may be prepared by repeating the S_N Ar reaction and reduction of nitro group followed by a reported procedure to close down the ring (PCT Int. Appl., 2013068376). Ligand 22016 and Ligand 28348 may be prepared by Pd-mediated C-N coupling between Intermediate-3 and bromophenylpyrazole derivative (U.S. Pat. Appl. Publ., 20160276603) and Intermediate-6 and bromophenylbenzimidazole (Angew. Chem. Int. Ed. 2012, 51, 8012), followed by Cadogen cyclization in the presence of PPh3, respectively. Compound 22016 and Compound 28348 may then be synthesized by typical platination procedures (Adv. Mater. 2016, 29, 1605002; Adv. Mater. 2014, 26, 7116).

Synthesis of Compound 271817738

Synthesis of 5-(4-(tert-butyl)pyridin-2-yl)-3-(3-chlorophenoxy)-7-methyl-5H-benzo[d]benzo[4,5]imidazole dazo[1,2-alimidazole

[0139] A mixture of 3-bromo-5-(4-(tert-butyl)pyridin-2-yl)-7-methyl-5H-benzo[d]benzo[4,5]imidazo[1,2-a]imidazole (2.78 g, 6.42 mmol), copper(I) iodide (0.244 g, 1.283 mmol), picolinic acid (0.316 g, 2.57 mmol), and potassium phosphate (2.72 g, 12.83 mmol) was vacuumed and backfilled with nitrogen. 3-chlorophenol (0.711 ml, 6.74 mmol) and dimethyl sulfoxide (DMSO) (35 ml) was added to the reaction mixture and heated at 130° C. for 48 hours. The mixture was cooled down and water was added. The resulting solid was collected by filtration and washed with

 $NH_4OH(aq)$ and dissolved in dichloromethane (DCM). The product was coated on Celite and chromatographed on silica (DCM/EA=30/1) (67% yield).

Synthesis of 3-[[1,1':3',1"-terphenyl]-2'-yl-2,2",3,3", 4,4",5,5",6,6"-d10)-1-(3-((5-(4-(tert-butyl)pyridin-2-yl)-7-methyl-5H-benzo[d]benzo[4,5]imidazo[1,2-a] imidazol-3-yl)oxy)phenyl)-1H-benzo[d]imidazol-3-ium chloride

[0140] N1-([1,1':3',1"-terphenyl]-2'-yl-2,2",3,3,4,4",5,5,6,6"-d0)-N2-(3-((5-(4-(tert-butyl)pyridin-2-yl)-7-methyl-5H-benzo[d]benzo[4,5]imidazo[1,2-a]imidazol-3-yl)oxy) phenyl)benzene-1,2-diamine (0.98 g, 1.239 mmol) was dissolved in triethoxymethane (8.24 ml, 49.6 mmol) and hydrogen chloride (0.122 ml, 1.487 mmol) was added. The reaction mixture was heated at 80° C. for 18 hours, then cooled down and removed most solvent and the solid was washed with hexane and filtered and dried in the vacuum oven (80% yield).

Synthesis of Compound 271817738

[0141] A mixture of 3-([1,1':3',1"-terphenyl]-2'-yl-2,2",3, 3"",4,4",5,5"",6,6"-d10)-1-(3-((5-(4-(tert-butyl)pyridin-2-yl)-7-methyl-5H-benzo[d]benzo[4,5]imidazo[1,2-a]imidazol-3-yl)oxy)phenyl)-1H-benzo[d]imidazol-3-ium chloride (830 mg, 0.991 mmol) and silver oxide (115 mg, 0.496 mmol) was stirred in 1,2-dichloroethane (12 ml) at R.T. for 18 hours. After removing 1,2-dichloroethane, Pt(COD)Cl₂ (371 mg, 0.991 mmol) was added and the reaction mixture was vacuumed and back-filled with nitrogen. 1,2-dichlorobenzene (12 ml) was added and heated at 205° C. for 60 hours. The solvent was then removed and coated on Celite and chromatographed on silica (DCM/Hep=5/2). The product was triturated in MeOH and dried in the vacuum oven (29% yield).

TABLE 1

Compound	Structure	Dihedral angle (indicated by *)	
254629586 (L _{X212192} , L _{Y26} , L _{Z13})	N N * N N N N N N N N N N N N N N N N N	2.28°	446

TABLE 1-continued

	TABLE 1-continued		
Compound	Structure	Dihedral angle (indicated by *)	Calculated T ₁ (nm)
254678878 (L _{X212233} , L _{Y28} , L _{Z16})	Pt N * N CD3	4.83°	449
254630336 ($L_{X212192}$, L_{Y26} , L_{Z38})	N N N N N N N N N N N N N N N N N N N	0.41°	434
254679568 ($L_{X212233}$, L_{Y28} , L_{Z39})	N * * N CD3	2.79°	442

TABLE 1-continued

Compound	Structure	Dihedral angle (indicated by *)	Calculated T ₁ (nm)
271817738 (L _{X79253} , L _{Y28} , L _{Z42})		4.17°	433 (exp: 444)
Comparative Example 1	N N * *	13.67°	474
Comparative Example 2	CD ₃ N Pt N * N * * * * * * * * * *	15.66°	481

[0142] Table 1 shows the calculated dihedral angle and T_1 for inventive Compounds 254629586, 254678878, 254630336, 254679568, and 271817738, as well as Comparative Example 1 and 2. Geometry optimization calculations were performed within the Gaussian 09 software

package using the B3LYP hybrid functional and CEP-31G basis set which includes effective core potentials. Excited state energies were computed with TDDFT at the optimized ground state geometries. Excitation calculations include a simulated tetrahydrofuran solvent using a self-consistent

reaction field. The calculated T_1 's of all inventive compounds are much bluer as compared to those of comparative examples, indicating their excellent potential for blue emitting material in PhOLED application. The dihedral angle between the pyridine ring and benzimidazole or carbazole (as indicated by * in Table 1) are much smaller for all invented compounds. The small dihedral angles represent less distortion of their square planar geometries, which is always desired to achieve better chemical stability, hence OLEDs incorporating such compounds will exhibit better device lifetime.

[0143] The calculations obtained with the above-identified DFT functional set and basis set are theoretical. Computational composite protocols, such as the Gaussian09 with B3LYP and CEP-31G protocol used herein, rely on the assumption that electronic effects are additive and, therefore, larger basis sets can be used to extrapolate to the complete basis set (CBS) limit. However, when the goal of a study is to understand variations in HOMO, LUMO, S1, T1, bond dissociation energies, etc. over a series of structurallyrelated compounds, the additive effects are expected to be similar. Accordingly, while absolute errors from using the B3LYP may be significant compared to other computational methods, the relative differences between the HOMO, LUMO, S1, T1, and bond dissociation energy values calculated with B3LYP protocol are expected to reproduce experiment quite well. See, e.g., Hong et al., Chem. Mater. 2016, 28, 5791-98, 5792-93 and Supplemental Information (discussing the reliability of DFT calculations in the context of OLED materials). Moreover, with respect to iridium or platinum complexes that are useful in the OLED art, the data obtained from DFT calculations correlates very well to actual experimental data. See Tavasli et al., J. Mater. Chem. 2012, 22, 6419-29, 6422 (Table 3) (showing DFT calculations closely correlating with actual data for a variety of emissive complexes); Morello, G. R., J. Mol. Model. 2017, 23:174 (studying of a variety of DFT functional sets and basis sets and concluding the combination of B3LYP and CEP-31G is particularly accurate for emissive complexes).

[0144] OLED Device Fabrication:

[0145] OLEDs were grown on a glass substrate pre-coated with an indium-tin-oxide (ITO) layer having a sheet resistance of 15- Ω /sq. Prior to any organic layer deposition or coating, the substrate was degreased with solvents and then treated with an oxygen plasma for 1.5 minutes with 50W at 100 mTorr and with ultra violet (UV) ozone for 5 minutes. The devices in Tables 1 were fabricated in high vacuum $(<10^{-6} \text{ Torr})$ by thermal evaporation. The anode electrode was 750 Å of ITO. The device example had organic layers consisting of, sequentially, from the ITO surface, 100 Å thick Compound A (HIL), 250 Å layer of Compound B (HTL), 50 Å of Compound C (EBL), 300 Å of Compound D doped with 10% of Emitter (EML), 50 Å of Compound E (BL), 300 Å of Compound G doped with 35% of Compound F (ETL), 10 Å of Compound G (EIL) followed by 1,000 Å of Al (Cathode). All devices were encapsulated with a glass lid sealed with an epoxy resin in a nitrogen glove box (<1 ppm of H₂O and O₂) immediately after fabrication with a moisture getter incorporated inside the package. The doping percentages are in volume percent.

[0146] The structures of the compounds used in the experimental devices are shown below:

Compound B

Compound D

Compound E

Compound G

[0147] It is understood that the various embodiments described herein are by way of example only, and are not intended to limit the scope of the invention. For example, many of the materials and structures described herein may be substituted with other materials and structures without deviating from the spirit of the invention. The present invention as claimed may therefore include variations from the particular examples and preferred embodiments described herein, as will be apparent to one of skill in the art. It is understood that various theories as to why the invention works are not intended to be limiting.

We claim:

1. A compound selected from the group consisting of:

Formula I

Formula II

$$\mathbb{R}^{D}$$
 \mathbb{C}
 $\mathbb{C$

TABLE 2

Device Data								
	_			at 1,00	0 nit			
	1931	CIE	λ max	FWHM	Voltage	LE	EQE	PE
Device	x	у	[nm]	[nm]	[V]	[cd/A]	[%]	[lm/W]
Compound 271817738	0.138	0.161	459	46	4.2	16.9	13.4	12.8

Formula III

-continued

wherein,

A, B, C, D, and F are each independently a 5-membered or 6-membered aromatic ring;

ring B may or may not be present;

M is selected from the group consisting of Pt, Pd, Cu, and Au;

Z¹, Z², Z³, Z⁴, Z⁵, Z⁶, and Z⁷ are each independently selected from the group consisting of C and N;

m1, m2 and m3 are each independently an integer of 0 or 1; when m2 is 0, each m1 and m3 is 1; when m2 is 1, each m1 and m3 can be 0 or 1;

when m1 is 0, L¹ is not present; when m2 is 0, L² is not present; when m3 is 0, L³ is not present;

L¹, L², and L³ each independently selected from the group consisting of a direct bond, BR, NR, PR, O, S, Se, C=O, S=O, SO₂, CRR', SiRR', GeRR', alkyl, cycloalkyl, and combinations thereof;

each R^A , R^B , R^C , R^D , and R^E represents monoto maximum possible number of substitutions, or no substitution:

each R^A, R^B, R^C, R^D, R^E, R and R' is independently a hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, boryl, and combinations thereof; and

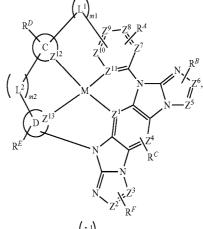
any two substituents can be joined or fused into a ring, provided that, in Formula I, if ring C is a 5-membered aromatic ring, L^2 is present and is a direct bond, then at least one pair of R^D , one pair of R^E , or one R^D and one R^E are joined together to form a fused ring.

- 2. The compound of claim 1, wherein M is Pt.
- 3. The compound of claim 1, wherein one of Z^6 and Z^7 is nitrogen, and the other one of Z^6 and Z^7 is carbon.
- **4**. The compound of claim **1**, wherein one of Z^6 and Z^7 is a neutral carbene carbon, and the other one of Z^6 and Z^7 is an anionic carbon.
- **5**. The compound of claim **1**, wherein rings A, B, C, D, and E are each independently selected from the group consisting of phenyl, pyridine, pyrimidine, triazine, pyrazole, triazole, imidazole, and imidazole derived carbene.
- **6**. The compound of claim **1**, wherein L³ and Z⁴ are fused to form a 5-membered or 6-membered carbocyclic or heterocyclic ring.

7. The compound of claim 1, wherein L³ is present and is selected from the group consisting of O, S, and CRR'.

8. The compound of claim **1**, wherein the compound is Formula I and ring A is pyridine with N coordinating to M.

9. The compound of claim 1, wherein the compound is selected from the group consisting of:



$$\begin{array}{c|c}
\mathbb{R}^{D} & \mathbb{R}^{D} \\
\mathbb{C} & \mathbb{Z}^{10} \\
\mathbb{C} & \mathbb{Z}^{10}
\end{array}$$

$$\begin{array}{c|c}
\mathbb{R}^{D} & \mathbb{Z}^{8} & \mathbb{R}^{A} \\
\mathbb{Z}^{7} & \mathbb{Z}^{7} \\
\mathbb{Z}^{7} & \mathbb{Z}^{7}
\end{array}$$

$$\begin{array}{c|c}
\mathbb{R}^{E} & \mathbb{Z}^{11} & \mathbb{Z}^{11} \\
\mathbb{R}^{E} & \mathbb{Z}^{2} & \mathbb{Z}^{2}
\end{array}$$

$$\begin{array}{c|c}
\mathbb{R}^{E} & \mathbb{Z}^{2} & \mathbb{Z}^{3} \\
\mathbb{Z}^{2} & \mathbb{Z}^{3} & \mathbb{Z}^{3}
\end{array}$$

-continued

$$L^{1}_{m1}$$
 $Z^{11} - Z^{10} R^{4}$
 Z^{12}
 $Z^{13} - Z^{10} R^{4}$
 $Z^{13} - Z^{10} R^{4}$
 $Z^{13} - Z^{10} R^{4}$
 $Z^{13} - Z^{10} R^{4}$
 $Z^{14} - Z^{10} R^{4}$
 $Z^{10} -$

 $\begin{array}{l} \text{wherein,} \\ Z^1,\,Z^2,\,Z^3,\,Z^4,\,Z^5,\,Z^6,\,Z^7,\,Z^8,\,Z^9,\,Z^{10},\,Z^{11},\,Z^{12},\,Z^{13},\,Z^{14},\\ \text{and } Z^{15} \text{ are each independently C or N;} \end{array}$

R^F represents mono- to maximum possible number of substitutions, or no substitution; and

each R^F is independently a hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, boryl, and combinations thereof; and any two substituents can be joined or fused into a ring.

10. The compound of claim 9, wherein the compound has the structure:

$$\mathbb{R}^{Y}$$
 \mathbb{R}^{Z}
 \mathbb{R}^{A}
 \mathbb{R}^{B}
 \mathbb{R}^{B}
 \mathbb{R}^{B}

wherein R^{Y} represents mono- to tetra-substitutions, or no substitution:

wherein any two substituents can be joined or fused into a ring;

wherein R^Y is a hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, boryl, and combinations thereof; and

wherein R^Z is selected from the group consisting of alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, silyl, aryl, heteroaryl, boryl, partially or fully deturated variants thereof, partially or fully fluorinated variants thereof, and combinations thereof.

11. The compound of claim 1, wherein at least one of R^A , R^B , R^C , R^D , R^E , R^F , R and R' comprises a chemical group containing at least three 6-membered aromatic rings that are not fused next to each other.

12. The compound of claim 10, wherein at least one of \mathbb{R}^Y and \mathbb{R}^Z comprises a chemical group containing at least three 6-membered aromatic rings that are not fused next to each other.

13. The compound of claim 1, wherein the compound is the compound x having the formula $(L_{\chi_i})Pt(L_{\chi_i})(L_{Zk})$;

wherein,

 L_{x_i} is a bidentate ligand;

 L_{yi} is a monodentate ligand;

 L_{Zk} is a monodentate ligand;

 L_{Xi} is linked to L_{Zk} by a linking group L^3 ;

 L_{Zk} is linked to L_{Yj} by a direct bond;

x=30(k-1)+j+1200(i-1), i is an integer from 1 to 212258,j is an integer from 1 to 30, and k is an integer from 1 to

40; when k=41, 42, or 43, x=25(k-41)+j+75(i-1)+254709600, i is an integer from 1 to 212258,j is an integer from 1 to 25;

 L_{Xi} is selected from the group consisting of L_{X1} to $L_{X212258}$ whose structures are defined as follows:

 $L_{X212258}$ whose structures are defined as follows: Ar1, R1 \mathbb{L}_{Xi} Structure of Lx wherein wherein $Ar^{1} = Am$ and $R^{1} = y = 330(m - 1) + n$ L_{X1} to L_{X9900} have the structure Rn, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and wherein $Ar^{1} = Am$ and $R^{1} = y = 330(m - 1) + n +$ wherein L_{X9901} - L_{X19800} Rn,9900 have the structure wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and

wherein L_{X19801} - L_{X29700} have the structure R^1 wherein $Ar^1 = Am$ and $R^1 = y = 330(m-1) + n + Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and

wherein $Ar^1 = Am$ and $R^1 = y = 330(m-1) + n + Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and

-continued						
L_{Xi}	Structure of L_{Xi}	Ar^1, R^1 i				
wherein L_{X39601} - L_{X49500} have the structure	R ¹	wherein $Ar^1 = Am$ and $R^1 = y = 330(m-1) + n + Rn$, 39600 wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and				
wherein L_{X49501} - L_{X59400} have the structure	Ar ¹	wherein $Ar^1 = Am$ and $R^1 = y = 330(m-1) + n + Rn$, 49500 wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and				
wherein L_{X59401} - L_{X69300} have the structure	Ar ¹	wherein $Ar^1 = Am$ and $R^1 = y = 330(m-1) + n + Rn$, 59400 wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and				
wherein L_{X69301} - L_{X79200} have the structure	Ar ¹ R N N	wherein $Ar^1 = Am$ and $R^1 = y = 330(m-1) + n + Rn$, 69300 wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and				
wherein L_{X79201} to L_{X79530} have the structure	* Ar'	wherein $R^1 = Rn$, $y = n + 79200$ wherein n is an integer from 1 to 330, and				

-continued

-continued						
L_{Xi}	Structure of L_{Xi}	Ar^1 , R^1	i			
wherein $L_{X79531}L_{X79860}$ have the structure	R ¹ N *	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 79530			
wherein L_{X79861} - L_{X80190} have the structure	R ¹ N *	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 79860			
wherein L_{X80191} - L_{X80520} have the structure	R ¹ N *	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 80190			
wherein L_{X80521} to L_{X90420} have the structure	CD ₃ R N Ar *	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 80520			
wherein L_{X90421} to $L_{X100320}$ have the structure	D ₃ C R ¹	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 90420			

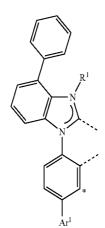
-continued			
\mathbb{L}_{Xi}	Structure of L_{Xi}	Ar ¹ , R ¹	i
wherein $\mathcal{L}_{X100321}$ to $\mathcal{L}_{X110220}$	CD ₃ R N N Ar Ar *	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an have the structure integer from 1 to 330, and	y = 330(m-1) + n + 100320
wherein $\mathcal{L}_{X110221}$ to $\mathcal{L}_{X120120}$ have the structure	D_3C D_3C N N Ar^1	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 is an integer integer from 1 to 330, and	y = 330(m-1) + n + 110220
wherein $L_{X120121}$ to $L_{X130020}$ have the structure	Ar ¹	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 120120
wherein	$^{\mathrm{CD_{3}}}$	wherein $Ar^1 = Am$ and $R^1 = Rn$	y = 330(m-1) + n + 130020

wherein $L_{X130021}$ to $L_{X139920}$ have the structure

wherein $Ar^1 = Am$ and $R^1 = y = 330(m-1) + n - Rn$, 130020 wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and

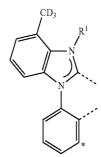
Continuos			
L_{Xi}	Structure of L_{Xi}	Ar^1 , R^1	i
wherein $L_{X139921}$ to $L_{X149820}$ have the structure	D ₃ C N *	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 139920
wherein $L_{X149821}$ to $L_{X159720}$ have the structure	D ₃ C N Ar ¹	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 149820

wherein $L_{X159721}$ to $L_{X169620}$ have the structure



wherein $Ar^1 = Am$ and $R^1 = y = 330(m-1) + n + Rn$, 159720 wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and

wherein $L_{X169621}$ to $L_{X169950}$ have the structure



wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and

y = n + 169620

-continued

\mathbb{L}_{Xi}	Structure of L_{Xi}	Ar ¹ , R ¹	i
wherein $\mathcal{L}_{X169951}$ to $\mathcal{L}_{X170280}$ have the structure	D ₃ C N	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 169950
wherein ${\cal L}_{X170281}$ to ${\cal L}_{X170610}$ have the structure	D ₃ C	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 170280
wherein $L_{X170610}$ to $L_{X170940}$ have the structure	R ^I N *	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 170610
wherein $L_{X170941}$ to $L_{X171270}$ have the structure	N R I	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 170940
wherein $L_{X171271}$ to $L_{X171600}$ have the structure		wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 171270

-continued

	-conti	inued
\mathbb{L}_{Xi}	Structure of L_{Xi}	Ar^1 , R^1 i
wherein $\mathcal{L}_{X171601}$ to $\mathcal{L}_{X181500}$ have the structure	D R ¹	wherein $Ar^1 = Am$ and $R^1 = y = 330(m-1) + n + Rn$, 171600 wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and
wherein ${\rm L}_{X181501}$ to ${\rm L}_{X191400}$ have the structure	$D \longrightarrow N$ N Ar^{1}	wherein $Ar^1 = Am$ and $R^1 = y = 330(m-1) + n + Rn$, 181500 wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and
wherein ${\cal L}_{X191401}$ to ${\cal L}_{X191730}$ have the structure	D R ¹ N *	wherein $R^1 = Rn$, $y = n + 191400$ wherein n is an integer from 1 to 330, and
wherein ${\cal L}_{X191731}$ to ${\cal L}_{X192060}$ have the structure	D ₃ C R ¹	wherein $R^1 = Rn$, $y = n + 191730$ wherein n is an integer from 1 to 330, and
wherein ${\cal L}_{X192061}$ to ${\cal L}_{X201960}$ have the structure	D ₃ C R ¹ N Ar ¹ *	wherein $Ar^1 = Am$ and $R^1 = y = 330(m-1) + n + Rn$, 192060 wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and

-continued

\mathbb{L}_{Xi}	Structure of L_{Xi}	Ar^1, R^1	i
wherein $L_{X201961}$ to $L_{X211860}$ have the structure	D ₃ C R ¹ N Ar ¹	wherein $Ar^1 = Am$ and $R^1 = Rn$, wherein m is an integer from 1 to 30 and n is an integer from 1 to 330, and	y = 330(m-1) + n + 201960
wherein $L_{X211861}$ to $L_{X212190}$ have the structure	D ₃ C R ¹ N *	wherein $R^1 = Rn$, wherein n is an integer from 1 to 330, and	y = n + 211860

L_{3/21/21/92}

$$L_{3/21/21/92}$$

$$L_{3/21/21/92}$$

$$L_{3/21/21/92}$$

 $\mathcal{L}_{X212200}$

 $\rm L_{\it X212195}$

-continued

L_{X212196}

 $\rm L_{\it X212197}$

L_{X212198}

 $L_{X2\,12\,199}$

 $L_{X212201}$

 $L_{X212202}$

 $L_{X212204}$

 $L_{X212210}$

 $L_{X212211}$

 $L_{X212212}$

L_{X212213}

L_{X212214}

-continued

 $\mathcal{L}_{X212205}$

 $\mathcal{L}_{X212206}$

-continued

L_{X212207}

L_{X212208}

 $L_{X212215}$

 $L_{X212226}$

-continued

 $L_{X212231}$

L_{X212232}

$$L_{X212228}$$

$$\mathcal{L}_{X212229}$$

$$L_{X212235}$$

L_{X212236}

$$L_{\lambda 212241}$$

 $L_{X212246}$

-continued

 $\mathrm{L}_{X212247}$

 $\mathcal{L}_{X212248}$

 $L_{X212249}$

 $\mathcal{L}_{X212250}$

 $L_{X212251}$

L_{X212254}

 $L_{X212253}$

L_{X212255}

L_{X212256}

wherein A1 to A30 have the following structures:

Al ,

-continued

D, D,

A4

A5

CF₃ , A6

A7

A8

A9

A10

A11 Me,

iPr,

A13

A12

tBu,

A14

A15

A16

A18

-continued

A23

$$\begin{array}{c} A24 \\ \\ D \\ D \\ D \end{array}$$

$$\begin{array}{c} \text{A30} \\ \text{D} \end{array}$$

R1 to R330 have the following structures:

Et,

rPr,

 ${\rm R3} \\ {\rm tBu},$

R4

R5

R6

R7

 CF_3 ,

R9

R10

-continued

RI1

R12

 $\begin{array}{c} \text{R13} \\ \\ \text{D} \\ \\ \text{D} \\ \\ \text{D} \end{array},$

R14

R15

R16

R17

D D CF_3 ,

$$D_3C$$

$$CF_3$$
 D
 D
 D
 D

$$F = F$$

$$F$$

R97

-continued

$$\begin{array}{c} D \\ D \\ D \\ D \end{array}$$
 R109

R115

R116

R117

R118

-continued

R125

R133

R165

-continued

-continued

R179

R201

R235

R240

R241

-continued

R246

R247

R252

R253

R263

R270

R276

R289

-continued

R287

R288

R293

R303

R304

R309

R310

R311

R312

R325

R326

-continued

-continued

 L_{yj} is selected from the group consisting of:

$$L_{76}$$

$$\begin{array}{c} L_{\gamma_{14}} \\ \\ \\ \\ N \\ \\ \end{array}$$

 $\rm L_{Y18}$

 \mathcal{L}_{Y19}

 L_{Y23}

-continued

L_{Y17}

$$L_{129}$$

 L_{Zk} is selected from the group consisting of:

$$\begin{array}{c} **\\ *\\ N\\ N\\ N\\ N\\ D_3C\\ \end{array},$$

$$L_{Z29}$$

-continued

and the * of L_{Zk} attaches to the * of L_{Xi} , and the ** of L_{Zk} attaches to the ** of L_{Yj} .

14. The compound of claim 19, wherein x=5(k-41)+(j-25)+15(i-1)+270628950, i is an integer from 1 to 212258,j is an integer from 26 to 30, and k is an integer from 41 to 43.

15. The compound of claim 1, wherein the compound is selected from the group consisting of:

16. An organic light emitting device (OLED) comprising: an anode;

a cathode; and

an organic layer, disposed between the anode and the cathode, comprising a compound selected from the group consisting of:

Formula I

$$\begin{array}{c}
\mathbb{R}^{D} & \mathbb{L}^{1} \\
\mathbb{R}^{D} & \mathbb{L}^{1} \\
\mathbb{R}^{D} & \mathbb{R}^{D} \\
\mathbb{R}^{D} & \mathbb{R$$

wherein,

A, B, C, D, and F are each independently a 5-membered or 6-membered aromatic ring;

ring B may or may not be present;

M is selected from the group consisting of Pt, Pd, Cu, and

 Z^1 , Z^2 , Z^3 , Z^4 , Z^5 , Z^6 , and Z^7 are each independently selected from the group consisting of C and N;

m1, m2 and m3 are each independently an integer of 0 or 1; when m2 is 0, each m1 and m3 is 1; when m2 is 1, each m1 and m3 can be 0 or 1;

when m1 is 0, L¹ is not present; when m2 is 0, L² is not present; when m3 is 0, L³ is not present;

L¹, L², and L³ each independently selected from the group consisting of a direct bond, BR, NR, PR, O, S, Se, C=O, S=O, SO₂, CRR', SiRR', GeRR', alkyl, cycloalkyl, and combinations thereof;

each R^A , R^B , R^C , R^D , and R^E represents monoto maximum possible number of substitutions, or no substitution:

each R^A, R^B, R^C, R^D, R^E, R and R' is a hydrogen or a substituent independently selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, boryl, and combinations thereof; and

any two substituents can be joined or fused into a ring, provided that, in Formula I, if ring C is a 5-membered aromatic ring, L^2 is present and is a direct bond, then at least one pair of R^D , one pair of R^E , or one R^D and one R^E are joined together to form a fused ring.

17. The OLED of claim 16, wherein the organic layer further comprises a host, wherein the host comprises at least one chemical group selected from the group consisting of triphenylene, carbazole, dibenzothiphene, dibenzofuran, dibenzoselenophene, azatriphenylene, azacarbazole, azadibenzothiophene, aza-dibenzofuran, and aza-dibenzoselenophene.

18. The OLED of claim 17, wherein the host is selected from the group consisting of:

-continued

and combinations thereof.

19. The OLED of claim 16, wherein the compound is a sensitizer; wherein the device further comprises an acceptor; and wherein the acceptor is selected from the group consisting of fluorescent emitter, delayed fluorescence emitter, and combination thereof.

20. A consumer product comprising an organic light-emitting device (OLED) comprising:

an anode;

a cathode; and

an organic layer, disposed between the anode and the cathode, comprising a compound selected from the group consisting of:

Formula I

$$\begin{array}{c|c}
R^{D} & C & L^{1} \\
C & A & R^{A} \\
L^{2}_{m2} & N & T^{7} & B
\end{array}$$

$$\begin{array}{c|c}
R^{B} & R^{B}, \\
C & Z^{1} & N & Z^{6} & B
\end{array}$$

$$\begin{array}{c|c}
R^{B} & R^{B}, \\
C & Z^{3} & Z^{4} & Z^{5} \\
R^{C} & R^{C} & R^{C}
\end{array}$$

Formula II

Formula III $\begin{array}{c}
\mathbb{R}^{D} \\
\mathbb{C} \\
\mathbb{C}$

wherein

A, B, C, D, and F are each independently a 5-membered or 6-membered aromatic ring;

ring B may or may not be present;

M is selected from the group consisting of Pt, Pd, Cu, and Au;

Z¹, Z², Z³, Z⁴, Z⁵, Z⁶, and Z⁷ are each independently selected from the group consisting of C and N;

m1, m2 and m3 are each independently an integer of 0 or 1; when m2 is 0, each m1 and m3 is 1; when m2 is 1, each m1 and m3 can be 0 or 1;

when m1 is 0, L¹ is not present; when m2 is 0, L² is not present; when m3 is 0, L³ is not present;

L¹, L², and L³ each independently selected from the group consisting of a direct bond, BR, NR, PR, O, S, Se, C=O, S=O, SO₂, CRR', SiRR', GeRR', alkyl, cycloalkyl, and combinations thereof;

each R^A , R^B , R^C , R^D , and R^E represents monoto maximum possible number of substitutions, or no substitution:

each R^A, R^B, R^C, R^D, R^E, R and R' is a hydrogen or a substituent independently selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, arylalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, boryl, and combinations thereof; and

any two substituents can be joined or fused into a ring, provided that, in Formula I, if ring C is a 5-membered aromatic ring, L^2 is present and is a direct bond, then at least one pair of R^D , one pair of R^E , or one R^D and one R^E are joined together to form a fused ring.

* * * * *



专利名称(译)	有机电致发光材料和器件		
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[标]申请(专利权)人(译)	环球展览公司		
申请(专利权)人(译)	通用显示器公司		
当前申请(专利权)人(译)	通用显示器公司		
[标]发明人	CHEN HSIAO FAN SILVERSTEIN DANIEL W WOLOHAN PETER FLEETHAM TYLER BROOKS JASON NEELARAPU RAGHUPATHI ROHLFING KATARINA WILLIAMS DOUGLAS		
发明人	CHEN, HSIAO-FAN SILVERSTEIN, DANIEL W. WOLOHAN, PETER FLEETHAM, TYLER BROOKS, JASON STANTON, III, CHARLES J. TRETYAK, OLEXANDR NEELARAPU, RAGHUPATHI ROHLFING, KATARINA WILLIAMS, DOUGLAS		
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摘要(译)

公开了一种具有基于苯并咪唑的结构的新型化合物,其选自以下结构之一:该化合物可用于改善OLED的光物理性能。

