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Inventor(s)	Fleetham; Tyler et al.

Organic electroluminescent materials and devices

Abstract

Provided are organoboron compounds having Formula I: ##STR00001##
Also provided are formulations comprising these organoboron compounds. Further provided are OLEDs and related consumer products that utilize these organoboron compounds.

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Background/Summary

(1) This application claims priority under 35 U.S.C. § 119(e) to United States Provisional Application No. 63/105,845, filed on Oct. 26, 2020, and to United States Provisional Application No. 63/107,244, filed on Oct. 29, 2020, the entire contents of both applications are incorporated herein by reference.

FIELD

(1) The present disclosure generally relates to organometallic compounds and formulations and their various uses including as emitters/hosts in devices such as organic light emitting diodes and related electronic devices.

BACKGROUND

(2) Opto-electronic devices that make use of organic materials are becoming increasingly desirable for various 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.

(3) 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.

(4) 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 emissive layer (EML) device or a stack structure. Color may be measured using CIE coordinates, which are well known to the art.

SUMMARY

(5) In one aspect, the present disclosure provides a compound of Formula I:

(6) ##STR00002##

wherein each of Y^{sup.A}, Y^{sup.B}, and Y^{sup.C} is independently O, S, Se, CRR', or SiRR'; n is 0 or 1, with Y^{sup.C} being not present when n=0, while X^{sup.7} and X^{sup.8} are both C when n=1; each of X^{sup.1}-X^{sup.11} is independently C or N; each of R^{sup.A}, R^{sup.B}, and R^{sup.C} independently represents zero, mono, or up to the maximum allowed number of substitutions to its associated ring; each of R, R', R^{sup.A}, R^{sup.B}, and R^{sup.C} is independently a hydrogen or a substituent selected from the group consisting of the general substituents defined herein; and any two adjacent R, R', R^{sup.A}, R^{sup.B}, or R^{sup.C} can be joined or fused together to form a ring, wherein at least one of R^{sup.A}, R^{sup.B}, and R^{sup.C} comprises an N-containing moiety with each N atom forming three σ bonds with its adjacent atoms, and all the three σ bonds being within one or more cyclic groups.

(7) In another aspect, the present disclosure provides a formulation of a compound of Formula I as described herein.

(8) In yet another aspect, the present disclosure provides an OLED having an organic layer comprising a compound of Formula I as described herein.

(9) In yet another aspect, the present disclosure provides a consumer product comprising an OLED with an organic layer comprising a compound of Formula I as described herein.

Description

BRIEF DESCRIPTION OF THE DRAWINGS

(1) FIG. 1 shows an organic light emitting device.

(2) FIG. 2 shows an inverted organic light emitting device that does not have a separate electron transport layer.

DETAILED DESCRIPTION

A. Terminology

(3) Unless otherwise specified, the below terms used herein are defined as follows:

(4) 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.

(5) 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.

(6) 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.

(7) 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.

(8) 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.

(9) 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.

(10) The terms “halo,” “halogen,” and “halide” are used interchangeably and refer to fluorine, chlorine, bromine, and iodine.

(11) The term “acyl” refers to a substituted carbonyl radical (C(O)—R.sub.s).

(12) The term “ester” refers to a substituted oxycarbonyl (—O—C(O)—R.sub.s or —C(O)—O—R.sub.s) radical.

(13) The term “ether” refers to an —OR.sub.s radical.

(14) The terms “sulfanyl” or “thio-ether” are used interchangeably and refer to a —SR.sub.s radical.

(15) The term “selenyl” refers to a —SeR.sub.s radical.

(16) The term “sulfinyl” refers to a —S(O)—R.sub.s radical.

(17) The term “sulfonyl” refers to a —SO.sub.2—R.sub.s radical.

(18) The term “phosphino” refers to a —P(R.sub.s).sub.3 radical, wherein each R.sub.s can be same or different.

(19) The term “silyl” refers to a —Si(R.sub.s).sub.3 radical, wherein each R.sub.s can be same or different.

- (20) The term “germyl” refers to a $\text{—Ge(R.sub.s).sub.3}$ radical, wherein each R.sub.s can be same or different.
- (21) The term “boryl” refers to a —B(R.sub.s).sub.2 radical or its Lewis adduct —B(R.sub.s).sub.3 radical, wherein R.sub.s can be same or different.
- (22) In each of the above, R.sub.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.sub.s is selected from the group consisting of alkyl, cycloalkyl, aryl, heteroaryl, and combination thereof.
- (23) 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 may be optionally substituted.
- (24) 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 may be optionally substituted.
- (25) 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 may be optionally substituted.
- (26) 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 may be optionally substituted.
- (27) The term “alkynyl” refers to and includes both straight and branched chain alkyne radicals. Alkynyl groups are essentially alkyl groups that include at least one carbon-carbon triple bond in the alkyl chain. Preferred alkynyl groups are those containing two to fifteen carbon atoms. Additionally, the alkynyl group may be optionally substituted.
- (28) 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 may be optionally substituted.
- (29) 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 hetero-non-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.
- (30) The term “aryl” refers to and includes both single-ring aromatic hydrocarbonyl 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 hydrocarbonyl 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 may be optionally substituted.

(31) 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 aza-analogs thereof. Additionally, the heteroaryl group may be optionally substituted.

(32) 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.

(33) 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.

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

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

(36) In some instances, the preferred general substituents are selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, alkoxy, aryloxy, amino, silyl, boryl, aryl, heteroaryl, sulfanyl, and combinations thereof.

(37) In yet other instances, the more preferred general substituents are selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, aryl, heteroaryl, and combinations thereof.

(38) The terms “substituted” and “substitution” refer to a substituent other than H that is bonded to the relevant position, e.g., a carbon or nitrogen. For example, when R^{sup.1} represents mono-substitution, then one R^{sup.1} must be other than H (i.e., a substitution). Similarly, when R^{sup.1}

represents di-substitution, then two of R.sup.1 must be other than H. Similarly, when R.sup.1 represents zero or no substitution, R.sup.1, for example, can be a 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.

(39) 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.

(40) 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 aromatic ring can be replaced by a nitrogen atom, for example, and without any limitation, azatriphenylene encompasses both dibenzo[f,h]quinoxaline and dibenzo[f,h]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.

(41) 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.

(42) 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.

(43) In some instance, a pair of adjacent substituents can be optionally joined or fused into a ring. The preferred ring is a five, six, or seven-membered carbocyclic or heterocyclic ring, includes both instances where the portion of the ring formed by the pair of substituents is saturated and where the portion of the ring formed by the pair of substituents is unsaturated. As used herein, “adjacent” means that the two substituents involved can be on the same ring next to each other, or on two neighboring rings having the two closest available substitutable positions, such as 2,2' positions in a biphenyl, or 1, 8 position in a naphthalene, as long as they can form a stable fused ring system.

B. The Compounds of the Present Disclosure

(44) In one aspect, the present disclosure provides a compound of Formula I:

(45) ##STR00003## wherein: each of Y.sup.A, Y.sup.B, and Y.sup.C is independently O, S, Se, CRR', or SiRR'; n is 0 or 1, with Y.sup.C being not present when n=0, while X.sup.7 and X.sup.8

are both C when n=1; each of X.sup.1-X.sup.11 is independently C or N; each of R.sup.A, R.sup.B, and R.sup.C independently represents zero, mono, or up to the maximum allowed number of substitutions to its associated ring; each of R, R', R.sup.A, R.sup.B, and R.sup.C is independently a hydrogen or a substituent selected from the group consisting of the general substituents defined herein; and any two adjacent R, R', R.sup.A, R.sup.B, or R.sup.C can be joined or fused together to form a ring, wherein at least one of R.sup.A, R.sup.B, and R.sup.C comprises an N-containing moiety with each N atom forming three a bonds with its adjacent atoms, and all the three σ bonds being within one or more cyclic groups.

(46) In some embodiments, each of R, R', R.sup.A, R.sup.B, and R.sup.C can be independently hydrogen or a substituent selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof.

(47) In some embodiments, one R.sup.A can comprise an N-containing moiety with each N atom forming three a bonds with its adjacent atoms, and all the three σ bonds being within one or more cyclic groups.

(48) In some embodiments, one R.sup.B can comprise an N-containing moiety with each N atom forming three a bonds with its adjacent atoms, and all the three σ bonds being within one or more cyclic groups.

(49) In some embodiments, the N-containing moiety can be attached to Formula I through a direct bond, or a linking group.

(50) In some embodiments, the linking group can be selected from the group consisting of an atom, a monocyclic ring, a bicyclic fused ring, a tricyclic fused ring, and combinations thereof. In some embodiments, the linking group can be selected from the group consisting of:

(51) ##STR00004##

and combinations thereof, wherein Y.sup.D, Y.sup.E and Y.sup.F are each independently selected from the group consisting of O, S, NR, CRR', SiRR', GeRR', wherein R and R' are as previously defined above; and each of R.sup.1, and R.sup.2 is independently a hydrogen or a substituent selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof.

(52) In some embodiments, the linking group can be selected from the group consisting of:

(53) ##STR00005##

and combinations thereof, wherein Y.sup.a can be O, S, NR, CRR', or SiRR', wherein R and R' are as previously defined above.

(54) In some embodiments, two linking groups can be employed to link Formula I with the N-containing moiety. In some embodiments, the two linking groups can be the same. In some embodiments, the two linking groups can be different.

(55) In some embodiments, the N-containing moiety may comprise a structure selected from the group consisting of:

(56) ##STR00006## ##STR00007##

wherein each of Y.sup.D, and Y.sup.E are each independently selected from the group consisting of O, S, NR, CRR', SiRR', GeRR', wherein R and R' are as previously defined above.

(57) In some embodiments, n can be 0. In some embodiments, n can be 1.

(58) In some embodiments, two of Y.sup.A, Y.sup.B, and Y.sup.C can be O. In some embodiments, each of Y.sup.A, Y.sup.B, and Y.sup.C can be independently O.

(59) In some embodiments, each of X.sup.1-X.sup.3 can be independently C. In some embodiments, one of X.sup.1-X.sup.3 can be N. In some embodiments, each of X.sup.4-X.sup.7 can be independently C. In some embodiments, one of X.sup.4-X.sup.7 can be N. In some embodiments, each of X.sup.8-X.sup.11 can be independently C. In some embodiments, one of X.sup.8-X.sup.11 can be N. In some embodiments, each of X.sup.1-X.sup.11 can be independently

C. In some embodiments, one of X^{sup.1}-X^{sup.11} can be N. In some embodiments, two of X^{sup.1}-X^{sup.11} can be N. In some embodiments, three of X^{sup.1}-X^{sup.11} can be N.

(60) In some embodiments, two adjacent R^{sup.A} substituents can be joined to form a fused ring. In some embodiments, two adjacent R^{sup.B} substituents can be joined to form a fused ring. In some embodiments, the fused ring can be benzene, pyridine, pyrimidine, pyridazine, pyrazine, imidazole, pyrazole, pyrrole, oxazole, furan, thiophene, or thiazole.

(61) In some embodiments, the compound can be selected from the group consisting of:

(62) ##STR00008## ##STR00009##

wherein moiety D^{sup.G} is an electron-donating group, and the remaining variables are the same as previously defined. In some embodiments, the electron-donating group can be one of the N-containing moieties as described herein. In some embodiments, the electron-donating group can be selected from others. In some embodiments, the electron-donating group comprises a structure selected from the group consisting of:

(63) ##STR00010## ##STR00011## ##STR00012##

(64) In some embodiments, the compound can be selected from the group consisting of:

(65) ##STR00013## ##STR00014## ##STR00015## ##STR00016## ##STR00017##

wherein i, j, k, l, and m are each an integer from 1 to 5 where Y₁ is O, Y₂ is S, Y₃ is Se, Y₄ is CMe_{sub.2} and Y₅ is SiPh_{sub.2} and wherein n is an integer from 1 to 50 where each D_n is defined as shown below:

(66) ##STR00018## ##STR00019## ##STR00020##

(67) In some embodiments, the compound can be selected from the group consisting of:

(68) ##STR00021## ##STR00022## ##STR00023## ##STR00024##

(69) In some embodiments, the compound having Formula I described herein can be at least 30% deuterated, at least 40% deuterated, at least 50% deuterated, at least 60% deuterated, at least 70% deuterated, at least 80% deuterated, at least 90% deuterated, at least 95% deuterated, at least 99% deuterated, or 100% deuterated. As used herein, percent deuteration has its ordinary meaning and includes the percent of possible hydrogen atoms (e.g., positions that are hydrogen, deuterium, or halogen) that are replaced by deuterium atoms.

C. The OLEDs and the Devices of the Present Disclosure

(70) In another aspect, the present disclosure also provides an OLED device comprising an organic layer that contains a compound as disclosed in the above compounds section of the present disclosure.

(71) In some embodiments, the organic layer comprises a compound of Formula I:

(72) ##STR00025##

wherein each of Y^{sup.A}, Y^{sup.B}, and Y^{sup.C} is independently O, S, Se, CRR', or SiRR'; n is 0 or 1, with Y^{sup.C} being not present when n=0, while X^{sup.7} and X^{sup.8} are both C when n=1; each of X^{sup.1}-X^{sup.11} is independently C or N; each of R^{sup.A}, R^{sup.B}, and R^{sup.C} independently represents zero, mono, or up to the maximum allowed number of substitutions to its associated ring; each of R, R', R^{sup.A}, R^{sup.B}, and R^{sup.C} is independently a hydrogen or a substituent selected from the group consisting of the general substituents defined herein; and any two adjacent R, R', R^{sup.A}, R^{sup.B}, or R^{sup.C} can be joined or fused together to form a ring, wherein at least one of R^{sup.A}, R^{sup.B}, and R^{sup.C} comprises an N-containing moiety with each N atom forming three σ bonds with its adjacent atoms, and all the three σ bonds being within one or more cyclic groups.

(73) In some embodiments, the compound may be a host, and the organic layer may be an emissive layer that comprises a phosphorescent emitter.

(74) In some embodiments, the phosphorescent emitter may be a transition metal complex having at least one ligand or part of the ligand if the ligand is more than bidentate selected from the group consisting of:

(75) ##STR00026## ##STR00027## wherein: T is selected from the group consisting of B, Al, Ga,

and In; each of Y^{sup.1} to Y^{sup.13} is independently selected from the group consisting of carbon and nitrogen; Y' is selected from the group consisting of BR.sub.e, NR.sub.e, PR.sub.e, O, S, Se, C=O, S=O, SO.sub.2, CR.sub.eR.sub.f, SiR.sub.eR.sub.f, and GeR.sub.eR.sub.f; R.sub.e and R.sub.f can be fused or joined to form a ring; each R.sub.a, R.sub.b, R.sub.c, and R.sub.d independently represent zero, mono, or up to a maximum allowed number of substitutions to its associated ring; each of R.sub.a1, R.sub.b1, R.sub.c1, R.sub.d1, R.sub.a, R.sub.b, R.sub.c, R.sub.d, R.sub.e and R.sub.f is independently a hydrogen or a substituent selected from the group consisting of the general substituents defined herein; and any two adjacent R.sub.a, R.sub.b, R.sub.c, R.sub.d, R.sub.e and R.sub.f can be fused or joined to form a ring or form a multidentate ligand.

(76) In some embodiments, the compound may be an acceptor, and the OLED may further comprise a sensitizer selected from the group consisting of a delayed fluorescence emitter, a phosphorescent emitter, and combination thereof.

(77) In some embodiments, the compound may be a sensitizer, and the OLED may further comprise an acceptor selected from the group consisting of a delayed fluorescence emitter, a fluorescent emitter, and combination thereof.

(78) In some embodiments, the compound may be a fluorescent emitter, a delayed fluorescence emitter, or a component of an exciplex that is a fluorescent emitter or a delayed fluorescence emitter.

(79) In yet another aspect, the OLED of the present disclosure may also comprise an emissive region containing a compound as disclosed in the above compounds section of the present disclosure.

(80) In some embodiments, the emissive region may comprise a compound of Formula I:

(81) ##STR00028##

wherein each of Y^{sup.A}, Y^{sup.B}, and Y^{sup.C} is independently O, S, Se, CRR', or SiRR'; n is 0 or 1, with Y^{sup.C} being not present when n=0, while X^{sup.7} and X^{sup.8} are both C when n=1; each of X^{sup.1}-X^{sup.11} is independently C or N; each of R^{sup.A}, R^{sup.B}, and R^{sup.C} independently represents zero, mono, or up to the maximum allowed number of substitutions to its associated ring; each of R, R', R^{sup.A}, R^{sup.B}, and R^{sup.C} is independently a hydrogen or a substituent selected from the group consisting of the general substituents defined herein; and any two adjacent R, R', R^{sup.A}, R^{sup.B}, or R^{sup.C} can be joined or fused together to form a ring, wherein at least one of R^{sup.A}, R^{sup.B}, and R^{sup.C} comprises an N-containing moiety with each N atom forming three σ bonds with its adjacent atoms, and all the three σ bonds being within one or more cyclic groups.

(82) In some embodiments, at least one of the anode, the cathode, or a new layer disposed over the organic emissive layer functions as an enhancement layer. The enhancement layer comprises a plasmonic material exhibiting surface plasmon resonance that non-radiatively couples to the emitter material and transfers excited state energy from the emitter material to non-radiative mode of surface plasmon polariton. The enhancement layer is provided no more than a threshold distance away from the organic emissive layer, wherein the emitter material has a total non-radiative decay rate constant and a total radiative decay rate constant due to the presence of the enhancement layer and the threshold distance is where the total non-radiative decay rate constant is equal to the total radiative decay rate constant. In some embodiments, the OLED further comprises an outcoupling layer. In some embodiments, the outcoupling layer is disposed over the enhancement layer on the opposite side of the organic emissive layer. In some embodiments, the outcoupling layer is disposed on opposite side of the emissive layer from the enhancement layer but still outcouples energy from the surface plasmon mode of the enhancement layer. The outcoupling layer scatters the energy from the surface plasmon polaritons. In some embodiments this energy is scattered as photons to free space. In other embodiments, the energy is scattered from the surface plasmon mode into other modes of the device such as but not limited to the organic waveguide mode, the substrate mode, or another waveguiding mode. If energy is scattered to the non-free space mode of

the OLED other outcoupling schemes could be incorporated to extract that energy to free space. In some embodiments, one or more intervening layer can be disposed between the enhancement layer and the outcoupling layer. The examples for intervening layer(s) can be dielectric materials, including organic, inorganic, perovskites, oxides, and may include stacks and/or mixtures of these materials.

(83) The enhancement layer modifies the effective properties of the medium in which the emitter material resides resulting in any or all of the following: a decreased rate of emission, a modification of emission line-shape, a change in emission intensity with angle, a change in the stability of the emitter material, a change in the efficiency of the OLED, and reduced efficiency roll-off of the OLED device. Placement of the enhancement layer on the cathode side, anode side, or on both sides results in OLED devices which take advantage of any of the above-mentioned effects. In addition to the specific functional layers mentioned herein and illustrated in the various OLED examples shown in the figures, the OLEDs according to the present disclosure may include any of the other functional layers often found in OLEDs.

(84) The enhancement layer can be comprised of plasmonic materials, optically active metamaterials, or hyperbolic metamaterials. As used herein, a plasmonic material is a material in which the real part of the dielectric constant crosses zero in the visible or ultraviolet region of the electromagnetic spectrum. In some embodiments, the plasmonic material includes at least one metal. In such embodiments the metal may include at least one of Ag, Al, Au, Ir, Pt, Ni, Cu, W, Ta, Fe, Cr, Mg, Ga, Rh, Ti, Ru, Pd, In, Bi, Ca alloys or mixtures of these materials, and stacks of these materials. In general, a metamaterial is a medium composed of different materials where the medium as a whole acts differently than the sum of its material parts. In particular, we define optically active metamaterials as materials which have both negative permittivity and negative permeability. Hyperbolic metamaterials, on the other hand, are anisotropic media in which the permittivity or permeability are of different sign for different spatial directions. Optically active metamaterials and hyperbolic metamaterials are strictly distinguished from many other photonic structures such as Distributed Bragg Reflectors (“DBRs”) in that the medium should appear uniform in the direction of propagation on the length scale of the wavelength of light. Using terminology that one skilled in the art can understand: the dielectric constant of the metamaterials in the direction of propagation can be described with the effective medium approximation. Plasmonic materials and metamaterials provide methods for controlling the propagation of light that can enhance OLED performance in a number of ways.

(85) In some embodiments, the enhancement layer is provided as a planar layer. In other embodiments, the enhancement layer has wavelength-sized features that are arranged periodically, quasi-periodically, or randomly, or sub-wavelength-sized features that are arranged periodically, quasi-periodically, or randomly. In some embodiments, the wavelength-sized features and the sub-wavelength-sized features have sharp edges.

(86) In some embodiments, the outcoupling layer has wavelength-sized features that are arranged periodically, quasi-periodically, or randomly, or sub-wavelength-sized features that are arranged periodically, quasi-periodically, or randomly. In some embodiments, the outcoupling layer may be composed of a plurality of nanoparticles and in other embodiments the outcoupling layer is composed of a plurality of nanoparticles disposed over a material. In these embodiments the outcoupling may be tunable by at least one of varying a size of the plurality of nanoparticles, varying a shape of the plurality of nanoparticles, changing a material of the plurality of nanoparticles, adjusting a thickness of the material, changing the refractive index of the material or an additional layer disposed on the plurality of nanoparticles, varying a thickness of the enhancement layer, and/or varying the material of the enhancement layer. The plurality of nanoparticles of the device may be formed from at least one of metal, dielectric material, semiconductor materials, an alloy of metal, a mixture of dielectric materials, a stack or layering of one or more materials, and/or a core of one type of material and that is coated with a shell of a

different type of material. In some embodiments, the outcoupling layer is composed of at least metal nanoparticles wherein the metal is selected from the group consisting of Ag, Al, Au, Ir, Pt, Ni, Cu, W, Ta, Fe, Cr, Mg, Ga, Rh, Ti, Ru, Pd, In, Bi, Ca, alloys or mixtures of these materials, and stacks of these materials. The plurality of nanoparticles may have additional layer disposed over them. In some embodiments, the polarization of the emission can be tuned using the outcoupling layer. Varying the dimensionality and periodicity of the outcoupling layer can select a type of polarization that is preferentially outcoupled to air. In some embodiments the outcoupling layer also acts as an electrode of the device.

(87) In yet another aspect, the present disclosure also provides a consumer product comprising an organic light-emitting device (OLED) having an anode; a cathode; and an organic layer disposed between the anode and the cathode, wherein the organic layer may comprise a compound as disclosed in the above compounds section of the present disclosure.

(88) In some embodiments, the consumer product comprises an organic light-emitting device (OLED) having an anode; a cathode; and an organic layer disposed between the anode and the cathode, wherein the organic layer may comprise a compound of Formula I:

(89) ##STR00029##

wherein each of Y^{sup}.A, Y^{sup}.B, and Y^{sup}.C is independently O, S, Se, CRR', or SiRR'; n is 0 or 1, with Y^{sup}.C being not present when n=0, while X^{sup}.7 and X^{sup}.8 are both C when n=1; each of X^{sup}.1-X^{sup}.11 is independently C or N; each of R^{sup}.A, R^{sup}.B, and R^{sup}.C independently represents zero, mono, or up to the maximum allowed number of substitutions to its associated ring; each of R, R', R^{sup}.A, R^{sup}.B, and R^{sup}.C is independently a hydrogen or a substituent selected from the group consisting of the general substituents defined herein; and any two adjacent R, R', R^{sup}.A, R^{sup}.B, or R^{sup}.C can be joined or fused together to form a ring, wherein at least one of R^{sup}.A, R^{sup}.B, and R^{sup}.C comprises an N-containing moiety with each N atom forming three σ bonds with its adjacent atoms, and all the three σ bonds being within one or more cyclic groups.

(90) In some embodiments, the consumer product can be one of a flat panel display, a computer monitor, a medical monitor, a television, a billboard, a light for interior or exterior illumination and/or signaling, a heads-up display, a fully or partially transparent display, a flexible display, a laser printer, a telephone, a cell phone, tablet, a phablet, a personal digital assistant (PDA), a wearable device, a laptop computer, a digital camera, a camcorder, a viewfinder, a micro-display that is less than 2 inches diagonal, a 3-D display, a virtual reality or augmented reality display, a vehicle, a video wall comprising multiple displays tiled together, a theater or stadium screen, a light therapy device, and a sign.

(91) 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.

(92) 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.

(93) 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.

(94) 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.

(95) 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.

(96) 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.sub.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, electrically-conductive, 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.

(97) 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**.

(98) 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 present disclosure 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.

(99) 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.

(100) 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 are 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.

(101) Devices fabricated in accordance with embodiments of the present disclosure 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 non-polymeric material

consists essentially of polymeric silicon and inorganic silicon.

(102) Devices fabricated in accordance with embodiments of the present disclosure 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 present disclosure 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, heads-up 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, a light therapy device, and a sign. Various control mechanisms may be used to control devices fabricated in accordance with the present disclosure, 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° C.), but could be used outside this temperature range, for example, from -40 degree C. to +80° C.

(103) 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.

(104) 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.

(105) 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.

(106) 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.

(107) 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). 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 ligands. 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.

(108) 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.

(109) According to another aspect, a formulation comprising the compound described herein is also disclosed.

(110) 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.

(111) 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.

(112) 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 can also be incorporated into the supramolecule complex without covalent bonds.

D. Combination of the Compounds of the Present Disclosure with Other Materials

(113) 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.

(114) a) Conductivity Dopants:

(115) 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.

(116) 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, WO06081780, WO2009003455, WO2009008277, WO2009011327, WO2014009310, US2007252140, US2015060804, US20150123047, and US2012146012.

(117) ##STR00030## ##STR00031##

b) HIL/HTL:

(118) A hole injecting/transporting material to be used in the present disclosure 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 monomer derived from compounds such as phosphoric acid and silane derivatives; a metal oxide derivative, such as MoO₃; a p-type semiconducting organic compound, such as 1,4,5,8,9,12-Hexaazatriphenylenehexacarbonitrile; a metal complex, and a cross-linkable compounds.

(119) Examples of aromatic amine derivatives used in HIL or HTL include, but not limit to the following general structures:

(120) ##STR00032##

(121) Each of Ar^{sup.1} to Ar^{sup.9} 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, 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 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, sulfinyl, sulfonyl, phosphino, and combinations thereof.

(122) In one aspect, Ar^{sup.1} to Ar^{sup.9} is independently selected from the group consisting of:

(123) ##STR00033##

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

(124) Examples of metal complexes used in HIL or HTL include, but are not limited to the

following general formula:

(125) ##STR00034##

wherein Met is a metal, which can have an atomic weight greater than 40; (Y.sup.101-Y.sup.102) is a bidentate ligand, Y.sup.101 and Y.sup.102 are independently selected from C, N, O, P, and S; L.sup.101 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.

(126) In one aspect, (Y.sup.101-Y.sup.102) is a 2-phenylpyridine derivative. In another aspect, (Y.sup.101-Y.sup.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.sup.+ / Fc couple less than about 0.6 V.

(127) 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, DE102012005215, EP01624500, EP01698613, EP01806334, EP01930964, EP01972613, EP01997799, EP02011790, EP02055700, EP02055701, EP1725079, EP2085382, EP2660300, EP650955, JP07-073529, JP2005112765, JP2007091719, JP2008021687, JP2014-009196, KR20110088898, KR20130077473, TW201139402, US06517957, US20020158242, US20030162053, US20050123751, US20060182993, US20060240279, US20070145888, US20070181874, US20070278938, US20080014464, US20080091025, US20080106190, US20080124572, US20080145707, US20080220265, US20080233434, US20080303417, 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.

(128) ##STR00035## ##STR00036## ##STR00037## ##STR00038## ##STR00039##
##STR00040## ##STR00041##

c) EBL:

(129) 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.

(130) d) Hosts:

(131) The light emitting layer of the organic EL device of the present disclosure 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.

(132) Examples of metal complexes used as host are preferred to have the following general formula:

(133) ##STR00042##

wherein Met is a metal; (Y.sup.103-Y.sup.104)) is a bidentate ligand, Y.sup.103 and Y.sup.104 are independently selected from C, N, O, P, and S; L.sup.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.

(134) In one aspect, the metal complexes are:

(135) ##STR00043##

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

(136) In another aspect, Met is selected from Ir and Pt. In a further aspect, (Y.sup.103Y.sup.104) is a carbene ligand.

(137) In one aspect, the host compound contains at least one of the following groups 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.

(138) In one aspect, the host compound contains at least one of the following groups in the molecule:

(139) ##STR00044## ##STR00045##

wherein R.sup.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.sup.101 to X.sup.108 are independently selected from C (including CH) or N. Z.sup.101 and Z.sup.102 are independently selected from NR.sup.101, O, or S.

(140) 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, WO2004093207, WO2005014551, 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,

(141) ##STR00046## ##STR00047## ##STR00048## ##STR00049## ##STR00050##
##STR00051##

e) Additional Emitters:

(142) 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.

(143) 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. Pat. Nos. 6,699,599, 6,916,554, 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, US20090039776, US20090108737, US20090115322, 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.

(144) ##STR00052## ##STR00053## ##STR00054## ##STR00055## ##STR00056##
##STR00057## ##STR00058## ##STR00059## ##STR00060## ##STR00061## ##STR00062##
##STR00063## ##STR00064## ##STR00065## ##STR00066## ##STR00067## ##STR00068##
##STR00069## ##STR00070## ##STR00071## ##STR00072##

f) HBL:

(145) 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.

(146) In one aspect, compound used in HBL contains the same molecule or the same functional groups used as host described above.

(147) In another aspect, compound used in HBL contains at least one of the following groups in the molecule:

(148) ##STR00073##

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

g) ETL:

(149) 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.

(150) In one aspect, compound used in ETL contains at least one of the following groups in the molecule:

(151) ##STR00074##

wherein R^{sup.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. A^{sup.1} to A^{sup.3} has the similar definition as Ar's mentioned above. k is an integer from 1 to 20. X^{sup.101} to X^{sup.108} is selected from C (including CH) or N.

(152) In another aspect, the metal complexes used in ETL contains, but not limit to the following general formula:

(153) ##STR00075##

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

(154) 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, 8,415,031, WO2003060956, WO2007111263, WO2009148269, WO2010067894, WO2010072300, WO2011074770, WO2011105373, WO2013079217, WO2013145667, WO2013180376, WO2014104499, WO2014104535,

(155) ##STR00076## ##STR00077## ##STR00078## ##STR00079## ##STR00080##
##STR00081## ##STR00082## ##STR00083## ##STR00084##

h) Charge Generation Layer (CGL)

(156) 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.

(157) 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.

(158) 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.

E. Experimental Section

Synthesis of Compound 1

(159) ##STR00085## ##STR00086##

(160) To a 2 L flask under nitrogen was added 4-bromo-2,6-difluoroaniline (38.7 g, 186 mmol), K₂CO₃ (107 g, 778 mmol), copper (39.1 g, 616 mmol), 1-iodo-2-methoxybenzene (99 g, 423 mmol), and 1,2-dichlorobenzene (0.5 L). The reaction mixture was stirred and heated to 180° C. for 68 hours. After cooling to room temperature, the reaction mixture was filtered through a plug of celite eluted with DCM. The filtrate was concentrated under reduced pressure. The purple solid was triturated with heptane followed by MeOH to give 4-bromo-2,6-difluoro-N,N-bis(2-methoxyphenyl)aniline (46.18 g, 59% yield) as a purple solid that was used in the next step as is in the next step.

(161) To a 5 L flask under nitrogen was added 4-bromo-2,6-difluoro-N,N-bis(2-methoxyphenyl)aniline (46.18 g, 110 mmol) and dichloromethane (2113 mL). The reaction mixture was cooled to -78° C. and boron tribromide (21.30 mL, 225 mmol) was added slowly. The reaction mixture was allowed to slowly warm to room temperature and stirred for 2.5 hours. The reaction mixture was slowly poured into ice-cold water under stirring. The organic layer was separated, and the aqueous layer was extracted with DCM. The organic layer was dried over Na₂SO₄, filtered, and concentrated. 2,2'-((4-Bromo-2,6-difluorophenyl)azanediyl)diphenol (45.45 g) was obtained as a purple solid and was used as is in the next step.

(162) To a 5 L flask under nitrogen was added potassium carbonate (48.5 g, 351 mmol), 2,2'-((4-bromo-2,6-difluorophenyl)azanediyl)diphenol (45.45 g, 116 mmol) and DMF (2229 mL). The reaction mixture was heated to 100° C. and stirred for 16 hours. The mixture was then cooled to 10° C. and water (1.5 L) was added. The mixture warmed to 30° C. during the addition. The mixture was allowed to return to 10° C. and the solid was collected via suction filtration. The purple solid was triturated with MeOH. The solid was suspended in DCM and filtered through a mixed plug (silica gel/basic alumina). Fractions containing product were combined and concentrated to give 7-bromobenzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine (22.26 g, 54%) as a white solid.

(163) To a 1 L flask under nitrogen was added 7-bromobenzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine (22.26 g, 63.2 mmol) and THF (300 mL). The solution was cooled to -78° C. and 2.5 M n-butyllithium solution in hexane (27.8 mL, 69.5 mmol) was added slowly. The mixture was stirred for 1.5 h and a solution of 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (16.12 mL, 79 mmol) in THF (60.0 mL) was added slowly. The reaction mixture was allowed to slowly warm to room temperature and stirred for 17 hours. The reaction mixture was diluted with

NH₄Cl(aq), stirred, and the organic layer was separated. The aqueous layer was extracted with DCM. The organic layer was dried over Na₂SO₄, filtered, and concentrated. The crude material was filtered through a plug of silica gel and eluted with 25% DCM/heptane followed by 20% EtOAc/DCM. The pure fractions were combined and concentrated to obtain 7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine (19.96 g, 79%). (164) To a 1 L flask under nitrogen was added 4,6-dibromodibenzo[b,d]furan (38.8 g, 119 mmol), potassium carbonate (16.44 g, 119 mmol), tetrakis(triphenylphosphine)palladium(0) (2.20 g, 1.90 mmol), 7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine (19.0 g, 47.6 mmol), toluene (170 mL), ethanol (34.0 mL), and water (34.0 mL). The mixture was heated to reflux (74° C.) for 16 hours. After cooling to room temperature, the mixture was diluted with water and the solid was collected via suction filtration. The solid was sequentially triturated with MeOH, DCM and MeOH, and acetone, then recrystallized from refluxing toluene followed by refluxing CHCl₃ to obtain 7-(6-bromodibenzo[b,d]furan-4-yl)benzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine (8.82 g, 35.4%).

(165) To a 250 mL flask under nitrogen was added 7-(6-bromodibenzo[b,d]furan-4-yl)benzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine (9.3 g, 17.94 mmol), 7-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene (8.53 g, 21.53 mmol), potassium phosphate (11.42 g, 53.8 mmol), dicyclohexyl(2',4',6'-triisopropyl-[1,1'-biphenyl]-2-yl)phosphane (1.026 g, 2.153 mmol), Pd₂(dba)₃ (0.986 g, 1.076 mmol), toluene (100 mL), and water (10.00 mL). The mixture was heated to reflux (89° C.) and stirred for 17 hours. The reaction mixture was allowed to cool to room temperature and the precipitated solid was collected via suction filtration. The solid was washed with water followed by MeOH and then triturated with MeOH. The solid material was then suspended in toluene, heated to reflux, passed through a mixed plug (Al₂O₃/SiO₂) and eluted with boiling toluene. The fractions were concentrated and the precipitate was collected via suction filtration. The solid was sequentially triturated with EtOAc, acetone, DCM, THF and MeOH to give 7-(6-(5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracen-7-yl)dibenzo[b,d]furan-4-yl)benzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine (Compound 1) as a yellow solid (10.37 g, 82% yield).

Synthesis of Compound 2

(166) ##STR00087##

(167) To a 2 L flask under nitrogen was added K₂CO₃ (347 g, 2510 mmol), 1-bromo-3,5-difluorobenzene (96.90 g, 502 mmol) and NMP (640 mL). To the mixture was then added phenol (104 g, 1105 mmol). The reaction mixture was stirred and heated to 150° C. After 44 hours the reaction was allowed to cool to room temperature. The reaction mixture was poured into stirring ice water. The solid was collected via suction filtration. The solid was dissolved in DCM and dried over Na₂SO₄. The solution was filtered and concentrated. The resulting brown oil was slowly poured into stirring MeOH. The resulting white solid was collected via suction filtration (124.25 g, 72%).

(168) To a 500 mL flask under nitrogen was added ((5-bromo-1,3-phenylene)bis(oxy))dibenzene (25 g, 73.3 mmol) and THF (75 mL). The solution was cooled to -78° C. To the solution was added 2.5 M nBuLi solution in hexanes (30.8 mL, 77 mmol). The solution was stirred for 45 min. The solution was added to a solution of dimethoxydiphenylsilane (24.87 mL, 110 mmol) in THF (75 mL) at -78° C. After 30 min the reaction flask was removed from the cooling bath and stirred overnight. After stirring for 16 hours the reaction was quenched by adding saturated NH₄Cl(aq). The organic layer was separated, and the aqueous layer was extracted with DCM. The combined organic layers were dried over Na₂SO₄, filtered, and concentrated. The yellow-brown oil was filtered through a plug of silica gel eluted with DCM/heptane (10%-45%). Fractions containing product were combined and concentrated and filtered through another plug of silica gel eluted with toluene/heptane (30%-50%). Fractions containing only desired product were combined and concentrated to give a colorless oil (9.85 g, 28%).

(169) To a 500 mL flask under nitrogen was added 7-bromobenzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine (12.60 g, 35.8 mmol) and THF (126 mL). The solution was cooled to -78°C . To the solution was added 2.5 M nBuLi solution in hexanes (15.03 mL, 37.6 mmol). The solution was stirred for 1 hour. To the solution was added a solution of (3,5-diphenoxyphenyl)(methoxy)diphenylsilane (17.10 g, 36.0 mmol) in THF (126 mL) at -78°C . The reaction flask was stirred overnight as it warmed to room temperature. After 16 hours to the reaction mixture was added water. The organic layer was separated, and the aqueous layer was extracted with DCM. The combined organic layers were dried over Na_2SO_4 , filtered, and concentrated. The resulting brown oil was dissolved in DCM and filtered through a plug of silica gel eluted with DCM/heptane (0%-25%). The fractions were combined and concentrated. The solid product was triturated with MeOH giving a white-yellow solid (22.07 g, 86%).

(170) To a 500 mL flask under nitrogen was added 7-((3,5-diphenoxyphenyl)diphenylsilyl)benzo[5,6][1,4]oxazino[2,3,4-kl]phenoxazine (17.0 g, 23.75 mmol) and m-xylene (88 mL). The solution was cooled to -40°C . and 2.3 M hexyllithium in hexane (10.84 mL, 24.93 mmol) was added slowly. The reaction was removed from the cooling bath and allowed to cool to room temperature. The reaction mixture was then heated to 60°C . for 5 hours. The reaction mixture was then cooled to -30°C . and tribromoborane (2.58 mL, 27.3 mmol) was added slowly. The reaction mixture was removed from the cooling bath and stirred as it warmed to room temperature overnight. After stirring for 18 h the solution was cooled to 0°C . and N-ethyl-N-isopropylpropan-2-amine (10.37 mL, 59.4 mmol) was added slowly. The reaction mixture was heated to 127°C . for 6 h. The reaction mixture was cooled to 10°C . To the reaction mixture was added sat. NaOAc(aq) and brine. The mixture was extracted with DCM. The combined organic layers were dried over Na_2SO_4 , filtered, and concentrated. The brown oil was then purified sequentially by filtration through a mixed plug of SiO_2 and Al_2O_3 eluted with toluene/DCM, vacuum chromatography eluted with DCM/heptane (0%-15%), and trituration with DCM and MeOH to give Compound 2 as a yellow solid (2.52 g, 14%).

(171) The photophysical and electrochemical data for Compound 1 and Compound 2 were measured and are shown in Table 1. Solution cyclic voltammetry and differential pulsed voltammetry were performed using a CH Instruments model 6201B potentiostat using anhydrous dimethylformamide solvent and tetrabutylammonium hexafluorophosphate as the supporting electrolyte. Glassy carbon, and platinum and silver wires were used as the working, counter and reference electrodes, respectively. Electrochemical potentials were referenced to an internal ferrocene-ferroconium redox couple (Fc/Fc^+) by measuring the peak potential differences from differential pulsed voltammetry. The corresponding highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies were determined by referencing the cationic and anionic redox potentials to ferrocene (4.8 eV vs. vacuum) according to literature ((a) Fink, R.; Heischkel, Y.; Thelakkat, M.; Schmidt, H.-W. *Chem. Mater.* 1998, 10, 3620-3625. (b) Pommerehne, J.; Vestweber, H.; Guss, W.; Mahrt, R. F.; Bassler, H.; Porsch, M.; Daub, J. *Adv. Mater.* 1995, 7, 551). The T1 energy is obtained from the peak maximum of the gated emission spectrum of frozen sample in 2-MeTHF at 77 K. The gated emission spectra were collected on a Horiba Fluorolog-3 spectrofluorometer equipped with a Xenon Flash lamp with a flash delay of 10 milliseconds and a collection window of 50 milliseconds. All samples were excited at 300 nm.

(172) TABLE-US-00001 TABLE 1 Photophysical and electrochemical properties

Structure	HOMO	LUMO	T1
Compound 1	-5.10 eV	-2.65 eV	2.47 eV
Compound 2	-5.16 eV	-2.69 eV	2.66 eV

(173) The above data shows that Compounds 1 and 2 both have easily accessible HOMO and LUMO levels that make them good candidates as bipolar hosts for green or red OLEDs without the need for exocyclic C—N bonds.

Claims

1. A compound of Formula I ##STR00090## wherein: each of Y^{sup}.A, Y^{sup}.B, and Y^{sup}.C is independently O, S, Se, CRR', or SiRR'; n is 0 or 1, with Y^{sup}.C being not present when n=0, while X^{sup}.7 and X^{sup}.8 are both C when n=1; each of X^{sup}.1-X^{sup}.11 is independently C or N; each of R^{sup}.A, R^{sup}.B, and R^{sup}.C independently represents zero, mono, or up to the maximum allowed number of substitutions to its associated ring; each of R, R', R^{sup}.A, R^{sup}.B, and R^{sup}.C is independently a hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, selenyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and any two adjacent R, R', R^{sup}.A, R^{sup}.B, or R^{sup}.C can be joined or fused together to form a ring, wherein at least one of R^{sup}.A, R^{sup}.B, and R^{sup}.C comprises an N-containing moiety with each N atom forming three σ bonds with its adjacent atoms, and all the three σ bonds being within one or more cyclic groups.
2. The compound of claim 1, wherein each of R, R', R^{sup}.A, R^{sup}.B, and R^{sup}.C is independently hydrogen or a substituent selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof; and any two adjacent R, R', R^{sup}.A, R^{sup}.B, or R^{sup}.C can be joined or fused together to form a ring, wherein at least one of R^{sup}.A, R^{sup}.B, and R^{sup}.C comprises an N-containing moiety with each N atom forming three σ bonds with its adjacent atoms, and all the three σ bonds being within one or more cyclic groups.
3. The compound of claim 1, wherein one R^{sup}.A or one R^{sup}.B comprises an N-containing moiety with each N atom forming three σ bonds with its adjacent atoms, and all the three σ bonds being within one or more cyclic groups.
4. The compound of claim 1, wherein the N-containing moiety is attached to Formula I through a direct bond, or a linking group selected from the group consisting of an atom, a monocyclic ring, a bicyclic fused ring, a tricyclic fused ring, and combinations thereof.
5. The compound of claim 4, wherein the linking group is selected from the group consisting of: ##STR00091## and combinations thereof, wherein Y^{sup}.D, Y^{sup}.E and Y^{sup}.F are each independently selected from the group consisting of O, S, NR, CRR', SiRR', GeRR'; and each of R^{sup}.1 and R^{sup}.2 is independently a hydrogen or a substituent selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, boryl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof.
6. The compound of claim 4, wherein the linking group is selected from the group consisting of: ##STR00092## and combinations thereof, wherein Y^{sup}.a is O, S, NR, CRR', or SiRR'.
7. The compound of claim 1, wherein the N-containing moiety comprises a structure selected from the group consisting of: ##STR00093## ##STR00094## wherein each of Y^{sup}.D and Y^{sup}.E are each independently selected from the group consisting of O, S, NR, CRR', SiRR', GeRR'.
8. The compound of claim 1, wherein n is 0 or 1.
9. The compound of claim 1, wherein each of Y^{sup}.A, Y^{sup}.B, and Y^{sup}.C is independently O; or two of Y^{sup}.A, Y^{sup}.B, and Y^{sup}.C are O.
10. The compound of claim 1, wherein each of X^{sup}.1-X^{sup}.3 is independently C; or one of X^{sup}.1-X^{sup}.3 is N.
11. The compound of claim 1, wherein each of X^{sup}.4-X^{sup}.7 is independently C; or one of X^{sup}.4-X^{sup}.7 is N.
12. The compound of claim 1, wherein each of X^{sup}.8-X^{sup}.11 is independently C; or one of

X.sup.8-X.sup.11 is N.

13. The compound of claim 1, wherein the compound is selected from the group consisting of: ##STR00095## ##STR00096## ##STR00097## ##STR00098## wherein, each of R.sup.1 and R.sup.2 is independently a hydrogen or a substituent selected from the group consisting of deuterium, fluorine, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, alkenyl, cycloalkenyl, heteroalkenyl, aryl, heteroaryl, nitrile, isonitrile, sulfanyl, and combinations thereof; Y.sup.D, Y.sup.E and Y.sup.F are each independently selected from the group consisting of O, S, NR, CRR', SiRR', GeRR'; and moiety D.sup.G comprises a moiety selected from the group consisting of: ##STR00099## ##STR00100## ##STR00101##

14. The compound of claim 1, wherein the compound is selected from the group consisting of: ##STR00102## ##STR00103## ##STR00104## ##STR00105## ##STR00106## ##STR00107## ##STR00108## ##STR00109## ##STR00110## ##STR00111## ##STR00112## ##STR00113## ##STR00114## wherein i, j, k, l, and m are each an integer from 1 to 5, where Y1 is O, Y2 is S, Y3 is Se, Y4 is CMe.sub.2 and Y5 is SiPh.sub.2 and wherein n is an integer from 1 to 50 where each Dn is defined as shown below: ##STR00115## ##STR00116## ##STR00117## ##STR00118## ##STR00119## ##STR00120## ##STR00121## ##STR00122## ##STR00123##

15. The compound of claim 1, wherein the compound is selected from the group consisting of: ##STR00124## ##STR00125## ##STR00126## ##STR00127## ##STR00128## ##STR00129## ##STR00130## ##STR00131## ##STR00132##

16. An organic light emitting device (OLED) comprising: an anode; a cathode; and an organic layer disposed between the anode and the cathode, wherein the organic layer comprises a compound of Formula I ##STR00133## wherein: each of Y.sup.A, Y.sup.B, and Y.sup.C is independently O, S, Se, CRR', or SiRR'; n is 0 or 1, with Y.sup.C being not present when n=0, while X.sup.7 and X.sup.8 are both C when n=1; each of X.sup.1-X.sup.11 is independently C or N; each of R.sup.A, R.sup.B, and R.sup.C independently represents zero, mono, or up to the maximum allowed number of substitutions to its associated ring; each of R, R', R.sup.A, R.sup.B, and R.sup.C is independently a hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, alkoxy, aryloxy, amino, silyl, germlyl, boryl, selenyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and any two adjacent R, R', R.sup.A, R.sup.B, or R.sup.C can be joined or fused together to form a ring, wherein at least one of R.sup.A, R.sup.B, and R.sup.C comprises an N-containing moiety with each N atom forming three σ bonds with its adjacent atoms, and all the three σ bonds being within one or more cyclic groups.

17. The OLED of claim 16, wherein the compound is a host, and the organic layer is an emissive layer that comprises a phosphorescent emitter.

18. The OLED of claim 16, wherein the phosphorescent emitter is a transition metal complex having at least one ligand or part of the ligand if the ligand is more than bidentate selected from the group consisting of: ##STR00134## ##STR00135## ##STR00136## wherein: T is selected from the group consisting of B, Al, Ga, and In; each of Y.sup.1 to Y.sup.13 is independently selected from the group consisting of carbon and nitrogen; Y' is selected from the group consisting of BR.sub.e, NR.sub.e, PR.sub.e, O, S, Se, C=O, S=O, SO.sub.2, CR.sub.eR.sub.f, SiR.sub.eR.sub.f, and GeR.sub.eR.sub.f; R.sub.e and R.sub.f can be fused or joined to form a ring; each R.sub.a, R.sub.b, R.sub.c, and R.sub.d independently represent zero, mono, or up to a maximum allowed number of substitutions to its associated ring; each of R.sub.a1, R.sub.b1, R.sub.c1, R.sub.d1, R.sub.a, R.sub.b, R.sub.c, R.sub.d, R.sub.e and R.sub.f is independently a hydrogen or a substituent selected from the group consisting of deuterium, halide, alkyl, cycloalkyl, heteroalkyl, alkoxy, aryloxy, amino, silyl, germlyl, boryl, selenyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carbonyl, carboxylic acid, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; the general substituents defined herein; and any two adjacent

R.sub.a, R.sub.b, R.sub.c, R.sub.d, R.sub.e and R.sub.f can be fused or joined to form a ring or form a multidentate ligand.

19. A consumer product comprising an organic light-emitting device comprising: an anode; a cathode; and an organic layer disposed between the anode and the cathode, wherein the organic layer comprises a compound of Formula I: ##STR00137## wherein: each of Y^{sup.A}, Y^{sup.B}, and Y^{sup.C} is independently O, S, Se, CRR', or SiRR'; n is 0 or 1, with Y^{sup.C} being not present when n=0, while X^{sup.7} and X^{sup.8} are both C when n=1; each of X^{sup.1}-X^{sup.11} is independently C or N; each of R^{sup.A}, R^{sup.B}, and R^{sup.C} independently represents zero, mono, or up to the maximum allowed number of substitutions to its associated ring; each of R, R', R^{sup.A}, R^{sup.B}, and R^{sup.C} is independently a hydrogen or a substituent selected from the group consisting of deuterium, halogen, alkyl, cycloalkyl, heteroalkyl, heterocycloalkyl, alkoxy, aryloxy, amino, silyl, germyl, boryl, selenyl, alkenyl, cycloalkenyl, heteroalkenyl, alkynyl, aryl, heteroaryl, acyl, carboxylic acid, ether, ester, nitrile, isonitrile, sulfanyl, sulfinyl, sulfonyl, phosphino, and combinations thereof; and any two adjacent R, R', R^{sup.A}, R^{sup.B}, or R^{sup.C} can be joined or fused together to form a ring, wherein at least one of R^{sup.A}, R^{sup.B}, and R^{sup.C} comprises an N-containing moiety with each N atom forming three σ bonds with its adjacent atoms, and all the three σ bonds being within one or more cyclic groups.

20. A formulation comprising a compound according to claim 1.
