Aggregation-Induced Delayed Fluorescence Molecules with Mechanochromic Behaviors for Efficient Blue Organic Light-Emitting Diodes

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SUMMARY

Aggregation-induced delayed fluorescence (AIDF) materials combining the advantages of aggregation-induced emission and thermally activated delayed fluorescence, have attracted considerable attention. However, blue AIDF materials with satisfactory electroluminescence efficiencies are still few. In this work, two blue luminescent molecules (XT-DPDBA and XT-BDPDBA) with evident AIDF characteristics and high photoluminescence quantum yields are developed by using rigid electron acceptor xanthenone and weak electron donor 10-dihydrodibenzo[b,e][1,4]azasiline. Both molecules exhibit prominent mechanochromic luminescence (MCL) behaviors originating from conformational interconversion between quasi-axial and quasi-equatorial conformations. The quasi-equatorial conformation has small singlet–triplet energy splitting and thus delayed fluorescence characteristic. Efficient blue organic light-emitting diodes are fabricated based on both molecules, providing high external quantum efficiencies of up to 27.0% and small efficiency roll-offs. These blue AIDF molecules with MCL property have good application potentials in various optical and electronic devices.

INTRODUCTION

The development of high-efficiency organic light-emitting diodes (OLEDs) is of essential importance for commercial applications in both full-color displays and lighting industry.[1-3] In recent years, tremendous efforts have been devoted to improve the exciton utilization of the luminescent materials.[4-8] As promising purely organic emitters for OLEDs, thermally activated delayed fluorescence (TADF) materials can harvest singlet and triplet excitons simultaneously for radiative transition by the reverse intersystem crossing (RISC) process and thus reach the comparable external quantum efficiencies (η_{ext}s) to those of noble metal-containing phosphorescent materials. The singlet–triplet energy splitting (ΔE_{ST}) is a crucial parameter to evaluate TADF emitters. A small ΔE_{ST} can promote RISC process, which can be realized by the separation of the highest occupied molecular orbitals (HOMOs) and the lowest unoccupied molecular orbitals (LUMOs).[9-13] However, due to the long lifetimes of triplet excited states, most conventional TADF materials suffer from concentration quenching and triplet-triplet annihilation in pure films.[14-15] In consideration of this, guest-host doping technique is widely used to disperse luminescent materials into host matrix to alleviate emission and exciton quenching.[16-17]

Aggregation-induced delayed fluorescence (AIDF) materials, which possess the advantages of both high triplet exciton utilization and strong luminescence in solid states, have received increasing attention. The reported non-doped OLEDs based on AIDF emitters have high η_{ext}s and low efficiency roll-offs, which manifest their high application potential.[18-26] Thus far, the emission color of the high-performance OLEDs fabricated by AIDF materials are mostly yellow and green, while efficient blue AIDF materials are much less. Besides, blue-emitting materials play an indispensable role in the RGB (red, green and blue) display and white lighting engineering.[27-30] Hence, it is highly desired to develop robust blue AIDF emitters.

The carbonyl group has been widely used to design numerous luminescent materials as an electron acceptor, which can facilitate intersystem crossing by increasing spin-orbit coupling.[31-35] Thus, in this work, we adopt the xanthenone (XT) containing a carbonyl group as a weak acceptor. It has as a more planar and rigid configuration than benzophenone (BP) because of an oxygen bridge linking two phenyl rings of BP, which is favorable for improving photoluminescence quantum yield (Φ_{PL}) of the target molecules. Moreover, 5,10-dihydrodibenzo[b,e][1,4]azasiline (DPDBA), an analogue of 9,9-diphenyl-9,10-dihydroacridine (DPAC), is used as electron donor to create delayed fluorescence molecules with XT acceptor. The employment of Si atom in DPDBA can reduce the electron-donating ability and thus lead to blue-shifted emission.[36-40] Based on this design, molecules with XT as acceptor conjugated with unilateral and bilateral DPDBA (XT-DPDBA and XT-BDPDBA) are explored. They exhibit evident bicolor switching phenomena under mechanical force due to their conformational interconversion, and have apparent AIDF property and strong blue emission in neat films. Owing to these advantageous photophysical attributes, the OLEDs based on XT-DPDBA and XT-BDPDBA exhibit bright blue electroluminescence (EL) with a high η_{ext} of up to 27.0%. The results further indicate that the employment of DPDBA as donor can maintain comparable EL performance but blue-shifted emissions in comparison with the molecules with DPAC donors (Figure 1A).

RESULTS AND DISCUSSION

Synthesis and Characterization

The chemical structures and synthetic routes of XT-DPDBA and XT-BDPDBA are presented in Scheme S1 in Supporting Information. DPDBA was prepared according to the reported method.[40] The target molecules XT-DPDBA and XT-BDPDBA were obtained by the Buchwald−Hartwig amination of DPDBA with 3-bromo-9H-xanthen-9-one and 3,6-dibromo-9H-xanthen-9-one, respectively. The molecular structures were confirmed by ^{1}H and ^{13}C NMR and high-resolution mass spectrometry (HRMS), and the detailed synthetic procedures and characterization data are described in Supporting Information.

Single crystals of XT-DPDBA and XT-BDPDBA were obtained from a dichloromethane (DCM)-methanol system via slow solvent evaporation. As shown in Figure 1B, both XT-DPDBA and XT-BDPDBA adopt a quasi-axial (QA) conformation in crystals, in which DPDBA is highly twisted. It looks like DPDBA standing on XT plane. This kind of conformation occurs frequently in the molecules with acridan-analogous donors containing C-Si or C-S bonds, which can be attributed to the mismatch of the bridging bond lengths in each donor unit.[41-50] There are intramolecular π–π stacking formed between the phenyl rings in DPDBA and XT with distances of 3.64–3.84 Å, which are favored to stabilize such QA conformation. However, no obvious intermolecular π–π stacking is observed in their crystal packing mode (Figure S1). Taking XT-BDPDBA as an example, multiple C–H···π interactions and C=O···H hydrogen bonds with distances of 2.58–3.27 Å are observed, which can rigidify molecular structure and restrict intramolecular motions in the aggregated state, thus suppressing non-radiative decay of the excited state.

Thermal Stability and Electrochemical Behavior

The thermal stabilities of XT-DPDBA and XT-BDPDBA were examined by thermogravimetric analysis (TGA) at a heating rate of 10 ^{o}C min^{-1} under nitrogen atmosphere. They have good thermal stabilities (Figure 2A), with high decomposition temperatures (T_d, corresponding to 5% weight loss) of 347 and 459 ^{o}C for XT-DPDBA and XT-BDPDBA, respectively. The electrochemical properties of the molecules were characterized by cyclic voltammetry (Figure 2B). Both molecules have similar reversible oxidation and reduction processes, indicating their good electrochemical stability. The energy levels of highest occupied molecular orbitals (HOMOs) and lowest unoccupied molecular orbitals (LUMOs) are calculated from the onsets of the oxidation and reduction peaks. XT-DPDBA and XT-BDPDBA have similar HOMO energy levels of –5.52 and –5.51eV, and similar LUMOs energy levels of –2.80 and –2.94 eV, respectively.

Photophysical Properties

The XT-DPDBA and XT-BDPDBA exhibit similar absorption maxima at 337 nm. A weak absorption tail extending to 420 nm is observed (Figure 3A), mainly associated with intramolecular charge transfer (ICT) from DPDBA donor to XT acceptor. In dilute tetrahydrofuran (THF) solution, XT-DPDBA and XT-BDPDBA emit weak emissions with peaks at 501 and 508 nm, and low Φ_{PL} values of 16.2% and 16.7%, respectively. To study the emission property of the molecules in the aggregated state, their PL spectra in THF/water mixtures with different water fractions (f_{w}s) are measured. As shown in Figure 3B and Figure S2, the PL emission remains weak at low f_{w}s (0–70 vol%), which are attributed to the vigorous intramolecular motion that can quench the excited state in a nonradiative manner. But at high f_{w}s (80–99 vol%), the molecules tend to form aggregate and the PL emission is greatly enhanced due to restriction of intramolecular motions in the aggregated state.[51-52]

The transient PL decay spectra of the molecules were also measured in THF/water mixtures. Taking XT-DPDBA as an example (Figure 3C and Table S1), it shows short PL lifetime without obvious delayed component in THF. But with the increase of f_{w}, the PL lifetime of XT-DPDBA elongates sharply from 34 ns to 740 ns. At a f_{w} of 99 vol%, delayed component becomes apparent, with the lifetime and proportion reaching 1.81 μs and 40.0%, respectively. These findings indicate that both molecules possess evident AIDF property.

The neat films of XT-DPDBA and XT-BDPDBA show blue emission peaks at 472 and 480 nm and high Φ_{PL} values of 77% and 86%, respectively. They exhibit apparent delayed fluorescence with longer lifetimes of 2.82 and 2.40 μs, respectively. The improved delayed fluorescence in neat films again validates the AIDF property of both molecules. To further clarify the delayed fluorescence nature of XT-DPDBA and XT-BDPDBA in neat films, temperature-dependent transient PL decay spectra are measured in a range of 77 K to 300 K (Figure 3D and Figure S3) under nitrogen. As the temperature rises from 77 K to 300 K, both molecules exhibit more prominent delayed fluorescence (Table S2) owing to the facilitation of RISC at high temperatures, which demonstrates typical TADF characteristic. The fluorescence and phosphorescence spectra of the neat films are recorded at 77 K (Figure S4). The values of ΔE_{ST} are 0.063 eV for XT-DPDBA and 0.025 eV for XT-BDPDBA, calculated from the onsets of the fluorescence and phosphorescence spectra. Such small ΔE_{ST} values can ensure the occurrence of RISC and thus delayed fluorescence of the molecules. The temperature-dependent PL spectra of XT-DPDBA and XT-BDPDBA in diluted solutions and films are also measured (Figure S5). The PL intensity becomes weakened apparently as the increase of temperature, while the PL intensity changes slightly in films. This is because intramolecular motion is dominative in solution sate. At high temperatures, more active intramolecular motion dissipates more excited state energy and serves as a non-radiative decay channel, leading to serious emission quenching. On the other hand, the intramolecular motion is suppressed to a large degree in film state. Although high temperature facilitates intramolecular motion, it also promotes RISC process, which leads to the enhancement of delayed fluorescence. These competing effects make the PL intensity vary slightly along with the increase of temperature, which confirms the existence of delayed fluorescence as well.

Vacuum-deposited doped films of XT-DPDBA and XT-BDPDBA in bis[2-(diphenylphosphino)phenyl]ether oxide (DPEPO) host at a doping concentration of 30 wt% and 20 wt% are fabricated and investigated by the PL spectra and transient PL decay spectra (Figure S6). Based on all measured photophysical data, the rate constants of different excited state attenuation pathways can be calculated (Table 1 and Table S3, Support Information). The doped film of XT-DPDBA exhibits a higher Φ_{PL} of 97%, more delayed component (R_{delayed} = 49%), larger rate constant of RISC ($k_{\mathrm{RISC}} = 6.6 \times 10^5$ s^{-1}) and smaller ΔE_{ST} (0.026 eV) in comparison with neat film, ensuring a higher exciton utilization and excellent performance of the doped OLEDs based on XT-DPDBA. A similar trend can also be observed for XT-BDPDBA.

Electronic Structures

According to the previous reports, quasi-equatorial (QE) and QA conformations are supposed to result in two different conformers presenting delayed fluorescence and conventional fluorescence characteristics, respectively.[53-54] The effect of conformational interconversion in this system is visually observed in the PL spectra in various solvents with different polarities (Figure S7). The two molecules clearly display dual emissions consisting of a main peak at 470–570 nm (low-energy emission region) and a subsidiary peak at 400–420 nm (high-energy emission region) in polar solvents. As the polarity increases from *n*-hexane to *N*,*N*-dimethylformamide (DMF), both molecules show unconspicuous bathochromic shifts in PL peaks in high-energy emission region, indicating they result from their locally excited (LE) or mixed LE and intramolecular charge transfer (ICT). However, the PL peaks in low-energy emission region are associated with the ICT, as evidenced by the large bathochromic shifts with the increase of the polarity.

To gain in-depth insights into the electronic structures of both molecules, the computational simulation is performed using density functional theory (DFT) and time-dependent density functional theory. As shown in Figure 4, the optimized structures of both molecules in QA conformations are similar to their single crystal structures. The HOMOs and LUMOs are mostly overlapped on the acceptor moiety and present a dominating localized electronic transition characteristic in accordance with the measured high-energy emissions. The excessive overlaps between HOMOs and LUMOs lead to large theoretical ΔE_{ST} values of 0.72 eV and 0.54 eV for XT-DPDBA and XT-BDPDBA, respectively, which is unfavored for RISC process.

Since the conformational isomer of the molecules in QE conformation are not obtained directly from single crystal, computational simulation is carried out to obtain QE conformers as one of the energy-minimal conformers. Taking XT-DPDBA as an example, much larger torsion angles are estimated for its QE conformer and the free energy differences ($\Delta E_{\mathrm{Gibbs}}$) between the QA and QE conformers are estimated to be considerably small (2.4 kcal mol^{-1}), indicating that the QA conformer is thermodynamically preferable and interconvertible into QE conformer in dilute solution. As a symmetric donor-acceptor-donor (D-A-D) molecule, XT-BDPDBA justifiably adopts three possible conformers (QA-QA, QA-QE and QE-QE). Nevertheless, the Gibbs free energy of QE-QE conformer is 1287 kcal mol^{-1} higher than that of QA-QA conformer. Therefore, the QE-QE conformer is thermodynamically unpreferable and can hardly exist. The Gibbs free energy of (QE-QA) is only 0.21 kcal mol^{-1} higher than QA-QA, which allows coexistence of two conformers in solution at room temperature. Focusing on the HOMOs and LUMOs of QE conformers, there is inappreciable spatial overlaps of HOMOs and LUMOs, where the HOMOs and LUMOs are centered on DPDBA donors and XT acceptors, respectively, demonstrating apparent ICT characteristic in line with lower-energy broad emissions. Based on TD-DFT calculations, the ΔE_{ST} values of XT-DPDBA in QE conformation and XT-BDPDBA in QA-QE conformation are estimated to be 0.01 eV and 0.14 eV. Therefore, the higher- and lower-energy emissions originate from the QA and QE conformers, respectively, accountable for the solvent-dependent dual emissions.

Mechanochromic Luminescence

Conformational interconversion as a momentous mechanism of mechanochromic luminescence (MCL) is investigated extensively. As shown in Figure 5A, the pristine crystals of XT-DPDBA and XT-BDPDBA radiate deep blue lights with emission peaks at 421 and 439 nm, respectively.

When pristine crystals are treated by grinding, distinct emission changes from deep blue to sky-blue (421 nm to 480 nm for XT-DPDBA, and 439 nm to 492 nm for XT-BDPDBA) are observed. The MCL behaviors are further examined by powder X-ray diffraction (PXRD) measurement (Figure 5G and 5H). The PXRD pattern of the pristine crystals shows sharp and intense diffraction peaks in the range of 5^o to 35^o, disclosing high crystalline degree. After grinding, the diffraction peaks intensity is decreased but still remain diffraction peaks, indicating that the ground sample is still in crystalline state. Moreover, the MCL behaviors are reversible for XT-DPDBA. As shown in Figure 5B and 5D, after fuming with DCM vapor or heating at 200 ^{o}C for 1 hour, the sky-blue emission changes back to deep blue emission, and this behavior can be repeated for several circles. However, in comparison with XT-DPDBA, XT-BDPDBA shows inferior recovery ability (Figure 5C).

To further explore the cause of their MCL behaviors, photophysical properties of crystals and ground samples are investigated by the PL spectra at 77 K and transient PL decay spectra (Figure 5E, 5F and Figure S8). Before grinding, the transient PL attenuates rapidly with the lifetime of 4.0 ns for XT-DPDBA and 4.8 ns for XT-BDPDBA. The transient PL decay curves of ground sample can be well fitted by double exponential decay, corresponding to prompt and delayed fluorescence. The prompt and delayed lifetimes reach 37 ns and 3.36 μs for XT-DPDBA and 39 ns and 1.87 μs for XT-BDPDBA, respectively. Moreover, compared to the pristine crystals, the ΔE_{ST} values of the ground samples are reduced from 0.40 eV to 0.11 eV for XT-DPDBA, and from 0.28 eV to 0.09 eV for XT-BDPDBA, which facilitate RISC processes. The photophysical properties of pristine crystals reflect conventional fluorescence exactly corresponding to the theoretical calculation of QA conformers. The ground samples show bathochromic shifts and the characteristics of delayed fluorescence, which are associated to the QE conformers.

Luminescence properties of the two molecules are obviously changed from conventional fluorescence to delayed fluorescence by grinding. The change of molecular conformation should be the main reason of the mechanochromic behaviors.[55]

Carrier transport

The carrier transport property of both molecules is investigated in hole- and electron-only devices with the configurations of ITO/TAPC (10 nm)/XT-DPDBA or XT-BDPDBA (80 nm)/TAPC (10 nm)/Al and ITO/TmPyPB(10 nm)/XT-DPDBA or XT-BDPDBA (80 nm)/TmPyPB (10 nm)/LiF (1 nm)/Al, respectively, via space charge limited current method. As shown in Figure 6, at an electric field of 5.5×10^5 V cm^{-1}, the electron mobilities of XT-DPDBA and XT-BDPDBA are determined to be 3.11×10^{-3}, and 9.66×10^{-4} cm^2 V^{-1} s^{-1}, while the hole mobilities are 4.47×10^{-4} and 6.12×10^{-4} cm^2 V^{-1} s^{-1} respectively, which reveal the good bipolar carrier-transporting ability of XT-BDPDBA. In comparison with XT-DPDBA, XT-BDPDBA enjoys better balanced hole and electron transport ability, which is favorable for the fabrication of efficient OLEDs.

Electroluminescence

Benefiting from the prominent AIDF properties and high Φ_{PL} values in the neat films, the EL performance of the OLEDs using XT-DPDBA and XT-BDPDBA as emitting layers are investigated. The non-doped OLEDs possess a configuration of ITO/HATCN (5 nm)/TAPC (50 nm)/TCTA (5 nm)/mCP (5 nm)/EML (20 nm)/DPEPO (5 nm)/TmPyPB (30 nm)/LiF (1 nm)/Al (120 nm), where the neat film of XT-DPDBA and XT-BDPDBA serve as light-emitting layers (EML); indium-tin oxide (ITO) is the transparent anode; dipyrazino[2,3-f:2',3'-h]quinoxaline-2,3,6,7,10,11-hexacarbonitrile (HATCN) is hole-injecting material; 4,4'-(cyclohexane-1,1-diyl)bis(*N*,*N*-di-p-tolylaniline) (TAPC) and 1,3,5-tri(*m*-pyrid-3-yl-phenyl)benzene (TmPyPB) act as hole- and electron-transporting layers, respectively; 1,3-di(9H-carbazol-9-yl)benzene (mCP) and tris(4-(9H-carbazol-9-yl)phenyl)amine (TCTA) work as electron-blocking layers; bis[2-(diphenylphosphino)phenyl]ether oxide (DPEPO) serves as hole-blocking layers; and LiF/Al is cathode.

The non-doped device based on XT-DPDBA has a low turn-on voltage of 3.0 V and emits blue light at 472 nm with Commission Internationale de I'clairage coordinates ($\mathrm{CIE}_{x,y}$) of (0.151, 0.272) and maximum luminance ($L_{\max}$) of 4403 cd m^{-2}. Besides, the device shows the maximum current efficiency (η_C), power efficiency (η_P) and external quantum efficiency (η_{ext}) of 15.5 cd A^{-1}, 13.5 lm W^{-1} and 8.9%, respectively. Moreover, at a luminance of 1000 cd m^{-2}, the η_C, η_P, and η_{ext} retain 14.0 cd A^{-1}, 11.0 lm W^{-1}, and 8.0%, respectively, disclosing low efficiency roll-offs of this blue OLED (Figure S9 and Table 2). Compared with OLEDs of DPAC-XT in the previous literature[15]¸ this device exhibits a blue-shift from 488 nm to 472 nm, and the η_{ext} value at high luminance is better than those of DPAC-XT (η_{ext} = 5.9%). As for XT-BDPDBA, the non-doped OLEDs are turned on at a low voltage of 3.0 V and exhibits strong sky-blue EL emission with a peak at 488 nm and a high $L_{\max}$ of 9741 cd m^{-2}. The maximum η_C, η_P, and η_{ext} are increased to 30.1 cd A^{-1}, 29.6 lm W^{-1} and 13.1%, respectively.

To further evaluate the potential application of these molecules, doped OLEDs based on the doped films of the molecules are fabricated. The device configuration is ITO/HATCN (5 nm)/TAPC (50 nm)/TCTA (5 nm)/mCP (5 nm)/EML (20 nm)/DPEPO (5 nm)/TmPyPB (30 nm)/LiF (1 nm)/Al (120 nm). The EML is the doped film of the molecules in 2,8-bis (diphenylphosphoryl)dibenzo[b,d]furan (PPF) host or DPEPO host with varied doping concentrations of 20 and 30 wt%. The PPF doped OLEDs based on XT-DPDBA and XT-BDPDBA at doping concentrations of 20 and 30 wt%, respectively, show best performance and display low turn-on voltages of 3.2 and 3.0 V with EL peaks at 472 and 484 nm, respectively. The L_{max} values reach 9222 and 19319 cd m^{-2}, respectively (Figure 7, Figure S10 and Table 2). Moreover, high EL efficiencies of 33.6 cd A^{-1}, 33.0 lm W^{-1}, and 20.7% for XT-DPDBA and 55.0 cd A^{-1}, 57.5 lm W^{-1}, and 27.0% for XT-BDPDBA are acquired. Under the same device structure, at doping concentrations of 30 wt%, devices prepared by using another polar host material (DPEPO) also offers impressive EL performance with remarkable maximum current (η_{C}), power (η_{P}), and external quantum (η_{ext}) efficiencies of 31.2 cd A^{-1}, 30.6 lm W^{-1} and 18.0% for XT-DPDBA, and 51.2 cd A^{-1}, 47.3 lm W^{-1} and 26.4% for XT-BDPDBA.

In addition, OLEDs based on low-polar hosts are further fabricated with a configuration of ITO/HATCN (5 nm)/TAPC (50 nm)/TCTA (5 nm)/mCP (5 nm)/EML (20 nm)/DPEPO (5 nm) /TmPyPB (30 nm)/LiF (1 nm)/Al (120 nm), in which mCP and 3,3'-di(9H-carbazol-9-yl)-1,1'-biphenyl (mCBP) serve as hosts. The doped devices exhibit blue-shifted EL emissions with peaks in the range of 462 to 474 nm, and good EL performances with $\eta_{\mathrm{ext,max}}$, $\eta_{\mathrm{C,max}}$, and $\eta_{\mathrm{P,max}}$ of 8.7%, 12.5 cd A^{-1}, and 12.3 lm W^{-1} for XT-DPDBA, and 16.8%, 29.3 cd A^{-1}, and 28.8 lm W^{-1} for XT-BDPDBA (Figure 8 and Table 2). The decrease in EL efficiency may be attributed the larger ΔE_{ST} values of both molecules doped in low-polar host due to host tuning effect on ΔE_{ST}, which affects RISC process.[56] In comparison with the previously reported delayed fluorescence materials containing DPAC donors, both molecules containing DPDBA donors demonstrate comparable EL efficiencies but obviously blue-shifted EL emissions (Scheme 1). To the best of our knowledge, they are among the most efficient MCL-active TADF emitters (Table S4).[57-60]

Discussion

In conclusion, two molecules comprised of DPDBA donor and XT acceptor are designed and synthesized. They hold high thermal and electrochemical stabilities and exhibit AIDF characteristics. The rigid XT core and weak DPDBA donor enable the molecules to radiate intense blue-shifted emissions in comparison the analogous molecules with DPAC donors. By means of photophysical measurements, theory calculations and crystal structures, it is demonstrated that both molecules adopt two conformers (QA and QE) in dilute solution. They display remarkable mechanochromic behaviors with emissions changes from deep blue to sky-blue by grinding, which are associated with the conformational interconversion from QA to QE conformations. In comparison with QA conformers, the QE conformers have more separated HOMO and LUMOs and thus smaller ΔE_{ST} values, leading to the occurrence of delayed fluorescence. Efficient blue OLEDs are achieved based on the molecules, radiating apparently blue-shifted EL emissions in comparison with the analogous molecules containing DPAC donors as well. Their non-doped OLEDs provide good EL performance with η_{ext} values of up to 13.1% and small efficiency roll-offs. The doped OLEDs give excellent maximum η_C, η_P and η_{ext} of up to 55.0 cd A^{-1}, 57.5 lm W^{-1} and 27.0%, respectively. These results demonstrate that the utilizing of Si-containing weak electron-donor DPDBA offers a new avenue towards blue delayed fluorescence materials with MCL behaviors.

EXPERIMENTAL PROCEDURES

Resource availability

Lead contact

Further information and requests for resources and reagents should be directed to and will be fulfilled by the Lead Contact, Zujin Zhao (mszjzhao@scut.edu.cn)

Materials availability

The target molecules can be produced following the procedures in the section of the synthesis and characterization in Supporting Information

Data and code availability

All data supporting the findings of this study are available from the lead contact on request.

Supporting information

Supporting information can be found online at https://

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AUTHOR CONTRIBUTIONS

Z.Z. conceived of the study. J.H. synthesized the molecules and performed photophysical property measurements. H.C. and J.W. prepared and characterized devices. J.L. preformed theoretical computations. J.H. and Z.Z. wrote and revised the manuscript. Z.Z. and B.Z.T. supervised the project, and all authors contributed to writing and editing the document.

DECLARATION OF INTERESTS

The authors declare no competing interests.

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Figure Titles and Legends

Figure 1. Molecular and crystal structures

(A) The delayed fluorescence molecules containing DPAC and DPDBA donors and the EL data in doped OLEDs. (B) Single crystal structures of XT-DPDBA and XT-BDPDBA.

Figure 2. Thermal stability and electrochemical properties of the molecules

(A) TGA of XT-DPDBA and XT-BDPDBA, recorded under nitrogen atmosphere at a heating rate of 10 ^{o}C min^{-1}. T_d is the decomposition temperature. (B) Cyclic voltammograms of XT-DPDBA and XT-BDPDBA, measured in dichloromethane and *N*,*N*-dimethylformamide containing tetra-*n*-butylammonium hexafluorophosphate.

Figure 3. **Photophysical properties of the molecules**

(A) Absorption spectra of XT-DPDBA and XT-BDPDBA in THF solution (10^{-5} M) and PL spectra of XT-DPDBA and XT-BDPDBA in neat film. (B) PL spectra of XT-DPDBA in THF/water mixtures with different water fractions (f_w) (10^{-5} M), excited at 340 nm. (C) PL decay curves of XT-DPDBA in THF/water mixtures with different water fractions (f_w) (10^{-5} M), measured under nitrogen atmosphere at 300 K. (D) Temperature-dependent transient decay spectra of XT-DPDBA in neat film, measured under nitrogen atmosphere.

Figure 4. **Calculated frontier orbital distributions and energy levels of the molecules**

Calculated frontier orbital distributions (HOMOs and LUMOs) and energy levels for the ground-state QE and QA conformers of XT-DPDBA and XT-BDPDBA. Abbreviations: QA = quasi-axial; QE = quasi-equatorial; $\Delta E_{\mathrm{Gibbs}} = E_{\mathrm{QE}} - E_{\mathrm{QA}}$.

Figure 5. Mechanochromic behaviors of the molecules

(A) PL spectra of pristine crystals and ground samples. PL spectra of ground samples of (B) XT-DPDBA and (C) XT-BDPDBA in response to external stimuli (H: heating at 200 ^{o}C for 1 hour; F: fuming with CH_2Cl_2 for 1 hour; G: grinding with a mortar for 30 min). (D) Repeated mechanochromic behaviors of XT-DPDBA by grinding and heating (up layer), and grinding and fuming (bottom layer). Photographs of the samples under alternative grinding and heating (up layer), and grinding and fuming (bottom layer), taken under 365 nm irradiation. Transient PL decay curves of (E) XT-DPDBA and (F) XT-BDPDBA. PXRD patterns of the crystals and ground samples of (G) XT-DPDBA and (H) XT-BDPDBA.

Figure 6. Electric field-dependent carrier mobilities

(A) XT-DPDBA and (B) XT-BDPDBA. Carrier transport property of the molecules is measured in hole- and electron-only devices with the structures of ITO/TAPC (10 nm)/XT-DPDBA or XT-BDPDBA (80 nm)/TAPC (10 nm)/Al and ITO/TmPyPB(10 nm)/XT-DPDBA or XT-BDPDBA (80 nm)/TmPyPB (10 nm)/LiF (1 nm)/Al, respectively, via space charge limited current method.

Figure 7. Electroluminescence performance of XT-DPDBA and XT-BDPDBA in doped OLEDs with DPEPO and PPF hosts

EL spectra of (A) XT-DPDBA and (D) XT-BDPDBA at 10 mA cm^{-2}. Luminance–voltage–current density curves of (B) XT-DPDBA and (E) XT-BDPDBA. External quantum efficiency–luminance curves of (C) XT-DPDBA and (F) XT-BDPDBA. The device configuration is ITO/HATCN (5 nm)/TAPC (50 nm)/TCTA (5 nm)/mCP (5 nm)/EML (20 nm)/DPEPO (5 nm)/TmPyPB (30 nm)/LiF (1 nm)/Al (120 nm).

Figure 8. Electroluminescence performance of XT-DPDBA and XT-BDPDBA in doped OLEDs with mCP and mCPB hosts

EL spectra of (A) XT-DPDBA and (D) XT-BDPDBA at 10 mA cm^{-2}. Luminance–voltage–current density curves of (B) XT-DPDBA and (E) XT-BDPDBA. External quantum efficiency–luminance curves of (C) XT-DPDBA and (F) XT-BDPDBA. The device configuration is ITO/HATCN (5 nm)/TAPC (50 nm)/TCTA (5 nm)/mCP (5 nm)/EML (20 nm)/DPEPO (5 nm)/TmPyPB (30 nm)/LiF (1 nm)/Al (120 nm).

Tables and Table Titles and Legends

Table 1. The photophysical data of compounds.

molecule	soln[a]				film/doped film[b]					
	λ_{abs} (nm)	λ_{em} (nm)	Φ_{PL}[c] (%)	τ[d] (ns)	λ_{em} (nm)	Φ_{PL}[c] (%)	τ[d] (ns)	$\tau_{delayed}$[e] (ns)	$R_{delayed}$[f] (%)	ΔE_{ST}[g] (eV)
XT-DPDBA	337	501	16.2	34	472/477	77/97	1042/1472	2823/2956	36/49	0.063/0.026
XT-BDPDBA	337	508	16.7	40	480/486	86/91	1081/1313	2403/2259	44/57	0.025/0.020

[a] Measured in the THF solution (10^{-5} M) at room temperature.

[b] Vacuum-deposited 30 wt% doped film for XT-DPDBA and 20 wt% doped film for XT-BDPDBA with DPEPO host.

[c] Absolute PL quantum yield determined by a calibrated integrating sphere under nitrogen atmosphere at room temperature.

[d] Mean fluorescence lifetime.

[e] Lifetime of delayed component.

[f] Proportion of delayed component.

[g] Estimated from high-energy onsets of fluorescence and phosphorescence spectra at 77 K.

Table 2. Summary of device performance based on the blue molecules.[a]

EML	V_{on} (V)	L_{max} (cd m^{-2})	η_C (cd A^{-1})	η_P (lm W^{-1})	η_{ext} (%)	λ_{EL} (nm)	CIE (x, y)
			maximum value / at 1000 cd m^{-2}				
20 wt% XT-DPDBA : PPF	3.2	9222	33.6/24.7	33.0/16.9	20.7/15.2	472	(0.149,0.247)
30 wt% XT-DPDBA : PPF	3.2	11965	33.4/26.8	32.8/20.0	19.6/15.7	474	(0.148,0.260)
20 wt% XT-BDPDBA : PPF	3.2	14215	51.2/41.1	47.4/29.4	26.3/21.1	482	(0.158,0.324)
30 wt% XT-BDPDBA : PPF	3.0	19319	55.0/44.8	57.5/35.1	27.0/22.0	484	(0.158,0.341)
20 wt% XT-DPDBA : DPEPO	3.4	4903	26.4/22.0	21.6/14.4	16.7/14.0	470	(0.150,0.241)
30 wt% XT-DPDBA : DPEPO	3.0	6391	31.2/25.6	30.6/20.1	18.0/14.8	474	(0.149,0.262)
20 wt% XT-BDPDBA : DPEPO	3.4	6463	53.8/34.1	49.7/23.3	26.0/16.5	484	(0.167,0.341)
30 wt% XT-BDPDBA : DPEPO	3.2	8080	51.2/40.3	47.3/30.1	26.4/20.8	484	(0.167,0.357)
20 wt% XT-DPDBA : mCP	3.4	2255	8.0/4.4	7.4/2.7	6.0/3.3	462	(0.144,0.196)
30 wt% XT-DPDBA : mCP	3.4	3344	9.9/6.2	9.1/4.0	6.8/4.2	470	(0.144,0.207)
20 wt% XT-BDPDBA : mCP	3.2	9879	26.6/18.7	26.1/14.0	14.8/10.4	472	(0.146,0.277)
30 wt% XT-BDPDBA : mCP	3.0	12180	28.0/22.2	29.3/16.6	15.6/12.4	474	(0.147,0.285)
20 wt% XT-DPDBA : mCBP	3.4	3082	9.8/6.0	8.5/3.9	7.0/4.4	468	(0.145,0.206)

30 wt% XT-DPDBA : mCBP	3.2	4211	12.5/8.3	12.3/5.9	8.7/5.7	470	(0.141,0.218)
20 wt% XT-BDPDBA : mCBP	3.4	7237	26.6/17.8	24.6/12.7	15.9/10.6	472	(0.146,0.274)
30 wt% XT-BDPDBA : mCBP	3.2	11100	29.3/23.6	28.8/18.6	16.8/13.5	474	(0.148,0.293)
100 wt% XT-DPDBA	3.0	4403	15.5/14.0	13.5/11.0	8.9/8.0	472	(0.151,0.272)
100 wt% XT-BDPDBA	3.0	9741	30.1/25.1	29.6/20.8	13.1/11.0	488	(0.185,0.390)

[a] Abbreviations: EML = emitting layer; DC = doping concentration; V_{on} = turn-on voltage at 1 cd m^{-2}; $L_{\max}$ = maximum luminance; η_{C} = current efficiency; η_{P} = power efficiency; η_{ext} = external quantum efficiency; CIE = Commission Internationale de I'Eclairage coordinates; λ_{EL} = electroluminescence peak at 10 mA cm^{-2}.