

3,3'-Bicarbazole-Based Host Materials for High-Efficiency Blue Phosphorescent OLEDs with Extremely Low Driving Voltage

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High-performance organic light-emitting device (OLED) incorporating a phosphorescent emitter is one of the most promising candidates for energy-saving solid-state lighting and flat-display panel.^[1,2] Generally, a phosphorescent emitter is dispersed in a suitable host material to obtain a high photoluminescent quantum yield (η_{PL}) suppressing concentration quenching.^[3] Additionally, to realize a high η_{PL} for a blue phosphorescent emitter, a host material needs to have a triplet energy (E_{T}) over 2.75 eV. On the other hand, carrier balance is one of the most important factors to obtain a high efficiency OLED.^[4] For a better carrier balance between electrons and holes in an emissive layer (EML), it is considered to be important to adjust frontier molecular orbitals (FMO) of a host material with FMOs of a hole-transport layer (HTL) and an electron-transport layer (ETL). Therefore, OLED performance can be dramatically improved by using a suitable host material.

Among host materials, carbazole derivatives show superior performances in phosphorescent OLEDs. Because carbazole has a high E_{T} of over 3.0 eV and chemical compatibility of a phosphorescent emitter, a carbazole derivative can realize a high η_{PL} . Further, carbazole has a small singlet-triplet energy difference (ΔE_{ST}) of 0.48 eV, due to the reduced exchange energies involving $n-\pi^*$ transition.^[5] Thus, a carbazole-based host material potentially can reduce a driving voltage of OLED. Although a carbazole derivative has above mentioned advantages, a carbazole derivative without chemical modification shows strong excimer formation behavior leading to a significant loss of a triplet energy.^[6]

In this regard, 3,3'-bicarbazole (BCz), which is a dimer of carbazole, has not only a high E_{T} but also a small ΔE_{ST} of

0.46 eV.^[5] Very recently, Kim and co-workers also have predicted by DFT calculation that carbazole-based oligomer linked with 3,3'-position can possess a higher E_{T} than that of a common blue phosphorescent emitter, iridium(III) bis[(4,6-difluorophenyl)-pyridinate-*N,C2'*]picolate (FIRpic).^[7] Due to the sterically twisted structure, BCz derivatives can greatly reduce the host-host aggregation causing excimer formation, and a dimerization of carbazole can improve thermal and morphological stability of thin film. Additionally, the electronic properties of BCz derivatives can be tuned by chemical modification on the 9,9'-positions. These attractive features should promise tremendous opportunities as a host material in blue phosphorescent OLEDs. However, BCz derivative has not been used in blue phosphorescent OLED so far despite use in green phosphorescent OLEDs.^[8,9] In this study, we prepare and investigate a series of functionalized BCz derivatives as a host material for blue OLEDs. We can successfully develop a FIRpic-based OLED with a power efficiency ($\eta_{\text{p,100}}$) over 45 lm W^{-1} at 100 cd m^{-2} with an extremely low driving voltage at 3.1 V.

We investigated four types of functionalized 3,3'-bicarbazole derivatives, which are modified with triphenylamine (BCzTPA), triphenylphosphine oxide (BCzPO) and tetraphenylmethane (BCzTPM) and phenyl (BCzPh)^[10] moieties on the 9,9'-positions, respectively (Figure 1). For better hole-injection, triphenylamine (TPA) moieties were introduced. On the other hand, for better electron-injection, triphenylphosphine-oxide (PO) moieties were introduced. Prior to material preparation, we conducted the density functional theory (DFT) calculations. We used a common host material, *N,N'*-dicarbazolyl-3,5-benzene (mCP) as a reference. The calculated highest occupied molecular orbital (HOMO) energies of BCz derivatives were estimated to be between -5.15 and -5.44 eV, those are much shallower than that of mCP, depending on substituents on 9,9'-position. Among BCz derivatives, an electron-donating effect of TPA makes a HOMO energy shallower. While an electron-withdrawing inductive effect of PO deepens a HOMO energy. These results suggest that an enhanced hole-injection can be created by using BCz derivatives. On the other hand, the calculated lowest unoccupied molecular orbital (LUMO) energies were evaluated to be between -1.11 and -1.48 eV, those are much shallower than that of mCP except BCzPO, suggesting a poor electron-injection property. Whereas BCzPO is expected to have a much better electron-injection property than that of mCP. We also calculated E_{T} and E_{S} from TD-DFT calculation at the RB3LYP 6-31G(d) level. Although the conjugation length in a BCz derivative is longer than that of mCP, E_{T} levels were

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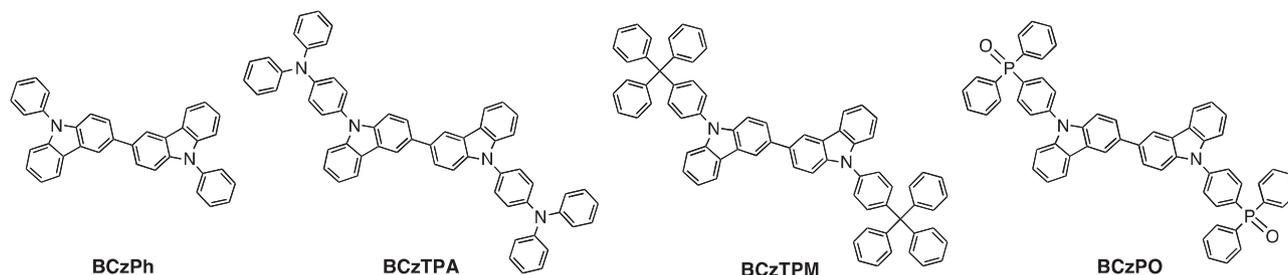


Figure 1. Chemical structure of BCz derivatives.

evaluated to be as high as around 3.00 eV, which is applicable in a blue phosphorescent OLED. E_S levels were calculated to be 3.57–3.96 eV, those are smaller than that of mCP. Compared with mCP and BCzPh, in the cases of BCzTPA and BCzPO, E_S levels were very small maintaining a high E_T over 3.00 eV, in other words, these BCz derivatives can possess very small ΔE_{ST} to reduce an operating voltage of a blue phosphorescent OLED. Considering HOMO/LUMO locations, this is because intramolecular charge-transfer (ICT) occurs in BCzTPA and BCzPO (see Supporting Information in detail). All the calculated data are summarized in Table 1.

The synthetic route of Bz derivatives was shown in Scheme 1. The precursor 3,3'-bicarbazole was prepared via an oxidation reaction of carbazole according to the literature.^[11] Then, a CuI/L-proline-catalyzed Ullmann coupling reaction of 3,3'-bicarbazole with a corresponding aryl halide gave the target BCz derivatives in 74–95% yield.^[12] Note that we also tried to prepare these materials via palladium-catalyzed Buchwald-Hartwig reaction, however we could not obtain sufficient amount of BCz derivatives probably due to the low solubility of 3,3'-bicarbazole in toluene or xylene.^[13] The characterization was established on the basis of NMR, mass spectrometry, and elemental analyses. The product was purified by train sublimation method before device fabrication. The purity of BCz derivatives thus obtained was confirmed to be >99.0% by HPLC analysis.

The thermal properties were measured by differential scanning calorimetry (DSC). The glass transition temperature (T_g) of functionalized BCz derivatives, such as BCzTPA and BCzPO were observed at over 136 °C, which is 30 °C higher than that of phenyl substituted BCzPh and more than double than that of mCP (60 °C). These results clearly promise excellent thermal

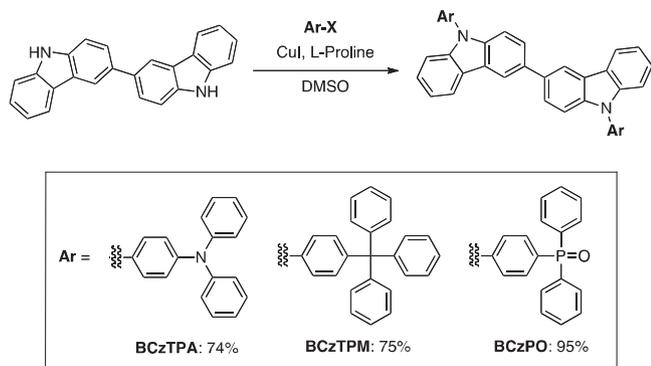
stability of thin solid film using BCz derivatives. The ionization potential (I_p) was measured by a photoelectron yield spectroscopy (PYS) under the vacuum ($\sim 10^{-3}$ Pa). As predicted from DFT calculation, BCz derivatives show a 0.4–0.5 eV shallower ionization potential around –5.65 eV by a photoelectron yield spectroscopy (PYS) compared with mCP (6.1 eV) in the solid state. Considering that I_p of BCzPh was observed at –5.67 eV, this is characteristic of 3,3'-bicarbazole skeleton. Among BCz derivatives, an electron-donating effect of TPA makes an I_p 0.06 eV shallower. While an electron-withdrawing inductive effect of PO slightly deepens the I_p of BCzPO (~ 0.02 eV), but the inductive effect is very small in the solid state. The electron affinity (E_a) was calculated to be around 2.30 eV by subtraction of the optical energy gap (E_g) from the I_p . Compared with mCP (–2.60 eV), these values are shallower indicating that electron-injection to EML should be improved in OLED. The phosphorescent spectrum of 3 wt%-BCz derivative doped PMMA film was measured by a streak camera at 5 K. We estimated E_T from the onset of phosphorescence in the solid state. The onset phosphorescence was observed at around 2.90 eV, which is comparable with that of mCP (3.00 eV), with almost no effect of substituents. From the perspective of ΔE_{ST} , all the BCz derivatives have very small ΔE_{ST} of 0.37–0.45 eV, which is even smaller than that of mCP (0.49 eV).^[14] Therefore, BCz derivatives are considered to be applicable for a blue phosphorescent OLED with a reduced operating voltage. All the physical properties are summarized in Table 2.

Prior to the device fabrication, photophysical properties of a 11wt% FIrpic-doped host film was evaluated. An η_{PL} was measured under N_2 flow using an integrating sphere excited 331 nm with a multichannel spectrometer as the optical detector. η_{PLS}

Table 1. Calculated HOMO, LUMO, ΔE_{H-L} , E_S , E_T and ΔE_{ST} values (eV).

Compound	HOMO ^{a)}	LUMO ^{a)}	ΔE_{H-L} ^{b)}	E_S ^{c)}	E_T ^{c)}	ΔE_{ST} ^{d)}
BCzPh	–5.31	–1.16	–4.15	3.96	3.02	0.97
BCzTPA	–5.15	–1.11	–4.04	3.67	3.00	0.67
BCzTPM	–5.26	–1.14	–4.12	3.73	3.02	0.71
BCzPO	–5.44	–1.48	–3.96	3.57	3.01	0.56
mCP	–5.80	–1.26	–4.54	4.01	3.18	0.83

^{a)} Calculated at RB3LYP 6-311+G(d,p)//RB3LYP 6-31G(d); ^{b)} ΔE_{H-L} = HOMO–LUMO; ^{c)} Lowest singlet (E_S) and triplet (E_T) energy from TD-DFT at RB3LYP 6-31G(d)//RB3LYP 6-31G(d); ^{d)} Energy difference between lowest singlet (E_S) and triplet (E_T) energy (ΔE_{ST} = E_S – E_T).



Scheme 1. Synthetic route of BCz derivatives.

of BCz/FIrpic films were estimated to be 62–74%. These values are 20% lower than that of mCP/FIrpic film.^[15] Among BCz derivatives, BCzTPM showed relatively high η_{PL} of 74% despite the similar E_{T} to the other BCz derivatives. In these highly doped films, emissions via the intermolecular energy transfer (ET) from host to FIrpic and/or via direct excitation of FIrpic should be involved. In the UV-vis spectrum of BCzTPM, smaller absorption at 331 nm can be observed than that in BCzTPA and BCzPO. Note that there are relatively small differences in the spectrum overlaps between the emission spectrum of BCz derivative and the absorption spectrum of FIrpic. (see Supporting information in detail). In the cases in BCzTPA and BCzPO, host material can absorb 331 nm light more effective than that in BCzTPM due to their strong $n-\pi^*$ absorption derived from the ICT. Thus, the efficient intermolecular ET from host to FIrpic should be more important to realize higher η_{PL} . However, considering the lower η_{PL} , the ET to FIrpic might be less efficient in BCzTPA and BCzPO. A transient PL decay curve of 11% FIrpic-doped film exhibited almost single-exponential decay at room temperature except BCzPh/FIrpic film (see Supporting information in detail). While in the case of BCzPh/FIrpic, a delayed component involving back energy transfer from FIrpic to BCzPh was observed. Here, in the molecular structure of BCz derivative, we should consider an E_{T} of each subunits,^[16] such as 3,3'-bicarbazole, phenyl, TPA, TPM and PO. In BCz derivative, a lowest E_{T} subunit is core 3,3'-bicarbazole skeleton. In BCzPh/FIrpic film, FIrpic can contact directly with 3,3'-bicarbazole skeleton because the phenyl groups are sterically compact. While in the other functionalized

BCz derivative, sterically bulky substituents, such as TPA, TPM and PO, can keep a FIrpic molecule away from a direct contact with 3,3'-bicarbazole skeleton, so the back energy transfer from FIrpic to 3,3'-bicarbazole skeleton is considered to be negligibly-small. Thus, a chemical modification of 9,9'-position of 3,3'-bicarbazole by sterically bulky functionalities can be an effective way to confine the triplet exciton of FIrpic. It should be noted that an aggregation induced concentration quenching of FIrpic is thought to be very small in these hosts compared with other symmetric tris-cyclometallated iridium complexes.^[17]

To investigate the function of BCz derivatives as a host material, a blue phosphorescent OLEDs using FIrpic as an emitter were fabricated. We used 1,1-bis[4-(*N,N*-di(*p*-tolyl)amino)phenyl]cyclohexane (TAPC) as a hole-transporting layer (HTL) and 3,3'',5,5''-tetra(3-pyridyl)-1,1';3',1''-terphenyl (B3PyPB)^[18] as an electron-transporting layer (ETL), these materials have higher E_{T} than that of FIrpic. Therefore, the triplet exciton quenching of FIrpic at the HTL/EML and/or EML/ETL interface(s) can be minimized. Then, we fabricated a blue phosphorescent OLED with a structure of [ITO (130 nm)/ TAPC (40 nm)/ FIrpic 11 wt% doped BCz derivative (10 nm)/ B3PyPB (50 nm)/ LiF (1 nm)/ Al (100 nm)]. EL spectra showed an emission only from FIrpic with no emission from neighboring materials (inset in Figure 2(b)). The current density–voltage–luminance (J – V – L) and the power efficiency–luminance (PE – L) characteristics are shown in Figure 2(a) and Figure 2(b), respectively. All the OLED performances are summarized in Table 3 (see also Supporting information).

By using BCzTPM and BCzPh, an OLED showed extremely reduced operating voltage of 3.1 V at 100 cd m^{-2} and gave an $\eta_{\text{p,100}}$ of over 45 lm W^{-1} at 100 cd m^{-2} presumably due to the superior carrier balance in EML. These are among the best performances in FIrpic-based OLEDs. Whereas in a OLED using mCP (–6.09 eV), an operating voltage of 3.7 V at 100 cd m^{-2} have been observed in the same device configuration.^[19] Among these hosts, BCzTPA with electron-donating TPAs showed a superior current density at a low driving voltage (<3.0 V). On the other hand, BCzPO with electron-accepting POs showed a less current density. In this FIrpic-based OLED, holes are preferably injected to host from TAPC ($I_{\text{p}} = -5.60$ eV) because of the much deeper I_{p} of FIrpic (–6.15 eV) than these hosts ($I_{\text{p}} = -5.67 \sim -5.72$ eV) from the viewpoint of a favorable density-of-state (DOS) overlap.^[20] Thus, a better hole-injection to EML is one of the critical factors in a FIrpic-based device.

Table 2. Physical properties of BCz derivatives.

Compound	$T_{\text{g}}/T_{\text{m}}/T_{\text{d5}}/^{\circ}\text{C}^{\text{a}}$	$I_{\text{p}}/E_{\text{a}}/E_{\text{g}}/\text{eV}^{\text{b}}$	$E_{\text{T}}/\text{eV}^{\text{c}}$	$\Delta E_{\text{ST}}/\text{eV}^{\text{d}}$	$\eta_{\text{PL}}/\%^{\text{e}}$
BCzPh	105/200/399	–5.67/–2.35/3.32	2.87	0.45	62
BCzTPA	157/239/526	–5.61/–2.20/3.31	2.91	0.40	63
BCzTPM	n.d./377/529	–5.72/–2.41/3.31	2.87	0.44	74
BCzPO	136/n.d./516	–5.69/–2.41/3.28	2.91	0.37	64
mCP ^f	60/187/341	–6.09/–2.60/3.49	3.00	0.49	80

^aGlass transition temperature (T_{g}) and melting point (T_{m}) determined by DSC measurement. Decomposition temperature with 5% weight loss (T_{d5}) obtained from TGA analysis; ^bIonization potential (I_{p}) obtained from PYS under the vacuum ($\sim 10^{-3}$ Pa). Energy gap (E_{g}) taken as the point of intersection of the normalized absorption spectra. Electron affinity (E_{a}) calculated using I_{p} and E_{g} ; ^cOnset of phosphorescence of 3 wt%-BCz derivative doped PMMA film measured by using a streak camera (C4334 from Hamamatsu Photonics); ^d $\Delta E_{\text{ST}} = E_{\text{g}} - E_{\text{T}}$; ^ePhotoluminescent quantum yield of 11 wt% FIrpic-doped film; ^fData from Ref[13].

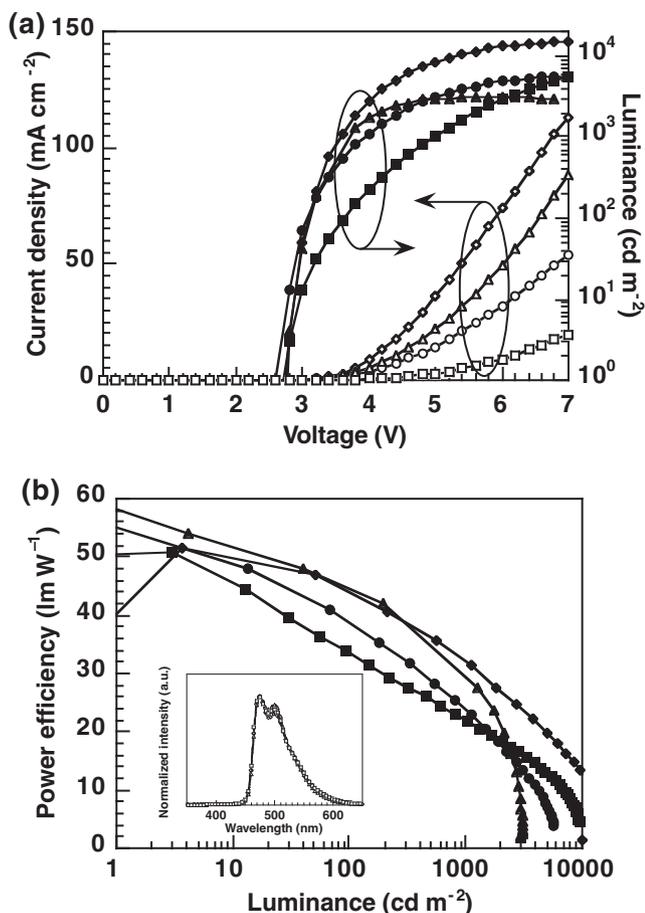


Figure 2. (a) J - V - L characteristics and (b) PE - L characteristics of blue OLEDs using BCzTPA (circle), BCzTPM (triangle), BCzPO (square) and BCzPh (diamond), respectively. Inset: EL spectra of the devices.

To get a better understanding into the carrier injection behaviors in this OLED, we compared three types of devices with an EML structure: (A) FIrpic 11wt% doped BCzTPA (10 nm), (B) BCzTPA (5 nm)/FIrpic 11wt% doped BCzTPA (5 nm), (C) 11wt% doped BCzTPA (5 nm)/BCzTPA (5 nm). The J - V and PE - L characteristics are shown in **Figure 3**. Compared with device (A), device (B) with non-doped BCzTPA at HTL interface showed much higher current density, while device (C)

Table 3. Summary of OLED performances.

Device	$\eta_{p,100}/\eta_{c,100}/V_{100}/EQE^a$	$\eta_{p,1000}/\eta_{c,1000}/V_{1000}/EQE^b$
	[lm W ⁻¹ /cd A ⁻¹ /V/%]	[lm W ⁻¹ /cd A ⁻¹ /V/%]
BCzTPA	39.3/38.2/3.1/16.6	23.8/29.7/3.9/12.9
BCzTPM	45.5/44.5/3.1/19.6	21.8/26.4/3.8/16.1
BCzPO	34.4/39.3/3.6/17.2	22.6/35.5/4.9/15.6
BCzPh	45.2/43.9/3.1/19.8	32.3/36.6/3.6/16.4
mCP ^c	28.7/33.9/3.7/16.6	21.5/30.1/4.4/13.8

^a) Power efficiency (η_p), current efficiency (η_c), voltage (V) and external quantum efficiency (η_{ext}) at 100 cd m⁻²; ^b) η_p , η_c , V and η_{ext} at 1000 cd m⁻²; ^c) Data from Ref [19].

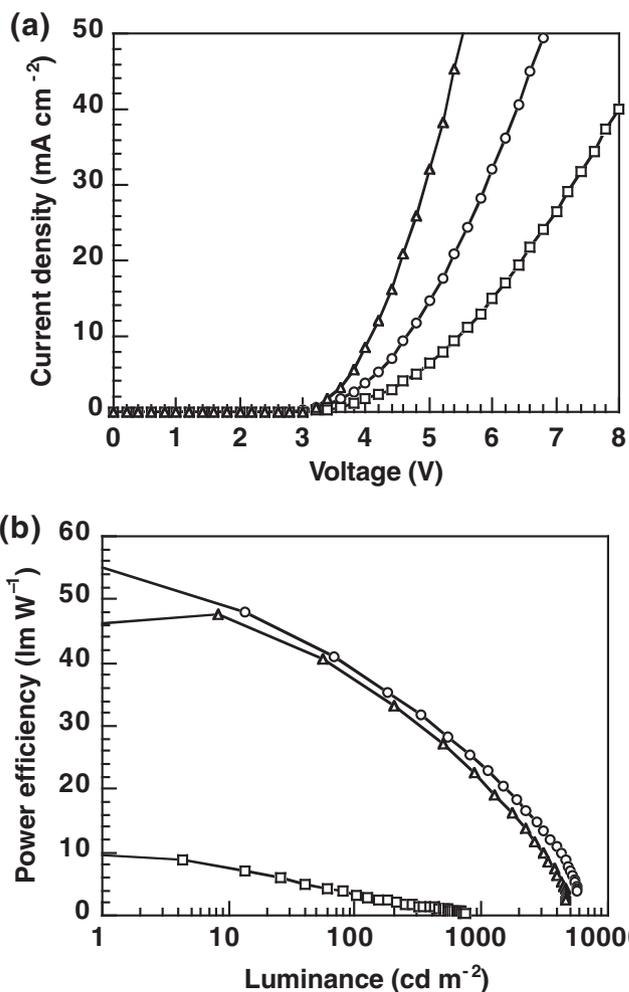


Figure 3. (a) J - V characteristics and (b) PE - L characteristics of BCzTPA-based OLEDs: device A (circle), B (triangle), C (square), respectively.

with non-doped BCzTPA at ETL interface showed much lower current density. Device (B) gave an $\eta_{p,100}$ of 38 lm W⁻¹ at 100 cd m⁻², which is comparable with the performance in device (A). On the other hand, device (C) showed much lower efficiency of under 10 lm W⁻¹. From these comparison, it can be considered that (i) better hole-injection to EML can be realized by using BCzTPA due to a favorable overlap of DOS distributions with HTL, (ii) electron-injection to EML can be greatly enhanced by carrier trapping of FIrpic, (iii) FIrpic prevents hole-injection and transport to EML due to the large difference in I_p levels between FIrpic and BCzTPA,^[21] (iv) electron-injection from ETL to BCzTPA is difficult without doping of FIrpic due to the shallow E_a level.

In conclusion, we prepared and investigated a series of functionalized BCz derivatives as a host material for blue phosphorescent OLEDs. DFT calculations predicted that a BCz derivative had (i) a shallower HOMO level than that of mCP to enhance hole-injection from HTL, (ii) a high E_T , which is applicable for a blue phosphorescent OLED and (iii) small ΔE_{ST} to reduce an operating voltage of an OLED. For the physical properties, BCz derivatives showed a 0.4–0.5 eV shallower

ionization potential around $-5.6 \sim -5.7$ eV by a PYS compared with a well-known carbazole derivative, mCP (-6.1 eV) in the solid state. An η_{PL} of a 11 wt%-doped FIrpic/BCz derivative film was observed to be moderate value of $\sim 74\%$ despite a high E_{T} probably due to the imperfect energy transfer from BCz derivative to FIrpic. A time-resolved photoluminescence analysis of a FIrpic-doped film revealed that a modification of 9,9'-position of BCz by sterically bulky functionalities is an effective way to confine the triplet exciton of FIrpic. Although a BCzTPM/FIrpic film showed a moderate η_{PL} of 74%, we successfully developed an OLED with high PE of 45.5 lm W^{-1} (44.5 cd A^{-1} , EQE 19.6%) with an extremely low driving voltage at 3.1 V at 100 cd m^{-2} . A BCzPh/FIrpic film showed a relatively low η_{PL} of 62%, a BCzPh-based blue OLED exhibited high PE of 45.2 lm W^{-1} (43.9 cd A^{-1} , EQE 19.7%) with an extremely low driving voltage at 3.1 V at 100 cd m^{-2} . These performances are the highest levels in the scientific literature. Investigation of the device performances showed that the hole-injection was greatly enhanced by using a BCz derivative and that the electron-injection was generated by carrier trapping process. Our results shows that a host material based on BCz is one of the most promising candidates for a high-performance blue phosphorescent OLED. Furthermore, these findings can also provide a powerful guideline to design a high-performance host material and a device architecture as well as a better understanding into the carrier injection process in a blue phosphorescent OLED.

Experimental Section

General Procedures: The optimized structures and single-point energies were calculated by Gaussian09 at the B3LYP 6-31G(d) and 6-311+G(d,p) levels, respectively. TD-DFT calculations for singlet and triplet energies were performed at the corresponding RB3LYP 6-31G(d) levels. NMR spectra were recorded on a JEOL 400 spectrometer (400 MHz for $^1\text{H-NMR}$ and 100 MHz for $^{13}\text{C-NMR}$). Mass spectra were obtained using a JEOL JMS-K9 mass spectrometer. Differential scanning calorimetry (DSC) was performed using a Perkin-Elmer Diamond DSC Pyris instrument under nitrogen atmosphere at a heating rate of $10 \text{ }^\circ\text{C min}^{-1}$. Thermogravimetric analysis (TGA) was undertaken using a SEIKO EXSTAR 6000 TG/DTA 6200 unit under nitrogen atmosphere at a heating rate of $10 \text{ }^\circ\text{C min}^{-1}$. UV-Vis spectra were measured using a Shimadzu UV-3150 UV-vis-NIR spectrophotometer. Photoluminescence spectra were measured using a FluroMax-4 (HORIBA Jobin-Yvon) luminescence spectrometer. The ionization potentials (I_{p}) were determined by an photoelectron yield spectroscopy (PYS) under the vacuum ($\sim 10^{-3}$ Pa). The phosphorescent spectra of 3 wt%-BCz derivative doped PMMA films were measured by using a streak camera (C4334 from Hamamatsu Photonics) at 5 K. All organic materials were purified by temperature-gradient sublimation in vacuum. The EL spectra were taken using an optical multichannel analyzer Hamamatsu Photonics PMA-11. The current density–voltage and luminance–voltage characteristics were measured using a Keithley source measure unit 2400 and a Minolta CS200 luminance-meter, respectively. External quantum efficiencies were calculated from the front luminance, current density and EL spectrum.

Synthesis of BCzTPA: 3,3'-Bicarbazole (1.00 g, 3.0 mmol) 4-bromo-triphenylamine (2.09 g, 9.0 mmol), L-proline (0.28 g, 2.5 mmol) and K_2CO_3 (2.8 g, 20.0 mmol) were added to a round bottom flask. DMSO (10 mL) was added and nitrogen bubbled through the mixture for 1 hour. Then, CuI (0.28 g, 1.5 mmol) was added and the resultant mixture was stirred for 18 hours at $140 \text{ }^\circ\text{C}$ under N_2 flow. The resulting mixture was cooled to room temperature, diluted with ethylacetate, washed with brine, dried over anhydrous MgSO_4 , filtered, and evaporated to dryness.

The resulting solid was purified by chromatography on silica gel (eluent: toluene/hexane = 1:4) to afford BCzTPA (1.82 g, 74%) as a pale yellow solid: $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 8.44 (d, 2H, $J = 1.8$ Hz), 8.23 (d, 2H, $J = 7.8$ Hz), 7.79 (dd, 2H, $J = 1.8, 7.8$ Hz), 7.55–7.43 (m, 8H), 7.35–7.21 (m, 26H), 7.09 (t, 4H, $J = 7.3$ Hz) ppm; $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 147.7, 147.2, 141.6, 140.3, 134.4, 131.5, 129.6, 127.9, 126.1, 125.9, 124.9, 124.1, 123.9, 123.5, 120.5, 119.0, 110.2, 110.1 ppm (several signals were superimposed); UV-vis (film): $\lambda_{\text{max}} = 310, 341$ nm; PL (film): $\lambda_{\text{max}} = 397, 418$ nm; MS (EI): $m/z = 820$ [$\text{M}+\text{H}$] $^+$; Anal. Calcd for $\text{C}_{60}\text{H}_{42}\text{N}_4$: C, 87.99; H, 5.17; N, 6.84%. Found: C, 87.86; H, 5.03; N, 6.81%.

BCzTPM: $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 8.42 (s, 2H), 8.22 (d, 2H, $J = 7.8$ Hz), 7.76 (dd, 2H, $J = 1.8, 8.7$ Hz), 7.57–7.40 (m, 16H), 7.34–7.25 (m, 30H) ppm; $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 146.7, 146.1, 141.3, 140.0, 135.6, 134.5, 132.7, 131.3, 127.8, 126.3, 126.1, 125.9, 125.8, 124.1, 123.7, 120.6, 120.1, 119.0, 110.3, 110.1 ppm (several signals were superimposed); UV-vis (film): $\lambda_{\text{max}} = 358$ nm; PL (film): $\lambda_{\text{max}} = 392, 412$ nm; MS (EI): $m/z = 969$ [M] $^+$; Anal. Calcd for $\text{C}_{74}\text{H}_{52}\text{N}_2$: C, 91.70; H, 5.41; N, 2.89%. Found: C, 91.67; H, 5.51; N, 2.80%.

BCzPO: $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 8.43 (s, 2H), 8.23 (d, 2H, $J = 7.3$ Hz), 7.95–7.90 (m, 4H), 7.82–7.76 (m, 14H), 7.63–7.51 (m, 16H), 7.45 (t, 2H, $J = 7.3$ Hz), 7.43 (t, 2H, $J = 7.3$ Hz) ppm; $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 141.4, 140.7, 139.4, 134.8, 134.0, 133.9, 132.7, 132.3, 132.2, 131.9, 131.7, 130.8, 128.9, 128.8, 126.6, 126.5, 126.1, 124.5, 124.0, 120.8, 120.7, 119.1, 110.1, 110.0 (several signals were superimposed); UV-vis (film): $\lambda_{\text{max}} = 308, 340$ nm; PL (film): $\lambda_{\text{max}} = 412$ nm; MS: $m/z = 885$ [M] $^+$; Anal. Calcd for $\text{C}_{60}\text{H}_{42}\text{N}_2\text{O}_2$: C, 81.43; H, 4.78; N, 3.17%. Found: C, 81.24; H, 4.82; N, 3.10%.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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