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Investigating blue phosphorescent iridium cyclometalated dopant with phenyl-imidazole ligands

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ABSTRACT

A blue phosphorescent emitter based on tris[1-(2,6-diisopropylphenyl)-2-phenyl-1H-imidazole]iridium(III), Ir(iprpmi)$_3$, as the dopant and 3,3′-bis(N-carbazolyl)biphenyl, mCBP, as the host have been evaluated in OLED devices. By optimizing the dopant concentration and the materials for the electron and hole-transport layers, external quantum efficiencies greater than 20% have been achieved. Improved device lifetimes over those using the classic light-blue dopant FIrpic have also been achieved. These improvements can be attributed to the control of the electron-hole recombination and emission regions within the emitter layer as well as the choice of material for the transport layers.

1. Introduction

A key advance in OLED technology can be attributed to the development of highly efficient phosphorescent OLEDs, known as PHOLEDs. Based on phosphorescent molecules as the emitter, including most notably the class of iridium(III) cyclometalated complexes [1–4], PHOLEDs with nearly 100% quantum efficiencies [5,6] across the visible spectrum have been demonstrated. In addition, excellent lifetime (>100,000 h) has been achieved for red and green PHOLEDs. However, the lifetime for blue PHOLEDs remains relatively short (typically less than 10,000 h) [7] and inadequate for most applications, such as display and lighting.

Considerable research efforts have focused on developing efficient and stable blue phosphorescent PHOLEDs [8]. However, there are few reports on the structure–property relationships for phosphorescent molecules as they pertain to device lifetime. Among the most studied phosphorescent molecules is bis(4,6-difluorophenyl-pyridinato-*N*,C2′) picolinate iridium(III), FIrpic. Used as a dopant in blue PHOLEDs, it is capable of achieving an external quantum efficiency (EQE) greater than 20% [9–14]. However, FIrpic doped PHOLEDs have been shown to be very unstable. Reported lifetimes are in the range of 0.1–110 h depending on the device architecture and test conditions [15–18]. In our tests, we have observed that the lifetime of FIrpic-based devices can vary from 5 min to 12 h depending on the choice of host and transport materials. The instability of FIrpic doped PHOLEDs has been largely attributed to the intrinsic instability of FIrpic molecules upon excitation. Both the ancillary picolinate ligand and the fluorine substituted phenyl-pyridyl ligands are susceptible to photo-induced dissociation [17,19,20]. It has also been reported that FIrpic is unstable to hole transport [21]. To avoid the

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detrimental structural features present in FIrpic, we have examined Ir complexes with phenyl-imidizole ligands, which reportedly can provide PHOLEDs with lifetimes as long as 10,000 h [22–29].

In this work we have performed a detailed study of one such dopant, tris[1-(2,6-diisopropylphenyl)-2-phenyl-1H-imidazole]iridium(III), $Ir(iprpmi)_3$. We will show that its performance as a blue phosphorescent dopant is not only related to its intrinsic photophysical properties, but also highly dependent on the compositions of the host matrix and the adjacent transport layers.

2. Material and methods

The following materials used in this study were purchased from Luminescence Technology Corporation and used as received, 3,3′-bis(N-carbazolyl)biphenyl (mCBP), tris[1-(2,6-diisopropylphenyl)-2-phenyl-1H-imidazole]iridium(III) ($Ir(iprpmi)_3$), and 1,3,5-tri(m-pyrid-3-yl-phenyl) benzene (TmPyPB). The following materials were obtained from Eastman Kodak Company, 4,4′-bis[N-(l-naphthyl)-N-phenyl-amino]-biphenyl (NPB), 1, 1-bis(di-4-tolylaminophenyl)cyclohexane (TAPC) and bis-(2-methyl-8-quinolinolate) -4-(phenylphenolate)aluminum (III) (BAlq). Fig. 1 shows the molecular structures and the energy level diagram (HOMO/LUMO) for all materials used in this work. Highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO) and triplet energy values for the following materials were based on reports in the literature, NPB [30,31], TAPC [32,33], mCBP [34], BAlq [35], and TmPyPB [36].

UV–Vis absorption spectra were obtained using a Perkin Elmer Lambda 750 spectrophotometer. PL spectra and phosphorescent spectra were recorded on a Hitachi F-4600 fluorescence spectrophotometer. Cyclic voltammetry (CV) was carried out on a CHI600 voltammetric analyzer at room temperature with a conventional three-electrode configuration consisting of a platinum disk working electrode, a platinum wire auxiliary electrode, and an Ag wire pseudo-reference electrode with ferrocenium–ferrocene (Fc^+/Fc) as the internal standard. Deaerated dichloromethane was used as solvent. UPS analyses were carried out with an unfiltered HeI (21.2 eV) gas discharge lamp and a hemispherical analyzer. DFT calculations were performed at the B3LYP level. The 6–31 g(d) basis set was employed for H, C, N atoms and a "double-ζ" quality basis set, LANL2DZ, was employed for the Ir(III) metal atom. All calculations were carried out using Gaussian 03 [37]. Tran-

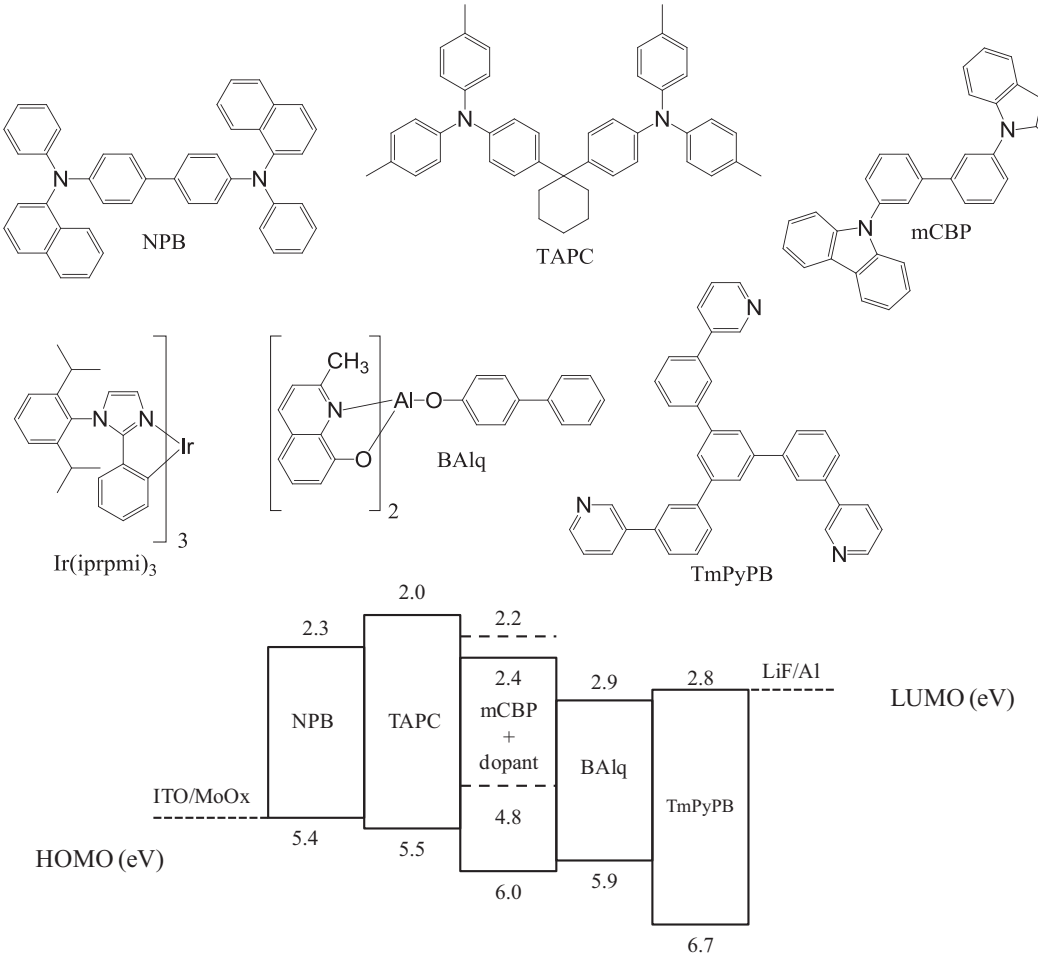

Fig. 1. Molecular structures and representative energy level diagram of the materials (values in eV).