

# Deep-Blue Narrowband Multi-Resonance Thermally Activated Delayed Fluorescent Emitters for Efficient Organic Light Emitting Diodes.

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## ABSTRACT

*In this study, we designed two new deep blue MR-type emitters TPD4PA and tBu-TPD4PA. Both emitters showed deep blue photo luminescent emissions of ~450nm and achieved very small  $\Delta E_{ST}$  and high rate of reverse intersystem crossing of  $\sim 2.5 \times 10^5 \text{ s}^{-1}$ . The TADF devices showed maximum external quantum efficiencies of 30.7 and 32.5% respectively.*

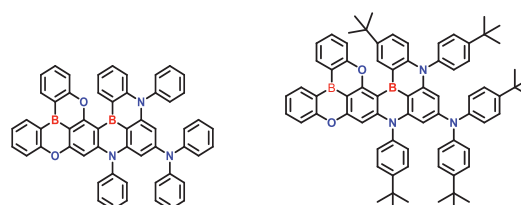
## 1 Introduction

In recent years, TADF emitters have drawn large attention because of 100% internal quantum efficiency (IQE) without using costly heavy metal. Conventional TADF molecules consist of donor-acceptor (D-A), spatially separate HOMO and LUMO to get small  $\Delta E_{ST}$ . Many groups have shown tremendous TADF-OLED performances due to their rigid molecular block and excellent intramolecular charge transfer (ICT) characteristics. However, this ICT nature of TADF materials causes structural relaxation in the excited state, and it shows a large stoke shift and broad emission spectra with a large full width half maximum (FWHM) which leads to poor color purity. To overcome this fatal issue and achieve BT2020 color coordinate of Blue (0.13, 0.05), multi-resonance (MR) type of boron based dopants are widely researched. Alternately aligned boron and nitrogen atom in rigid aromatic ring structure can separate HOMO and LUMO orbital atomically, so it shows not only small  $\Delta E_{ST}$  and large oscillator strength but also achieve high PLQY and narrow FWHM [1]. Recently, diboron embedded material, such as v-DABNA emitter, exhibits smaller  $\Delta E_{ST}$  value of 0.02eV and narrower FWHM 14nm spectrum in blue region due to strong MR effect compared to other single boron DABNA materials [2]. However, v-DABNA exhibited a sky-blue EL spectrum emission at 469nm with a CIE y coordinate of 0.11, which is deviated from the BT2020 color coordinate of blue (0.13, 0.05). Thereby it is required to develop deep blue MR- TADF

emitters which satisfy both high device efficiencies and color purity. Herein we present two new deep blue MR-TADF emitters, namely, TPD4PA and tBu-TPD4PA. Both emitters exhibit deep blue emission with high PLQY ~90%, small  $\Delta E_{ST}$  values, and fast  $k_{RISC}$  ( $2.5 \times 10^5 \text{ s}^{-1}$ ). Fabricated OLEDs with these emitters show excellent TADF performances with EQE<sub>max</sub> over 30% with CIE y coordinate of 0.06 (TPD4PA), 0.07 (tBu-TPD4PA), respectively.

## 2 Results and Discussion

We designed the emitter TPD4PA by amalgamating the high charge transfer (CT) characteristic moiety into MR type fragments towards efficient MR-TADF emitters with improved CT characteristics. Furthermore, we developed tBu-TPD4PA by adding an inert group (tert-butyl). We anticipate that incorporating tert-butyl groups in the molecules can effectively reduce the aggregation-caused self-quenching of excitons by inhibiting the intramolecular vibrational relaxation and the intermolecular  $\pi - \pi$  stacking.



**Fig. 1 The structure of TPD4PA, tBu-TPD4PA**

As you can see in Fig.2 (a), the room temperature photoluminescence (RTPL) spectra shows strong and narrow deep-blue emission maximum peaks at 445nm and 451nm for TPD4PA and tBu-TPD4PA. To confirm the clear TADF behavior, PLQY and time resolved photoluminescence (TRPL) measurements were carried out. The PLQY values are 88.1 and 90.3% for TPD4PA

and tBu-TPD4PA, respectively. Such high PLQY of these materials originated from their fully fused rigid molecular structure configuration. From the TRPL plot illustrated in Fig.2(b), prompt / delayed lifetimes of these materials are 7.82ns/4.69 $\mu$ s for TPD4PA and 8.07ns/5.55 $\mu$ s for tBu-TPD4PA. The short delayed lifetimes are originated from the small  $\Delta E_{ST}$  values and beneficial for good TADF performance.

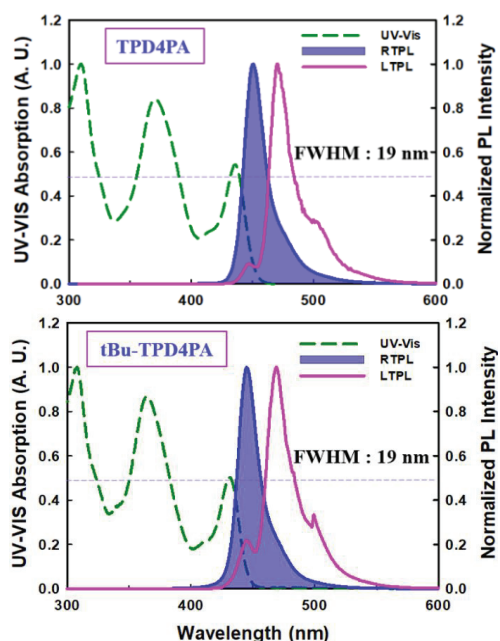


Fig. 2(a) Photophysical properties : UV-vis absorption, RTPL and LTPL

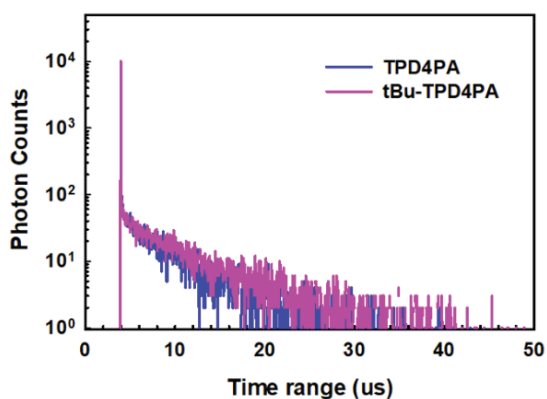


Fig. 2(b) Time resolved PL of TPD4PA and tBu-TPD4PA

To evaluate the electroluminescence (EL) properties of these materials, devices were fabricated. The EL performances of the devices are shown in Fig.3.

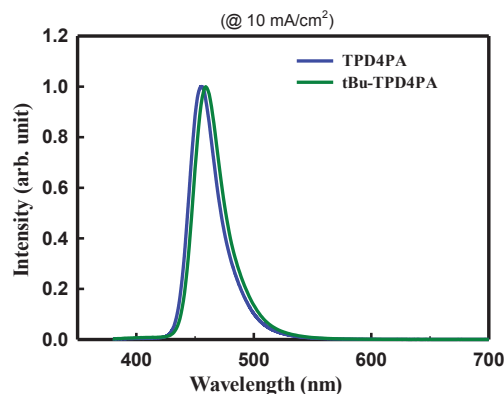


Fig. 3(a) EL spectra

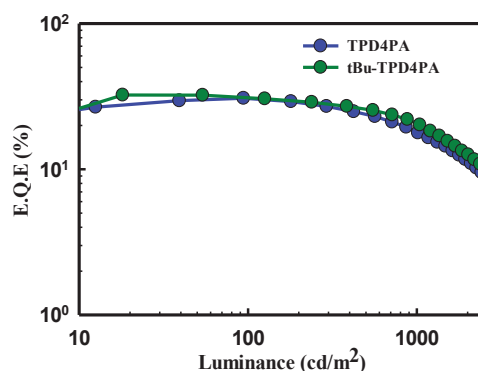


Fig. 3(b) EQE versus luminance

Both the devices emit deep blue color peaking at 455nm for TPD4PA and 460nm for tBu-TPD4PA, with narrow FWHM of 29nm for both materials. Furthermore, the devices exhibited the maximum EQE of 30.7 and 32.5% for TPD4PA and tBu-TPD4PA respectively. The detailed information will be discussed at the presentation.

### 3 Conclusions

In this work, we have developed two new, fully resonating  $\pi$ -extended double boron embedded multi resonant TADF emitters TPD4PA and tBu-TPD4PA. These materials exhibited a small  $\Delta E_{ST}$ , high PLQY and  $k_{RISC}$  of  $\sim 2.5 \times 10^5 \text{ s}^{-1}$ . The TADF devices based on TPD4PA and tBu-TPD4PA showed maximum EQEs of 30.7 and 32.5%, respectively. Furthermore, both devices exhibited narrow band deep blue emission, and corresponding CIE y coordinates match near NTSC and BT2020 blue color requirements. As for our knowledge, this is the first report in blue TADF OLED with high EQE over 30% and y coordinate below 0.07. Therefore, we believe that our design concepts provided in this study can guide the further exploration of narrowband systems with pure color emission capability and excellent TADF characteristics.

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**References**

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