

## ARTICLE

# Improving TADF Properties of Deep-Blue Multiple-Resonance Emitters by Strategic Oxygen–Sulfur Replacement

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An oxygen–sulfur replacement for improving the thermally activated delayed fluorescence (TADF) materials based on a multiple-resonance (MR) effect is reported. A comprehensive computational analysis of four possible isomers revealed that the precise placement of the sulfur atom is crucial to suppress undesired spectral red-shifts. Among them, a promising deep-blue emitter, **DOB2-DABNA-C-NP-S-1**, exhibits emission at 458 nm with a narrow full width at half maximum (FWHM) of 20 nm. Moreover, its reverse intersystem crossing rate constant ( $k_{\text{RISC}}$ ) of  $2.9 \times 10^6 \text{ s}^{-1}$  is three times larger than that of oxygen-based analog ( $9.0 \times 10^5 \text{ s}^{-1}$ ). An OLED device incorporating **DOB2-DABNA-C-NP-S-1** as an emitter achieves ultrapure deep-blue electroluminescence at 461 nm with Commission Internationale d'Éclairage (CIE) coordinates of (0.133, 0.077), satisfying the blue emitter standards set by the National Television System Committee (NTSC). The device demonstrates outstanding external quantum efficiencies (EQEs) of 24.3% (at maximum), 23.9% (at 1000  $\text{cd m}^{-2}$ ), and 18.7% (at 10000  $\text{cd m}^{-2}$ ), with the latter ranking the highest among the previously reported OLED devices employing deep-blue MR-TADF emitters.

## Introduction

Thermally activated delayed fluorescence (TADF) materials [1,2] have garnered significant attention in the field of organic light-emitting diodes (OLEDs)[3] due to their capability to utilize all excitons generated by electric field excitation. To enable highly efficient and color-pure TADF emission for advanced OLED technology, our group introduced a novel design principle in 2016, namely the multiple resonance (MR) effect [4]. This approach provides a powerful solution for simultaneously achieving both high photoluminescence quantum yield (PLQY) and narrow full width at half maximum (FWHM). Such attractive features originate from the unique electronic structure created by alternating electron-donating and electron-accepting atoms attached to a single benzene ring. This specific arrangement induces contrasting resonant features, effectively localizing the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) onto distinct carbon atoms. Consequently, MR-TADF emitters exhibit highly desirable narrow-band emission, enabling the realization of superior color purity in OLEDs without the need for energy-consuming color filtering. [5,6]

To improve the device performance of OLEDs fabricated with MR-TADF emitters, their reverse intersystem crossing (RISC) rate constant ( $k_{\text{RISC}}$ ) is a significant parameter because accumulated triplet excitons can lead to quenching processes such as triplet-triplet annihilation (TTA) and triplet-polaron annihilation (TPA). One of the most common strategies to enhance  $k_{\text{RISC}}$  is introducing heavy atoms into the MR framework.[7–9] For example, Shao, Wang, and coworkers first performed a direct comparison of oxygen- and sulfur-attached MR-TADF emitters and revealed the enhanced spin–orbit coupling (SOC) matrix element and accelerated RISC (Figure 1a).[10] Similarly, Park, Yasuda, and coworkers reported deep-blue MR-TADF emitters embedding sulfur atoms, whose  $k_{\text{RISC}}$  was up to 20 times higher than that of the oxygen-bridged analog (Figure 1b).[11] Although the heavy-atom effect of sulfur ( $Z_{\text{N}} = 16$ ) is considered to be not so significant, these results clearly prove the validity of oxygen–sulfur replacement. Stimulated by these pioneering works, many research studies have been conducted from both synthetic[12–25] and computational[26–28] approaches, attempting to improve the TADF property of MR-emitters. However, the incorporation of sulfur atoms often causes a red-shift in photoluminescence, especially in deep-blue emitters, thereby compromising the color purity of the original O-containing compounds (Table S7). For precise and strategic design of high-performance MR-TADF emitters, deeper understanding of the effect of oxygen-sulfur replacement is necessary.

With these circumstances in mind, herein, we focus on the improvement of **DOB2-DABNA-C-NP**, a  $\pi$ -extended MR-TADF material reported by our group (Figure 1c).[29] This compound, which contains four oxygen atoms, exhibits deep-blue

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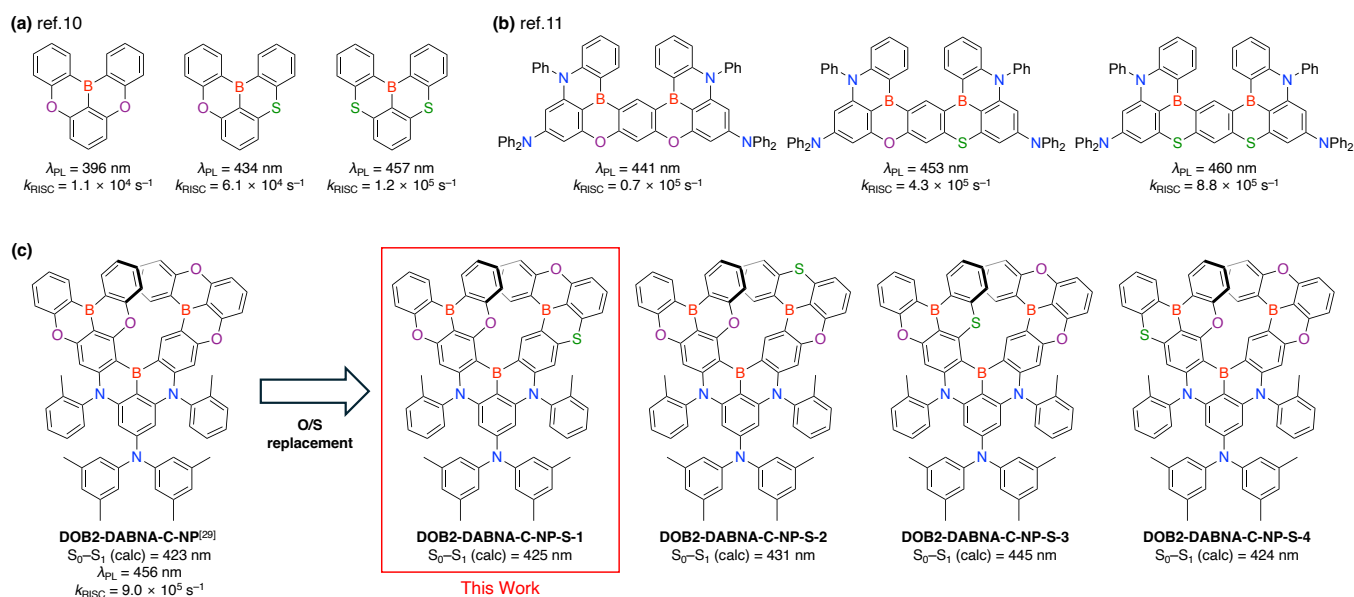
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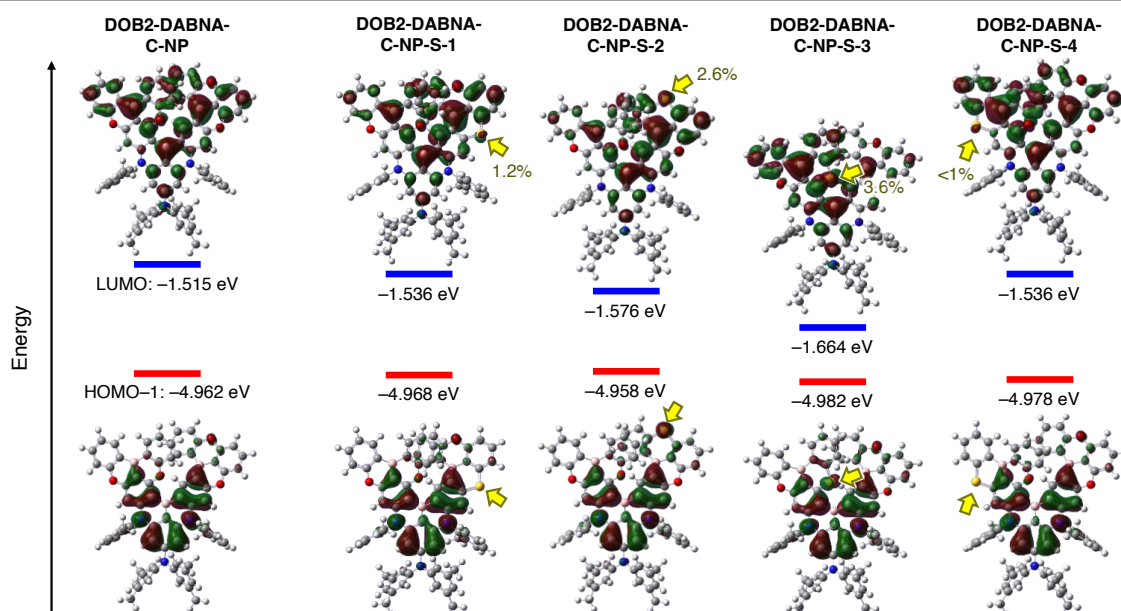
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**Fig. 1** (a)(b) Previous examples of the oxygen–sulfur replacement.[10,11] (c) Molecular structure of four O3S-type isomers and their predicted excitation wavelength of the  $S_0-S_1$  transition calculated at the B3LYP/6-31G(d) level of theory.



**Fig. 2** HOMO–1 and LUMO of DOB2-DABNA-C-NP and its sulfur-incorporated analogs. Yellow arrows show the position of the incorporated sulfur atom.

fluorescence (456–458 nm) and a fast  $k_{RISC}$  ( $0.8\text{--}1.1 \times 10^6 \text{ s}^{-1}$ ), leading to a remarkable OLED performance with an external quantum efficiency (EQE) of 20.8 % at  $1000 \text{ cd m}^{-2}$ . After a comprehensive computational analysis of all four candidates generated by oxygen–sulfur replacement of DOB2-DABNA-C-NP, we expect DOB2-DABNA-C-NP-S-1 to be a promising candidate for an improved deep-blue MR-TADF emitter. Motivated by this prediction, DOB2-DABNA-C-NP-S-1 was synthesized, and its photophysical properties were investigated, revealing an improved  $k_{RISC}$  ( $2.9 \times 10^6 \text{ s}^{-1}$ ) while maintaining pure blue emission (458 nm). The OLED device fabricated with DOB2-DABNA-C-NP-S-1 exhibited Commission Internationale d'Éclairage (CIE) coordinates of (0.133, 0.077), which satisfies the blue gamut standard defined by the National Television

System Committee (NTSC). Importantly, the efficiency roll-off is highly suppressed ( $\text{EQE}_{\text{max}} = 24.3\%/\text{EQE}_{1000} = 23.9\%$ ) because of the improved  $k_{RISC}$  value, indicating the validity of precisely selecting the sulfur incorporation position.

## Results and discussion

### Molecular design

Figure 2 shows the molecular orbitals of DOB2-DABNA-C-NP and its sulfur-incorporated analogs. Because the transition from HOMO–1 to LUMO is a main component of the  $S_0-S_1$  excitation in all cases (Table S2), these two molecular orbitals are discussed here. First, regarding the HOMO–1 energy level, only small differences were observed among all compounds. This

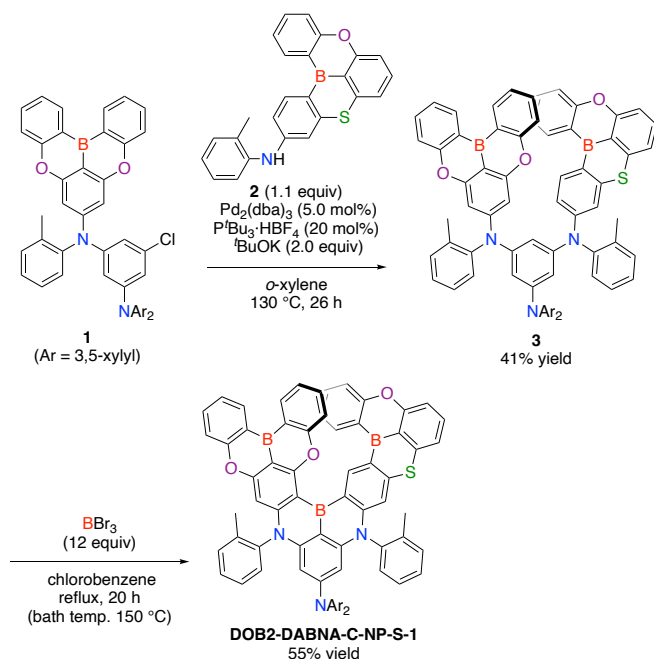


Fig. 3 Synthesis of DOB2-DABNA-C-NP-S-1.

can be attributed to a faint contribution of oxygen and sulfur atoms to HOMO–1. On the other hand, the LUMO energy is largely perturbed by the oxygen–sulfur replacement. Moreover, the extent of this perturbation strongly depends on the sulfur position. In DOB2-DABNA-C-NP-S-1 and DOB2-DABNA-C-NP-S-4, their LUMO energy was slightly stabilized from DOB2-DABNA-C-NP (0.021 eV). Much larger stabilization was observed in DOB2-DABNA-C-NP-S-2 (0.061 eV) and DOB2-DABNA-C-NP-S-3 (0.149 eV), which caused a red-shift characteristic of these two isomers (Figure 1c). Such a sulfur-position dependency can be rationalized by considering the anti-bonding character of two C–S bonds. While only one carbon atom adjacent to a sulfur atom shows a significant contribution to the LUMO in DOB2-DABNA-C-NP-S-1 and DOB2-DABNA-C-NP-S-4, clear nodes can be observed in both C–S bonds in DOB2-DABNA-C-NP-S-2 and DOB2-DABNA-C-NP-S-3, suggesting their contribution to LUMO as an anti-bonding component. In these two isomers, therefore, the replacement by sulfur strongly shifts the LUMO energy through the perturbation of an anti-bonding character. In other words, the position where sulfur is incorporated in DOB2-DABNA-C-NP-S-1 and DOB2-DABNA-C-NP-S-4 does not largely participate in LUMO, resulting in a small effect of the oxygen–sulfur replacement. These considerations are further supported by the population analysis, which proved that the contribution of a sulfur atom to the LUMO is larger in DOB2-DABNA-C-NP-S-2 (2.6%) and DOB2-DABNA-C-NP-S-3 (3.6%), thereby stabilizing their LUMO levels. Based on these results, we determined DOB2-DABNA-C-NP-S-1 to be a target molecule to achieve deep-blue emission and an improved OLED device performance.

## Synthesis

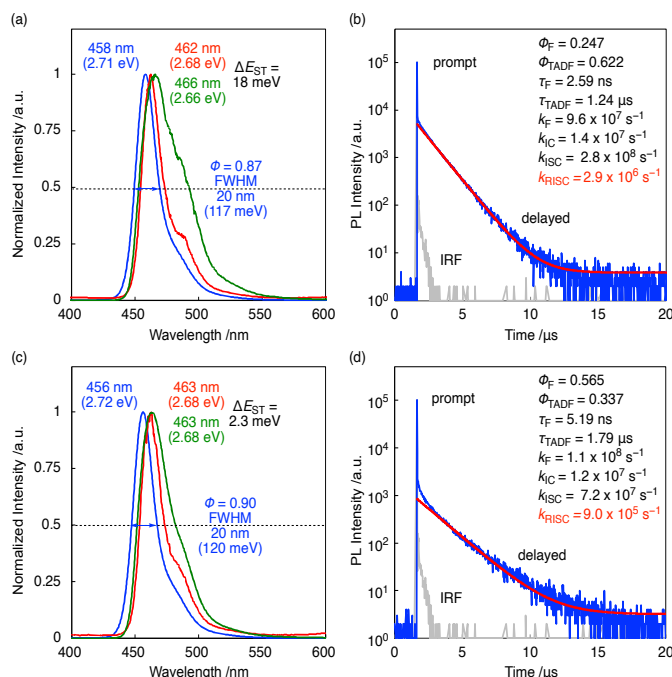
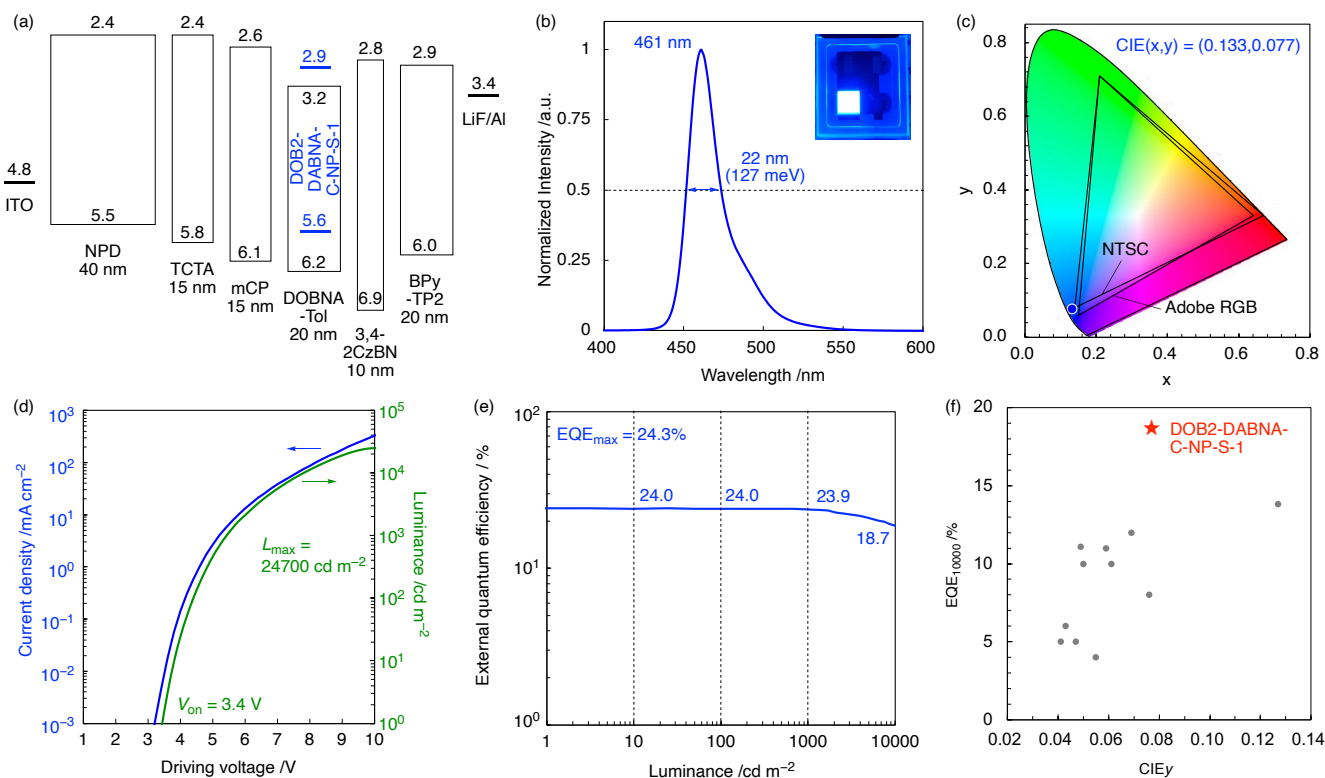


Fig. 4 Photophysical properties of (a,b) DOB2-DABNA-C-NP-S-1 and (c,d) DOB2-DABNA-C-NP in PS 1 wt.%-doped film. (a,c) Fluorescence spectra at 300 K (blue) and 77 K with (green) and without (red) a delay time of 25 ms. (b,d) Transient photoluminescence decay curve at 300 K and their relevant parameters. The red curve represents the single exponential fitting data (background = 3–4), and the gray curve represents an IRF curve.

The synthetic scheme of DOB2-DABNA-C-NP-S-1 is summarized in Figure 3. The procedure is totally the same as that for DOB2-DABNA-C-NP.[29] Starting from the previously reported compound 1, the sulfur-containing unit 2, which was synthesized in four steps from the commercially available materials, was introduced via Buchwald-Hartwig amination to afford 3 in 41% yield. After that, DOB2-DABNA-C-NP-S-1 was synthesized by one-shot borylation[30–32] in 55% yield. Along with DOB2-DABNA-C-NP, the introduction of steric methyl groups in an appropriate position allowed a moderate yield of the final borylation reaction.

## Photophysical properties

Next, the photophysical properties of DOB2-DABNA-C-NP-S-1 and DOB2-DABNA-C-NP were investigated in various conditions. To assess the impact of oxygen–sulfur replacement, toluene, poly(methyl methacrylate) (PMMA), and polystyrene (PS) were selected as matrices to mitigate specific intermolecular interactions with surrounding molecules (Table S6). Figure 4 summarizes representative photophysical properties measured in a 1 wt% DOB2-DABNA-C-NP-S-1-doped polystyrene (PS) film. As expected by the DFT calculation, DOB2-DABNA-C-NP-S-1 exhibited fluorescence maximum of 458 nm, which is only 2 nm red-shifted from DOB2-DABNA-C-NP (456 nm). The full width at half maximum (FWHM) and the energy difference between the  $S_1$  and  $T_1$  states ( $\Delta E_{ST}$ ) were 20 nm (117 meV) and 18 meV, respectively. These values are also comparable to those of DOB2-DABNA-C-NP, confirming little loss of its attractive deep-blue character. Nevertheless, a rate constant of reverse intersystem crossing ( $k_{RISC}$ ) of DOB2-DABNA-C-NP-S-1 ( $2.9 \times 10^6 \text{ s}^{-1}$ ) was 3.2 times larger than that of DOB2-DABNA-C-NP ( $9.0 \times$



**Fig. 5** OLED characteristics for the devices using **DOB2-DABNA-C-NP-S-1**. a) Device structures with the estimated energy levels in eV for each component. b) Normalized EL spectra. Inset: electroluminescence of the device. c) Commission Internationale de l'Éclairage (CIE) (x,y) coordinates. d) Current density-voltage ( $J$ - $V$ ) characteristics (blue) and luminance-voltage ( $L$ - $V$ ) characteristics (green). e) EQE-luminance (EQE- $L$ ) characteristics. f) Comparison of EQE values at 10000  $\text{cd m}^{-2}$  with reported blue OLEDs.

$10^5 \text{ s}^{-1}$ ). Thus, the oxygen-sulfur replacement effectively enhanced the TADF property. Measurements in toluene and PMMA exhibited consistent with those in PS (Figures S4 and S5). In addition, **DOB2-DABNA-C-NP-S-1** showed accelerated  $k_{\text{RISC}}$  and larger  $\Delta E_{\text{ST}}$  compared to **DOB2-DABNA-C-NP** in all conditions. Given that the increased  $\Delta E_{\text{ST}}$  is disadvantageous to the RISC process, the spin-orbit coupling (SOC) matrix should be enhanced by the oxygen-sulfur replacement. Although our computational SOC values largely depended on the conformation of the diphenylamine group, the higher  $k_{\text{RISC}}$  in **DOB2-DABNA-C-NP-S-1** could be reproduced by semi-classical Marcus equation (Figure S1 and Table S3).[33] Although intramolecular  $\pi$ - $\pi$  interaction was observed by noncovalent interaction (NCI) analysis (Figure S3),[34] the inclusion of Grimme's dispersion correlation parameters had a negligible effect on predicting the excited state properties (Tables S4 and S5). It should be noted that effects such as the Herzberg-Teller vibronic coupling should be included for a more accurate SOC calculation.[35] These results prove that a careful choice of the replacement position successfully suppresses the red-shift in fluorescence and contributes to realizing improved deep-blue emission.

### Electroluminescence properties

To evaluate the impact of the oxygen-sulfur replacement on OLED performance, a device using **DOB2-DABNA-C-NP-S-1** as an emitter was fabricated with the following structure: indium tin oxide (ITO, 50 nm); *N,N'*-di(1-naphthyl)-*N,N'*-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPD, 40 nm); tris(4-carbazolyl-9-

ylphenyl)amine (TCTA, 15 nm); 1,3-bis(*N*-carbazolyl)benzene (mCP, 15 nm); 1 wt% **DOB2-DABNA-C-NP-S-1** emitter and 99 wt% **DOBNA-Tol**[36] (20 nm); 3,4-di(9*H*-carbazol-9-yl)benzonitrile (3,4-2CzBN,[37] 10 nm); 2,7-bis(2,2'-bipyridine-5-yl)triphenylene (BPy-TP2,[38] 20 nm); LiF (1 nm); and Al (100 nm) (Figure 5a). The **DOB2-DABNA-C-NP-S-1**-fabricated device exhibited an ultrapure and narrow deep-blue emission ( $\lambda_{\text{EL}} = 461 \text{ nm}$ , FWHM = 22 nm) (Figure 5b). Its CIE coordinates were (0.133,0.077), which is extremely close to the blue gamut standard defined by NTSC (CIE(x,y) = (0.14,0.08)) (Figure 5c). This device had a turn-on voltage of 3.4 V, showing typical semiconducting properties (Figure 5d). While maintaining the desirable properties originally observed in the **DOB2-DABNA-C-NP**-fabricated device, the device performances, including EQE, current efficiency, power efficiency, and device lifetime were improved by sulfur incorporation. The EQEs of the **DOB2-DABNA-C-NP-S-1**-based device reached 24.3/24.0/23.9% at the maximum, 100, and 1000  $\text{cd m}^{-2}$ , respectively (Figure 5e). These values were improved from the 21.7/21.4/20.8% observed in the **DOB2-DABNA-C-NP**-based device. Notably, the efficiency roll-off at 1000  $\text{cd m}^{-2}$  was only 1.6%, an outstanding value compared to previous MR-emitter-based deep-blue OLED devices without a sensitizer (Table S8). The current and power efficiencies of the **DOB2-DABNA-C-NP-S-1**-based device at the maximum, 100, and 1000  $\text{cd m}^{-2}$  were 17.3/16.9/16.9  $\text{cd A}^{-1}$  and 16.9/12.1/9.8  $\text{lm W}^{-1}$ , respectively (Figure S13). These values also surpass those of the **DOB2-DABNA-C-NP**-based one (14.3/14.1/13.7  $\text{cd A}^{-1}$  and 13.5/9.8/7.5  $\text{lm W}^{-1}$ ). The half-

lifetime ( $LT_{50}$ ) with an initial luminance of  $500 \text{ cd m}^{-2}$  was 39 h, which is 3.3 times longer than that of the previously reported **DOB2-DABNA-C-NP** device (Figure S11). Notably, the  $EQE_{10000}$  (18.7%) ranks the highest among the previously reported OLED devices employing deep-blue MR-TADF emitters (Figure S5 and Table S9). Overall, the fast  $k_{RISC}$  of **DOB2-DABNA-C-NP-S-1**, benefiting from the oxygen–sulfur replacement, contributed to improved OLED performances while maintaining pure deep-blue electroluminescence.

## Conclusions

In this study, we present a molecular design strategy for enhancing the performance of MR-TADF emitters through targeted oxygen–sulfur replacement. Rather than simple replacement, we systematically evaluated four regioisomeric sulfur analogues to determine how the substitution position influences emission properties. Our analysis revealed that maintaining high excitation energy requires precise control over the LUMO level, which in turn depends critically on the sulfur atom's location. Among the candidates, **DOB2-DABNA-C-NP-S-1** emerged as a standout compound, exhibiting deep-blue photoluminescence at 458 nm with a narrow FWHM of 20 nm. These values are comparable to those of its oxygen-based counterpart, **DOB2-DABNA-C-NP**, thereby maintaining its desirable deep-blue character. Notably, the sulfur incorporation led to a threefold increase in the  $k_{RISC}$  compared to the oxygen-based emitter. The resulting OLED device delivered ultrapure deep-blue electroluminescence at 461 nm with CIE coordinates of (0.133, 0.077) and demonstrated excellent EQEs of 24.3%, 23.9%, and 18.7% at maximum, 1000, and 10000  $\text{cd m}^{-2}$ , respectively. Notably, the  $EQE_{10000}$  value surpasses all the previous OLED devices employing deep-blue MR-TADF emitters. These findings emphasize the importance of site-selective oxygen–sulfur replacement and offer valuable guidelines for the development of next-generation blue-emitting MR-TADF materials containing heavy atoms.

## Conflicts of interest

There are no conflicts to declare.

## Data availability

The data supporting this article have been included as part of the Supplementary Information.

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