



Triazolotriazine-based thermally activated delayed fluorescence sensitizer for narrowband red fluorescence OLEDs

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Abstract

The development of high-performance narrowband red organic light-emitting diodes (OLEDs) has garnered significant attention, offering both exciting opportunities and formidable challenges. In this study, we report the synthesis of a novel red thermally activated delayed fluorescence (TADF) molecule, 10,10',10''-([1,2,4]triazolo[1,5-a][1,3,5]triazine-2,5,7-triyltris(benzene-4,1-diyl))tris(10*H*-phenoxazine) (TPXZ-TAZTRZ), which integrates a highly electron-deficient triazolotriazine unit as the acceptor and three strongly electron-donating phenoxazine (PXZ) moieties as donors. TPXZ-TAZTRZ exhibits a small singlet-triplet energy gap, enabling a rapid reverse intersystem crossing rate. Additionally, it shows a broad emission spectrum peaking at 634 nm, spanning the yellow-to-red region. These features render TPXZ-TAZTRZ as an ideal TADF sensitizer for narrowband red fluorescent OLEDs. Accordingly, TPXZ-TAZTRZ was employed to sensitize the conventional fluorescent emitter DBP. The resulting TADF-sensitized fluorescence OLEDs (TSF-OLEDs) demonstrated efficient energy transfer from the TADF sensitizer to the emitter, effectively addressing the limitations previous encountered with TADF systems. The devices achieved high-performance pure red emission, with Commission International de l'Éclairage (CIE) coordinates of [0.67, 0.33], an emission peak at 612 nm, a narrow full width at half maximum (FWHM) of 27 nm, and a maximum external quantum efficiency of 16.2%.

Keywords: Organic light-emitting diodes, thermally activated delayed fluorescence, triazolotriazine; narrowband red emission

1. Introduction

Organic light-emitting diodes (OLEDs) are extensively utilized in applications such as flat panel displays and lighting due to their broad color spectrum, low energy consumption, and high flexibility. Achieving narrowband emission in OLEDs is essential for enhancing the accuracy and saturation of color performance and improving overall device display quality^[1-3]. This challenge has prompted widespread research into various types of narrowband OLED devices, which incorporate traditional fluorescence emitters, phosphorescence emitters, and thermally activated delayed fluorescence (TADF) emitters. Among these, multiple resonance (MR) TADF materials^[4-7] have shown promising results, especially in achieving high-performance blue^[8-17] and green^[18-27] narrowband emissions. However, compared to their blue and green OLEDs, high-performance narrowband red or pure red OLEDs remain few^[28-34]. Overall, due to the constraints imposed by the bandgap law, red OLED typically require a narrower energy gap. Therefore, this requires the larger π -conjugation and stronger intramolecular charge transfer properties of red OLED, which inevitably gives rise to a large structural relaxation in the excited state (S_1), along with substantial vibronic couplings between the S_1 and ground (S_0) states. As a result, the emission spectrum tends to broaden during electroluminescence, making it difficult to realize narrowband red emissions. Moreover, the development of red MR-TADF materials is further hampered by factors such as complex molecular architectures, lengthy and challenging synthesis routes, and generally low yields^[35,36].

Traditional fluorescence materials^[37,38] remain widely used in OLED applications due to their straightforward synthesis and structural diversity. For example, dibenzo[*l,l'*]-4,4',7,7'-tetraphenyl]diindeno[1,2,3-*cd*:1',2',3'-*lm*]perylene (DBP)^[39,40] (Figure 1a), a widely adopted red dye, is favored in OLEDs for its narrowband emission and high photoluminescence quantum yield (Φ_{PL}). However, conventional fluorescence emitters are inherently limited by a maximum internal quantum efficiency of 25%, as the remaining 75% of triplet excitons undergo non-radiative decay. To overcome these limitations, TADF-sensitized fluorescence (TSF)^[41,42], also referred to as



hyperfluorescence, has emerged as an effective strategy to boost OLED performance. By employing TADF materials as sensitizers to harvest triplet excitons, TSF-OLED devices exhibit improved performance^[43–46]. Nevertheless, several challenges remain for DBP-based TSF-OLEDs, including low external quantum efficiency (EQE), pronounced efficiency roll-off, and inadequate color purity^[40,41,47–51]. Therefore, the development of novel and highly efficient TADF sensitizers is crucial for advancing the performance of DBP-based TSF-OLED devices.

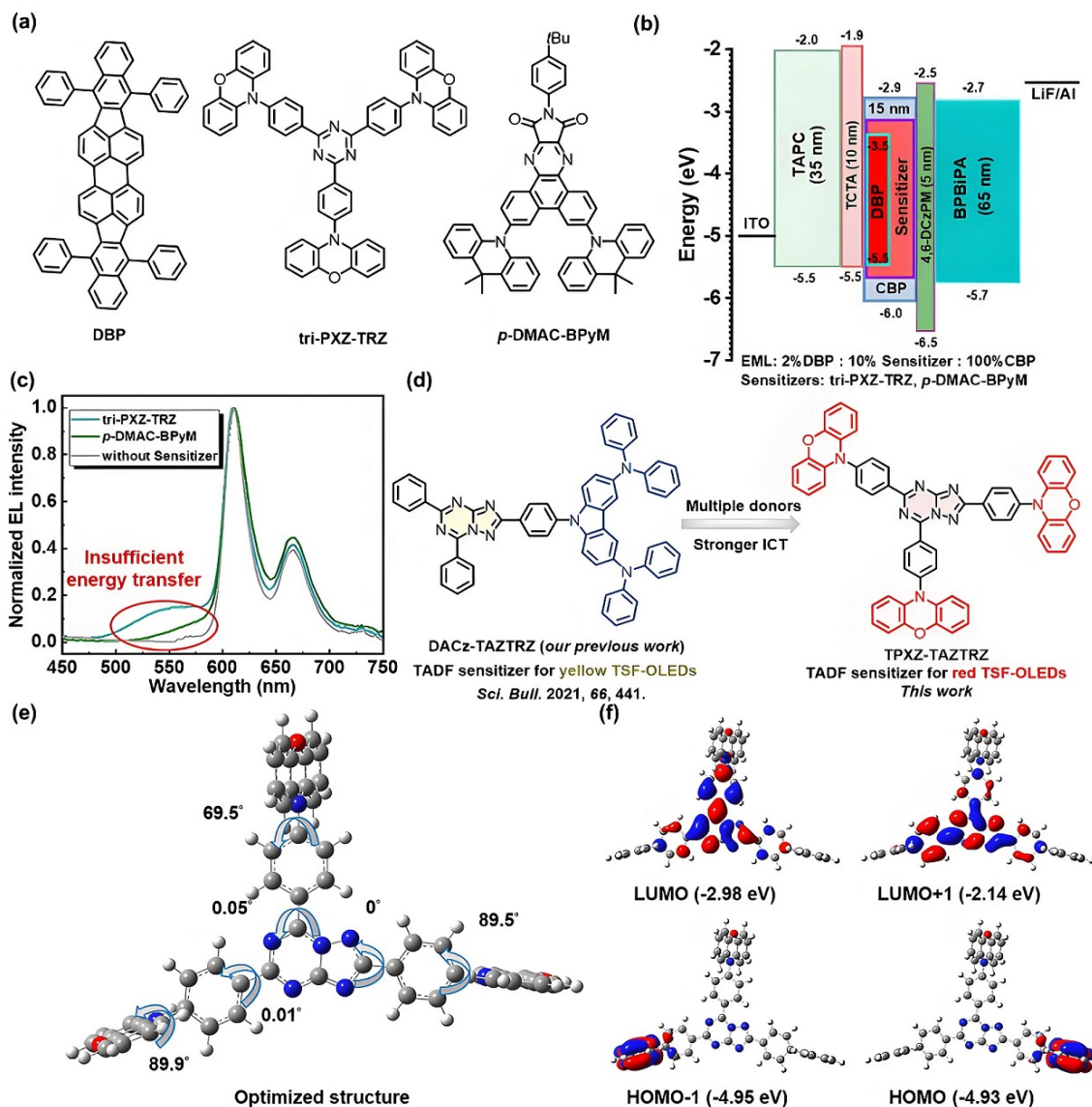


Figure 1. (a) Molecular structures of materials used in the emitting layer; (b) Device structure with energy level alignment; (c) EL spectra measured at 1,000 cd m⁻²; (d) Molecular design concept; (e) Optimized structures and (f) frontier molecular orbital distributions of TPXZ-TAZTRZ. EL: electroluminescence; TPXZ-TAZTRZ: 10,10',10''-([1,2,4]triazolo[1,5-a][1,3,5]triazine-2,5,7-triyltris(benzene-4,1-diyl))tris(10H-phenoxazine); DBP: dibenzo[[f,f']-4,4',7,7'-tetraphenyl]diindeno[1,2,3-cd:1',2',3'-lm]perylene; EML: emitting layer; CBP: 4,4'-bis(9-carbazolyl)-1,1'-biphenyl; LUMO: lowest unoccupied molecular orbital; HOMO: highest occupied molecular orbital; ITO: indium tin oxide; TAPC: 1,1-Bis(di-4-tolylaminophenyl)cyclohexane; TCTA: Tris(4-carbazoyl-9-ylphenyl)amine; ICT: intramolecular charge transfer.

Our initial experiments involved the fabrication of TSF-OLEDs using DBP and a previously reported tri-PXZ-TRZ sensitizer^[52,53] (Figure 1a,b). The optimized device architecture consisted of the following layered structure: indium-tin-oxide (ITO)/1,1-bis((di-4-tolylamino)phenyl)-cyclohexane (TAPC) (35 nm)/1,4,7-tris(acetato)-1,4,7-triazacyclon-onane (TCTA) (10 nm)/emitting layer (EML) (15 nm)/2,4,6-Tris(3-(9H-carbazol-9-yl)phenyl)-1,3,5-triazine (4,6-DCzPPM) (5 nm)/2,2'-[1,3-Phenylenebis(phenylphosphine oxide)]bis(1-phenyl-1H-benzimidazole) (BPBiPA) (65 nm)/LiF/Al. The EML comprised 2 wt% DBP, 10 wt% tri-PXZ-TRZ, 100 wt% 4,4'-bis(9-carbazolyl)-1,1'-biphenyl (CBP). The molecular structure of each functional material are illustrated in Figure S1. Although the electroluminescence (EL) spectra exhibited narrowband emission features, distinct emission peaks originating from the sensitizer were observed (Figure 1c), indicating incomplete energy transfer during the sensitization process. This shortcoming degraded the

color purity of the OLEDs, as reflected by the Commission International de l'Éclairage (CIE) coordinates of [0.56, 0.39]. To address this issue, we subsequently employed an orange TADF molecule previously developed by our group as a new sensitizer^[54,55]. While this adjustment improved color purity, as evidenced by a shift in the CIE coordinates to [0.63, 0.35], it still exhibited suboptimal energy transfer efficiency.

Building on these findings, we designed a highly efficient TADF sensitizer based on a triazolotriazine (TAZTRZ) acceptor, designated as TPXZ-TAZTRZ (Figure 1d). Compared to conventional triazine-based systems, triazolotriazine units feature higher electron deficiency and a flatter geometric structure, facilitating enhanced up-conversion rates and improved energy transfer. This improvements help suppresses residual sensitizer emission and enhance color purity. Additionally, the introduction of multiple donors strengthens the intermolecular charge-transfer characters, giving rise to a red TADF molecule and further enabling the red TSF-OLEDs with enhanced color purity.

2. Materials and Methods

2.1 Synthesis

Commercially available chemical reagents were used received without any further purification, unless otherwise specified. Solvents were dried and purified using an Innovative Technology PS-MD-5 solvent purification system. All reactions were conducted under a nitrogen atmosphere employing standard Schlenk techniques.

2.2 Measurements

High-resolution mass spectra were acquired using a Shimadzu LCMS-IT-TOF equipped with electrospray ionization. Nuclear magnetic resonance (NMR) spectra were recorded on an Agilent 400-MR DD2 spectrometer. Chemical shifts for the ¹H NMR (400 MHz) were referenced to CDCl₃ (δ = 7.26 ppm), and those for ¹³C NMR (100 MHz) were referenced to CDCl₃ (δ = 77.16 ppm). Fluorescence spectra and photoluminescence quantum yields were measured using a Horiba Jobin Yvon-Edison Fluoromax-3 fluorescence spectrometer equipped with a calibrated integrating sphere system. Phosphorescence spectra were obtained using both a HITACHI F-7100 fluorescence spectrophotometer and the Fluoromax-3. Transient photoluminescence (PL) decay curves were recorded using a Horiba FluoroHub single-photon counting controller in combination with a Horiba TBX picosecond photon detector. Cyclic voltammetry measurements were carried out using an LK2005A electrochemical 0.1 M tetrabutylammonium hexafluorophosphate (Bu₄NPF₆) in CH₂Cl₂ as the electrolyte. A ferrocene/ferrocenium (Fc/Fc⁺) redox couple was used as the internal reference. A three-electrode configuration was employed, consisting of a silver/silver chloride (Ag/Ag⁺) reference electrode, a platinum wire, a counter electrode, and a glassy carbon working electrode. Thermogravimetric analysis (TGA) was performed on a DTG-60(H) instrument under a nitrogen atmosphere at a heating rate of 10 °C min⁻¹.

2.3 OLED fabrication and characterization

ITO-coated glass substrates with a sheet resistance of 15 Ω /sq were used as the anode. The ITO substrates were cleaned using an alkaline detergent, followed by sequential treatments including boiling in deionized water, ultrasonication in deionized water, oven drying, and a 10-minute oxygen plasma treatment to enhance the surface work function. Organic layers were deposited at a rate of 0.1 nm·s⁻¹ in a high-vacuum chamber maintained below 2.0×10^{-4} Pa within an inert gas glovebox. Doped and co-doped layers were formed via co-evaporating of the dopant and host materials from separate sources, with doping concentrations by adjusting the respective evaporation rates. Current density-voltage-luminance (J-V-L) characteristics were measured using a KEYSIGHT B1500A semiconductor parameter analyzer. Luminance and electroluminescence spectra were recorded using a DLM-100Z photometer and an OPT2000 spectrophotometer.

3. Results and Discussion

3.1 Theoretical calculations

Density functional theory (DFT) and time-dependent DFT calculations were first performed to investigate the ground- and excited-state structures of the TPXZ-TAZTRZ molecule. The optimized geometry (Figure 1e) reveals that the benzene bridge and the TAZTRZ unit lie nearly in the same plane with small dihedral angles, likely due to intermolecular hydrogen bonding interactions. Additionally, the dihedral angles between the phenoxazine (PXZ) donors and their adjacent benzene bridges are 69.5°, 89.5°, and 89.9°, placing the donor and acceptor moieties in a nearly orthogonal configuration. The frontier molecular orbitals (FMOs) were further analyzed, as illustrated in Figure 1f. The highest occupied molecular orbitals (HOMO) and the next lowest (HOMO-1) are primarily located on the two separate PXZ donors with close energy levels of -4.93 eV and -4.95 eV respectively. In contrast, the lowest unoccupied molecular orbitals (LUMO) and the LUMO+1 are mainly distributed over the TAZTRZ acceptor and extend partially onto the π -bridge. Furthermore, the overlap integral of the FMOs was calculated to be 0.03877, indicating a relatively small singlet-triplet energy gap (ΔE_{ST}). The spatial separation between the HOMO and LUMO, together with the small FMO overlap, is favorable for achieving a low ΔE_{ST} and promoting an efficient up-conversion process.

3.2 Synthesis

The synthesis route for TPXZ-TAZTRZ is outlined in Figure 2. The process began with a nucleophilic substitution reaction between commercially available cyanuric chloride (1) and (4-bromophenyl) magnesium iodide Grignard reagent (2), yielding intermediate 3. A second nucleophilic substitution with hydrazine monohydrate afforded compound 4. Compound 4 then underwent dehydration followed by condensation with *para*-bromobenzaldehyde to give compound 5. Intramolecular oxidative cyclization was subsequently performed to generate compound 6. A Dimroth rearrangement was employed to convert compound 6 into compound 7. Finally, Buchwald-Hartwig amination with multiple PXZ donor units afforded the target molecule, TPXZ-TAZTRZ. More information about the synthesis route is available in Figure S2,S3,S4,S5,S6,S7.

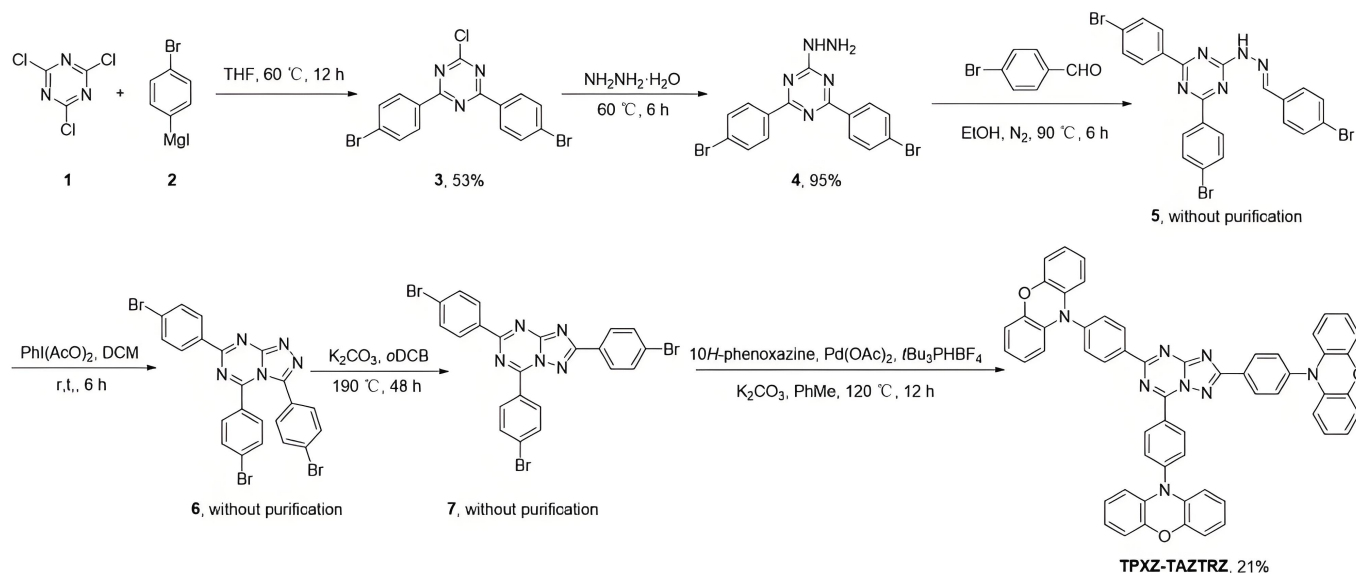


Figure 2. Synthetic route to TPXZ-TAZTRZ. TPXZ-TAZTRZ: 10,10',10''-([1,2,4]triazolo[1,5-a][1,3,5]triazine-2,5,7-triyl)tris(benzene-4,1-diyl)tris(10H-phenoxazine).

3.3 Photophysical properties

The PL characteristics of TPXZ-TAZTRZ are shown in Figure 3a and summarized in Table 1. TPXZ-TAZTRZ exhibits a sharp and intense absorption peaks at 326 nm in the ultraviolet region, attributed to an intramolecular localized excited transition. A broad and weaker absorption band centered at 458 nm indicates the presence of an intramolecular charge transfer (CT) transition. The room-temperature fluorescence spectrum of TPXZ-TAZTRZ in toluene displays a single broad emission peak at 634 nm, further confirming its predominantly CT emission character. Notably, the phosphorescence spectrum at 77 K shows a blue shift compared to the room-temperature fluorescence spectrum, likely due to geometric differences between the singlet and triplet excited states, which influence the energy levels under different thermal conditions. To explore this effect, we also recorded the low-temperature fluorescence spectrum of TPXZ-TAZTRZ in toluene at 77 K (Figure S8). Both the fluorescence and phosphorescence spectra at low temperature revealed an extremely small singlet-triplet energy gap (ΔE_{ST}). Moreover, the low-temperature fluorescence spectrum exhibited a pronounced blue shift relative to its room-temperature counterpart, possibly resulting from suppressed vibration at 77 K, in which leads to a small Stokes shift and blue shift emission. The singlet and triplet energy levels, estimated from the onset wavelengths of the fluorescence and phosphorescence spectra, were 2.53 eV and 2.51 eV, respectively, yielding a very small energy gap (ΔE_{ST}) of 0.02 eV. Such small measured values also indicate the rationality of theoretical analysis. This minimal ΔE_{ST} facilitates efficient reverse intersystem crossing processes (RISC), supported by computational findings (Figure 1f). As shown in Figure 3b, TPXZ-TAZTRZ exhibits pronounced TADF behavior in a CBP host matrix, with a prompt fluorescence lifetime (τ_p) of 24.1 ns and a delayed fluorescence lifetime (τ_d) of 1.2 μ s. In addition, TPXZ-TAZTRZ achieves a high Φ_{PL} of 68%. Accordingly, the radiative transition rate (k_R) and RISC rate (k_{RISC}) for TPXZ-TAZTRZ are calculated to be 1.9×10^7 s⁻¹ and 7.6×10^5 s⁻¹, respectively, as detailed in Table 1.

Subsequently, we evaluated the potential of TPXZ-TAZTRZ as a sensitizer for DBP. As shown in Figure 3c, the absorption spectra of DBP exhibits significant spectral overlap with the PL spectrum of TPXZ-TAZTRZ-based binary film (10 wt% TPXZ-TAZTRZ in CBP, excitation wavelength: 380 nm). This spectral overlap indicates that TPXZ-TAZTRZ is a suitable sensitizer for DBP, which is crucial for efficient Förster energy transfer (FET) during the sensitization process. Furthermore, the ternary film (excitation wavelength: 440 nm), containing 2% DBP and 10% TPXZ-TAZTRZ in a CBP matrix, showcased narrowband red emission predominantly from DBP, with an emission peak at 597 nm and full width at half maximum (FWHM) values of 20 nm, demonstrating the effective FET process between TPXZ-TAZTRZ sensitizer and DBP emitter. According to the transient PL decay curve (Figure 3d), the rates of FET (k_{FET}) and Dexter energy transfer (DET) rates (k_{DET}) for the ternary film were calculated and are summarized in Table S1. The fast k_{FET} ($\sim 10^8$ s⁻¹) and

relatively slow k_{DET} ($\sim 10^6 \text{ s}^{-1}$) promote the TSF process, contributing to the excellent color purity of the high-performance TSF-OLEDs. Additionally, the introduction of DBP reduces the exciton lifetime of the sensitizer due to energy transfer between the sensitizer and the emitter. This creates additional exciton decay pathways, ultimately shortening the overall exciton lifetime. The Förster radius (R_0) between the TPXZ-TAZTRZ sensitizer and the DBP emitter was estimated to be 34 nm, which is consistent with the characteristics of efficient Förster energy transfer, as shown in Table S2.

Prior to device fabrication, the HOMO and LUMO energy levels of TPXZ-TAZTRZ were determined from cyclic voltammetry measurements and the optical energy gap. The HOMO and LUMO levels were found to be -6.2 eV and -4.0 eV, respectively (Figure 3e, Table 1). In addition, TPXZ-TAZTRZ exhibited excellent thermal stability, as evidenced by a smooth TGA curve with a deposition temperature (corresponding to 5% weight loss) of 475 °C, as shown in Figure 3f.

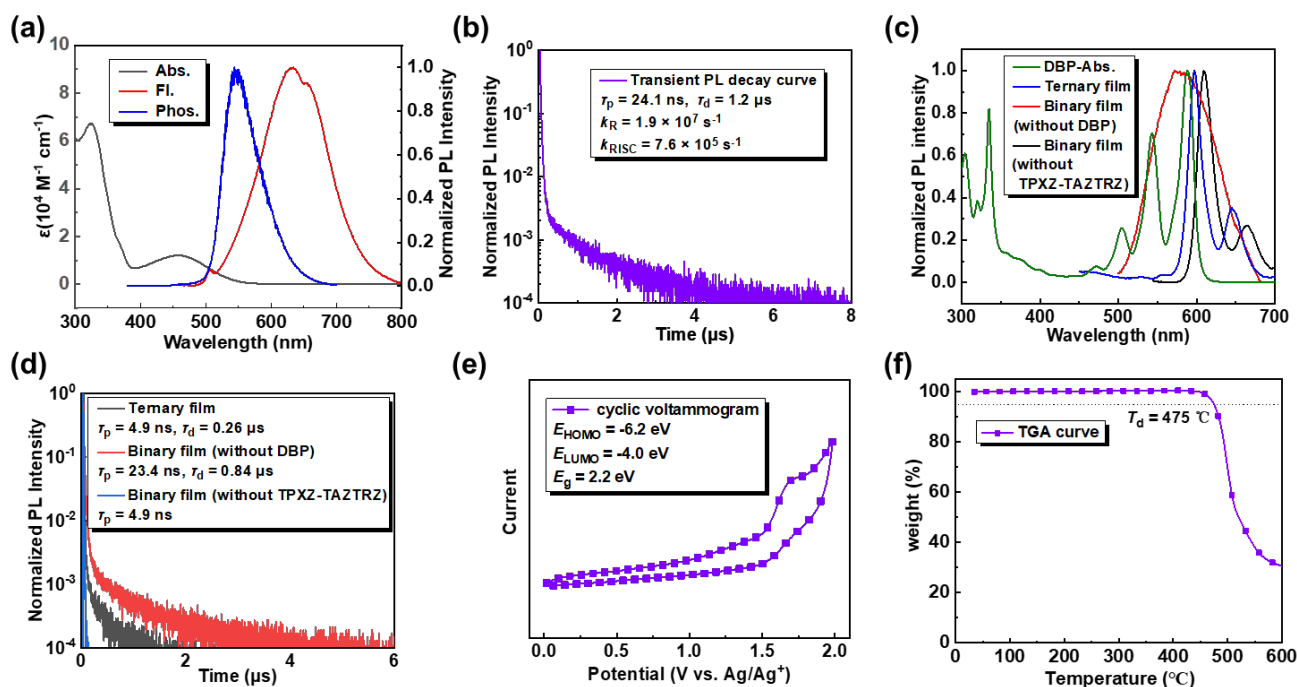


Figure 3. (a) Absorption spectra, normalized fluorescence spectra at room temperature, and phosphorescence spectra at 77K of TPXZ-TAZTRZ in toluene solution at $1.0 \times 10^{-5} \text{ mol L}^{-1}$; (b) Transient PL decay curve of TPXZ-TAZTRZ in 5 wt% film in CBP; (c) Normalized absorption spectrum of DBP and normalized fluorescence spectrum of TPXZ-TAZTRZ; (d) Transient PL decay curves of ternary and binary films; (e) Cyclic voltammogram of TPXZ-TAZTRZ in dry CH_2Cl_2 solution at $1.0 \times 10^{-3} \text{ mol L}^{-1}$; (f) Thermogravimetric analysis curve of TPXZ-TAZTRZ. Abs.: absorption spectra; Fl.: fluorescence spectra; Phos.: phosphorescence spectra; PL: photoluminescence; TPXZ-TAZTRZ: 10,10',10''-([1,2,4]triazolo[1,5-a][1,3,5]triazine-2,5,7-triyltris(benzene-4,1-diyl))tris(10H-phenoxazine); CBP: 4,4'-bis(9-carbazolyl)-1,1'-biphenyl; DBP: dibenzo[*h*,*j*]-4,4',7,7'-tetraphenyl]diindeno[1,2,3-*cd*:1',2',3'-*lm*]perylene; LUMO: lowest unoccupied molecular orbital; HOMO: highest occupied molecular orbital; TGA: thermogravimetric analysis.

Table 1. Thermal, electrochemical and photophysical data of TPXZ-TAZTRZ.

Compound	T_d^1 [°C]	HOMO ² [eV]	LUMO ³ [eV]	λ_{abs} [nm]	λ_{FL} [nm]	E_{S1} [eV]	E_{T1} [eV]
TPXZ-TAZTRZ	475	-6.2	-4.0	326, 458	634	2.53	2.51
Compound	ΔE_{ST} [eV]	Φ_{PL}^4 [%]	τ_p^4 [ns]	τ_d^4 [μs]	C_2^5 [%]	k_R^6 [10^7 s^{-1}]	k_{RISC}^7 [10^5 s^{-1}]
TPXZ-TAZTRZ	0.02	68	24.1	1.2	33.2	1.9	7.6

¹Deposition temperature with 5% weight loss calculated from thermogravimetric analysis curve (Figure 2f); ²calculated from cyclic voltammogram curve (Figure 2e). $E_{\text{HOMO}} = -4.8 - (E_{\text{ox}} - E_{\text{Fc}/\text{Fc}^+})$ (eV); ³calculated from the HOMO energy level and the energy gap from the absorption spectrum. $E_{\text{LUMO}} = E_g + E_{\text{HOMO}}$ (eV); ⁴measured in CBP host at 5 wt%; ⁵proportion of delayed component; ⁶ $k_R = C_1\Phi_{\text{PL}}/\tau_p$; ⁷ $k_{\text{RISC}} = C_2/[C_1\tau_d(1 - \Phi_{\text{PL}}C_1)]$; TPXZ-TAZTRZ: 10,10',10''-([1,2,4]triazolo[1,5-a][1,3,5]triazine-2,5,7-triyltris(benzene-4,1-diyl))tris(10H-phenoxazine); LUMO: lowest unoccupied molecular orbital; HOMO: highest occupied molecular orbital.

3.4 EL properties

Finally, TSF-OLEDs based on DBP were fabricated using the mentioned structure (Figure 1b). In these devices, the EML comprised 2 wt% DBP, 10 wt% TPXZ-TAZTRZ, and 100 wt% CBP. The device performance is presented in Figure 4 and summarized in Table 2. As

shown in the EL spectra (Figure 4a), the TSF-OLEDs exhibit no emission from the TADF sensitizer, indicating efficient energy transfer from the sensitizer to the emitter. The corresponding CIE chromaticity coordinates are [0.666, 0.332] (Figure 3b), closely matching the standard red defined by the NTSC, demonstrating the device's potential for display applications. Furthermore, the TSF-OLEDs exhibit excellent device performance, achieving a maximum EQE (EQE_{max}) of 16.2%, which is significantly higher than the 3.0% EQE_{max} observed in OLEDs without the TADF sensitizer. In addition, the introduction of sensitizers in TSF-OLEDs reduces turn-on voltage (V_{on}) from 3.7 V (without TPXZ-TAZTRZ) to 3.2 V (with TPXZ-TAZTRZ), and increases the maximum luminance (L_{max}) from 2,426 cd/m^2 to 12,276 cd/m^2 . However, the TSF-OLEDs exhibit severe efficiency roll-off, which may be attributed to the rigidity of the DBP emitter or an inadequate device structure. These issues may be addressed through the screening of alternative functional layer materials and the optimization of device architecture.

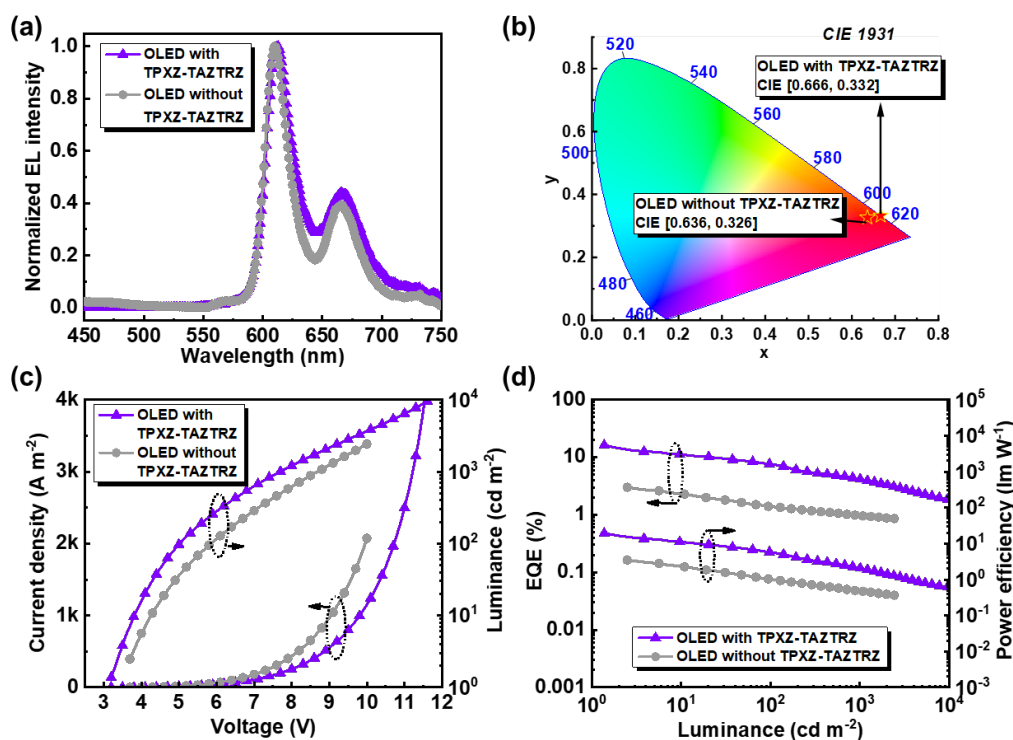


Figure 4. (a) EL spectra and (b) colour coordinates measured at 1,000 cd/m^2 ; (c) current density-voltage and luminance-voltage characteristics; (d) EQE-luminance and power efficiency-luminance curves of OLEDs. EL: electroluminescence; OLEDs: organic light-emitting diodes; EQE: external quantum efficiency; TPXZ-TAZTRZ: 10,10',10''-([1,2,4]triazolo[1,5-a][1,3,5]triazine-2,5,7-triyltris(benzene-4,1-diyl))tris(10H-phenoxazine); CIE: Commission International de l'Éclairage.

Table 2. Summary of EL performances.

Device	λ_{EL} [nm]	FWHM [nm]	CIE [x, y]	EQE_{max} [%]	EQE_{100} [%]	EQE_{1000} [%]	V_{on} [V]	Lum_{max} [cd/m^2]
TSF-OLED	612	27	[0.67, 0.33]	16.2	7.6	4.2	3.2	12,276
non TSF-OLED	610	25	[0.64, 0.33]	3.0	1.4	1.0	3.7	2,426

EL: electroluminescence; OLED: organic light-emitting diode; TSF-OLED: TADF-sensitized fluorescence OLED; CIE: Commission International de l'Éclairage; EQE: external quantum efficiency.

4. Conclusion

In summary, we have developed a novel red TADF molecule, TPXZ-TAZTRZ, which incorporates a highly electron-deficient TAZTRZ acceptor flanked by three strong electron-donating PXZ donors. TPXZ-TAZTRZ exhibits a fast RISC rate and significant spectral overlap with the narrowband red emitter DBP. As a result, TSF-OLEDs employing TPXZ-TAZTRZ as the sensitizer and DBP as the emitter demonstrated efficient energy transfer from the TADF sensitizer to the emitter, leading to pure red emission. The devices achieved CIE coordinates of [0.67, 0.33], an emission peak at 612 nm with a narrow FWHM of 27 nm, and a EQE_{max} of 16.2%. This study not only presents a promising TADF sensitizer for high-performance red TSF-OLEDs, but also highlights the critical role of a high RISC rate in facilitating efficient energy transfer from the sensitizer to the emitter.

Supplementary materials

The supplementary material for this article is available at: [Supplementary materials](#).

Declarations

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AI-assisted language editing was applied to improve the clarity and readability of the manuscript. The authors retain full responsibility for the scientific accuracy and integrity of the content.

Authors contribution

Tian Y, Zhang J: Performed the synthesis and characterization of the organic compounds, conducted OLEDs investigation, wrote the manuscript

Bin Z: Supervised the project, wrote the manuscript.

Conflict of interest

The authors declare no conflict of interest.

Ethical approval and consent

Not applicable.

Availability of data and materials

The data and materials could be obtained from the corresponding author upon request.

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