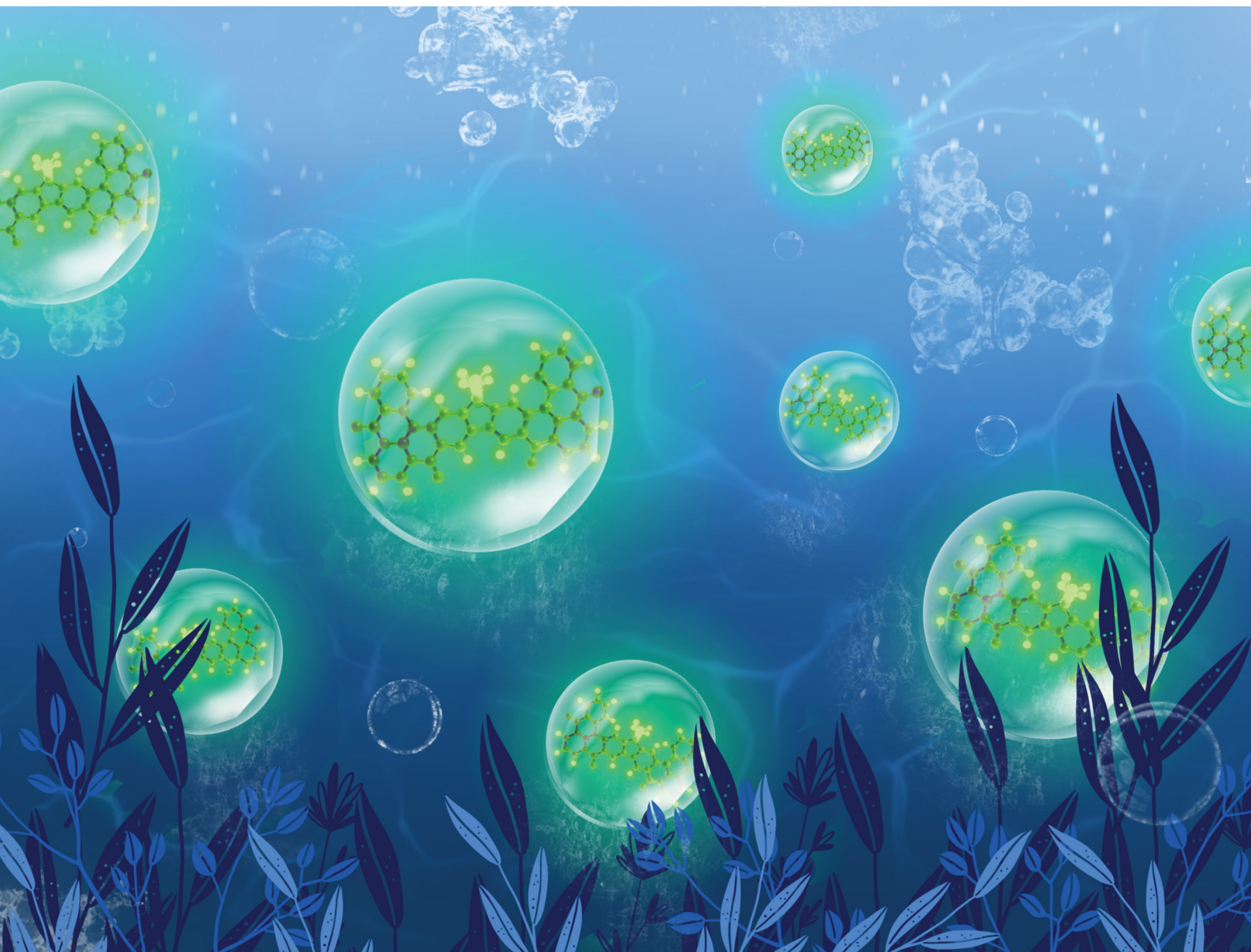


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A fluorene-bridged double carbonyl/amine multiresonant thermally activated delayed fluorescence emitter for efficient green OLEDs†‡

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Herein, we report a fluorene-bridged double carbonyl/amine-based MR TADF emitter DDiKta-F, formed by locking the conformation of the previously reported compound DDiKta. Using this strategy, DDiKta-F exhibited narrower, brighter, and red-shifted emission. The OLEDs with DDiKta-F emitted at 493 nm and showed an EQE_{max} of 15.3% with an efficiency roll-off of 35% at 100 cd m⁻².

Thermally activated delayed fluorescence (TADF) materials have demonstrated great potential as next-generation emitters in organic light-emitting diodes (OLEDs) due to their ability to harness 100% of the excitons to produce light without the need for noble metals, present in phosphorescent OLEDs. TADF compounds convert non-emission triplet excitons into emissive singlets by an endothermic upconversion reverse intersystem crossing (RISC) process.^{1–4} The efficiency of the RISC process is governed in part by the singlet-triplet energy gap, ΔE_{ST} .⁵ A strongly twisted structure that effectively reduces the conjugation between donor and acceptor moieties is one strategy to achieve a small ΔE_{ST} as the exchange integral of the frontier molecular orbitals (FMOs) is small.⁴ However, a twisted structure exhibits significant excited-state structural relaxation, resulting in a broad emission characterized by a full width at half maximum (FWHM) higher than 70 nm.⁶ To compensate for the

broad emission, filters or microcavities are required to improve color purity; however, this can, unfortunately, reduce the device efficiency.⁷

Multiresonant TADF (MR-TADF) emitters have emerged as a potential solution as these rigid structures exhibit narrowband emission. First reported by Hatakeyama *et al.*, these compounds are p- and n-doped polycyclic aromatic hydrocarbons (PAHs).⁸ By employing this approach, the singlet and triplet excited states possess an alternating pattern of increasing and decreasing electron density compared to the ground state, thus enabling a small exchange integral and consequently a small ΔE_{ST} .⁹ The rigid structure and the short-range charge transfer (SRCT) nature of the excited states endow the MR-TADF compounds with bright, narrowband emission. Since the first report of MR-TADF emitters used in OLEDs in 2016, there has been intense research focused on expanding the chemical space encompassed by this class of emitters.¹⁰ In the original works of Hatakeyama *et al.*, the n-dopants were boron atoms. It is possible to replace these with carbonyl groups, and the groups of Zysman-Colman¹¹ Zhang,¹² and Jiang and Liao¹³ were among the first to report examples of MR-TADF emitters containing this motif. Expanding the MR-TADF skeleton has been demonstrated to be an effective strategy for improving the performance of MR-TADF emitters,¹⁴ which has been less explored in carbonyl/amine systems.

We have shown that the dimerization of the MR-TADF emitter, DiKta, in DDiKta, leads to a modest red-shift of the emission and the OLED showed an improved performance.¹⁵ In an attempt to further improve the device performance and reduce the structural motion inherent in DDiKta, here, we envisioned annealing together two DiKta units through a central 9,9-dimethyl-9H-fluorene bridge, DDiKta-F. An analogue without the *tert*-butyl groups was also synthesized; however, purification proved too difficult owing to its poor solubility, likely due to its strong propensity to aggregate. Therefore, two *tert*-butyl groups were added to improve the solubility of this compound. DDiKta-F was found to be brighter (photoluminescence quantum yield, Φ_{PL} , of 78%) and emits with a narrower FWHM, of 49 nm compared to DDiKta (Φ_{PL} of 68% and FWHM of 59 nm) in 2 wt% doped films in 1,

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† Electronic supplementary information (ESI) available: ¹H and ¹³C-NMR spectra, HRMS, EA and HPLC of all target compounds; supplementary computational, photophysical device data. See DOI: <https://doi.org/10.1039/d3cc05761e>

‡ The research data supporting this publication can be accessed at <https://doi.org/10.17630/87972673-41de-4d34-9fd1-cfd23e633741>

§ Equal contribution.



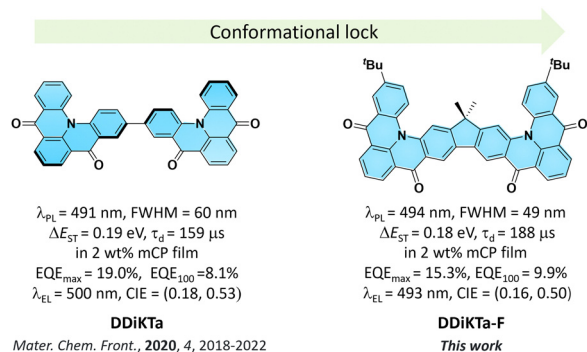


Fig. 1 Chemical structures, photophysical properties and device properties of **DDiKta** and **DDiKta-F**.

3-bis(carbazolyl)benzene (mCP). The device with **DDiKta-F** showed an EQE_{max} of 15.3% emitting at a λ_{EL} of 493 nm (FWHM of 46 nm) with an improved efficiency roll-off at 100 cd m⁻² of 35% compared to the devices with **DDiKta** (56%)¹⁵ and **DikTa** (44%) (Fig. 1).¹¹

Theoretical calculations were out to investigate the effect of the incorporation of the fluorene bridge on the optoelectrical properties of the emitter compared to those of the reference, **DikTa**. The geometry in the ground state was first optimized using density functional theory at the PBE0/6-31G(d,p) level. The frontier molecular orbitals (FMOs) are delocalized over the entire π -conjugated system, and the HOMO and LUMO show an alternating distribution pattern similar to that of **DDiKta**, which is emblematic of MR-TADF compounds.¹⁵ The calculated HOMO and LUMO levels of **DDiKta-F** are -5.94 and -2.32 eV, respectively. The HOMO–LUMO gap of 3.62 eV for **DDiKta-F** is smaller than that of **DDiKta** ($\Delta E_{HOMO-LUMO} = 3.70$ eV), reflecting an increased conjugation in the former. The locked structure of the molecule contributed to small geometric changes between the S_0 and S_1 states, as depicted in Fig. S15 (ESI[†]). Thus, it is expected that the emission spectrum will be narrow and that there will be a small Stokes shift. The emission spectra of both **DikTa** and **DDiKta-F** under vacuum were simulated using Frank–Condon analysis based on the S_1 – S_0 transition at the TDA-DFT-PBE0/6-31G(d,p) level (Fig. S16, ESI[†]). The simulated spectrum of **DikTa** shows an emission band peaking at $\lambda_{PL} = 428$ nm and a small FWHM = 14 nm, which closely aligns with the emission in hexane at $\lambda_{PL} = 436$ nm (FWHM = 21 nm). By contrast, the simulated emission spectrum of **DDiKta-F** is red-shifted at $\lambda_{PL} = 474$ nm and is slightly broader (FWHM = 18 nm). We previously demonstrated that DFT calculations do not accurately predict the excited-state properties of MR-TADF emitters.¹⁶ Here, we employed SCS-ADC(2)/cc-pVDZ calculations to accurately model the excited states of **DDiKta-F**.¹⁶ Difference density plots provide information on the changes in the electron density distribution in the excited states compared to that of the ground state. The difference density plots between S_0 and each of the S_1 and T_1 states, calculated for the S_0 optimized geometry, reveal that these excited states have SRCT characteristics typical of MR-TADF emitters. The calculated energies of the S_1 and T_1 states are 3.34 and 3.08 eV, respectively, which are lower than those of **DikTa** ($S_1/T_1 = 3.45/3.18$ eV) and **DDiKta** ($S_1/T_1 = 3.39/3.12$ eV), indicating that the emission in this compound should be red-shifted compared

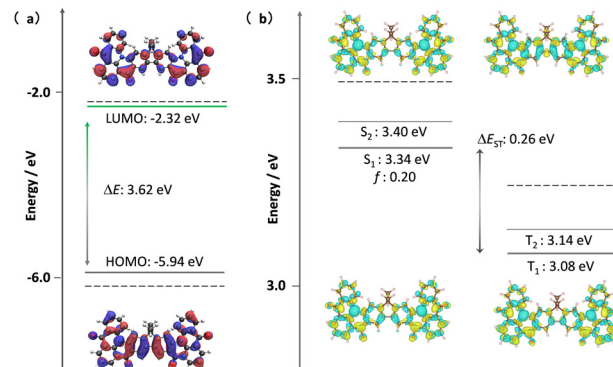


Fig. 2 (a) Distribution of FMOs of **DDiKta-F**, calculated at the PBE0/6-31G(d,p) level. (b) Difference density plots of S_1/S_2 and T_1/T_2 excited states, calculated at the SCS-ADC(2)/cc-pVDZ level for **DDiKta-F**, where f is the oscillator strength. The dashed lines in each figure reference the calculated values of **DikTa** at the same level of theory.¹⁷

to the two reference emitters. The calculated ΔE_{ST} for **DDiKta-F** is 0.26 eV, which is similar to those of **DikTa** (0.26 eV)¹⁷ and **DDiKta** (0.27 eV) (Fig. 2).¹⁵

The calculated spin–orbit coupling matrix element (SOCME) value between S_1 and T_1 is 0.37 cm^{-1} based on the T_1 -optimized geometry, while the SOCME values between S_1 and the four closely lying higher triplet excited states range from 0.07 to 5.93 cm^{-1} . In particular, the large $\langle S_1 | \hat{H}_{SOC} | T_3 \rangle$ value of 5.93 cm^{-1} is attributed to an n – π^* transition localized on the carbonyl groups (Fig. S18, ESI[†]).¹⁷ These closely lying intermediate triplet states can participate in the RISC mechanism between T_1 and S_1 mediated by spin-vibronic coupling.¹⁸

The electrochemical properties of **DDiKta-F** and **DikTa** were investigated using cyclic voltammetry (CV) and differential pulse voltammetry (DPV) in deaerated DCM with 0.1 M tetra-*n*-butylammonium hexafluorophosphate as the supporting electrolyte (Fig. S19, ESI[†]). The CV results show that the oxidation is irreversible while the reduction is a quasi-reversible process. The oxidation and reduction potentials, E_{ox} and E_{red} , determined, respectively, from the first oxidation and reduction peaks of the DPV, are 1.34 and -1.48 V vs. SCE. The corresponding HOMO/LUMO levels and energy gap (ΔE) are $-5.68/-2.86$ and 2.82 eV, respectively. The HOMO/LUMO are both destabilized compared to those of **DDiKta** ($-5.97/-3.07$ eV)¹⁵ and **DikTa** ($-6.10/-2.99$ eV), implying that the fluorene bridge acts as an electron donor. As a result, ΔE was smaller than those of **DDiKta** (2.90 eV) and **DikTa** (3.03 eV).

The absorption spectrum of the diluted toluene solution (10^{-5} M), shown in Fig. 3, exhibits two major bands. The band between 300 and 400 nm is linked to a π – π^* transition delocalized over the whole skeleton, and the band at 375 nm is associated with the absorption of the central fluorene unit, both assigned from analysis of the TDA-DFT calculations (Fig. S17, ESI[†]). The lower energy band at 453 nm and shoulder at 431 nm are characteristics of an SRCT excited state transition for MR-TADF emitters (Fig. S17, ESI[†]). The SRCT band of **DDiKta-F** is red-shifted and more intense ($\epsilon = 25 \times 10^3 \text{ M}^{-1} \text{ cm}^{-1}$) than those of **DDiKta** ($\lambda_{abs} = 440$ nm and $\epsilon = 10.4 \times 10^3 \text{ M}^{-1} \text{ cm}^{-1}$) and **DikTa** ($\lambda_{abs} = 433$ nm and $\epsilon = 21 \times 10^3 \text{ M}^{-1} \text{ cm}^{-1}$) due in part to its larger π -conjugation.¹⁵ The photoluminescence (PL) spectrum of **DDiKta-F** in toluene, shown in



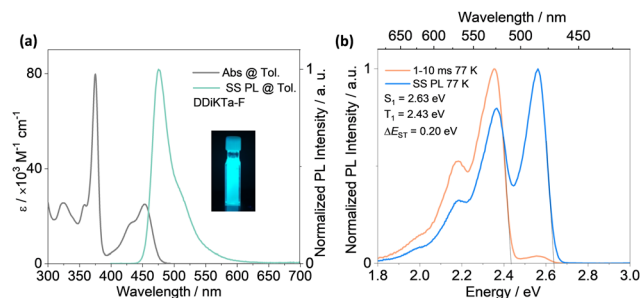


Fig. 3 (a) Absorption and SS PL spectra obtained in toluene at RT. Inset: Photograph of **DDiKta-F** in toluene and irradiated with a UV torch ($\lambda_{\text{exc}} = 365$ nm). (b) SS PL and delayed emission spectra (1–10 ms), collected in 2-MeTHF at 77 K ($\lambda_{\text{exc}} = 340$ nm).

Fig. 3a, has a peak maximum, λ_{PL} , of 476 nm, a shoulder at 511 nm, and an FWHM of 32 nm. The shoulder peak arises from the vibrational energy levels of the molecule, a typical characteristic of MR-TADF emitters.^{19,20} This emission is red-shifted compared to those of **DDiKta** ($\lambda_{\text{PL}} = 470$ nm) and **DikTa** ($\lambda_{\text{PL}} = 453$ nm).¹⁵ The emission of **DDiKta-F** shows a modest positive solvatochromism (Fig. S20, ESI[†]), which is consistent with the emissive excited state of SRCT. The energies of the S_1 and T_1 states, determined from the onsets of the steady-state PL and phosphorescence spectra at 77 K in 2-MeTHF glass are 2.63 and 2.43 eV, respectively (Fig. 3b); thus, $\Delta E_{\text{ST}} = 0.20$ eV. This value is similar in magnitude to those of **DikTa** (0.22 eV in frozen toluene) and **DDiKta** (0.21 eV in frozen toluene). The photoluminescence quantum yield, Φ_{PL} , in toluene is 34%, which decreases to 31% upon exposure to air (Fig. S21, ESI[†]). No delayed emission was observed in toluene and the lifetime of the emission decay, τ_{PL} , was 4.5 ns (Fig. S21, ESI[†]), which is similar to that of **DikTa** ($\tau_{\text{PL}} = 5.1$ ns).¹¹

With a view to employ **DDiKta-F** as an emitter in OLEDs and to cross-compare their device performance with those of **DDiKta** and **DikTa**, we next investigated the photophysical properties of this emitter as doped films in mCP. The 2 wt% doped film of **DDiKta-F** in mCP emits at 494 nm with a FWHM of 49 nm (Fig. 4a), an emission that is red-shifted compared to those of **DDiKta** ($\lambda_{\text{PL}} = 491$ nm) and **DikTa** ($\lambda_{\text{PL}} = 467$ nm) in 2 wt% doped films in mCP.¹⁷ We identified that 2 wt% doping provided the highest Φ_{PL} of 78%, while the Φ_{PL} decreased to 43% and the PL spectrum showed a pronounced red-shift from 491 to 507 nm when the doping concentration increased from 1 wt% to 10 wt% (Fig. S22, ESI[†]), implying that aggregation becomes an issue at this higher doping concentration. The Φ_{PL} of the 2 wt% doped film in mCP decreased to 65% in air. The Φ_{PL} of **DDiKta-F** is slightly higher than those of both **DikTa** ($\Phi_{\text{PL}} = 46\%$) and **DDiKta** ($\Phi_{\text{PL}} = 65\%$) in 2 wt% doped films in mCP. At the same doping concentration, the Φ_{PL} in the phosphine oxide-based hosts DPEPO and PPT are similar at 74 and 61% but the λ_{PL} are red-shifted at 510 and 511 nm, respectively, due to their higher polarity (Fig. S23, ESI[†]). The S_1/T_1 energies, determined from the onsets of the steady-state PL and delayed emission spectra at 77 K in the 2 wt% doped films in mCP, are 2.58/2.40 eV, resulting in a ΔE_{ST} of 0.18 eV (Fig. S26, ESI[†]), which

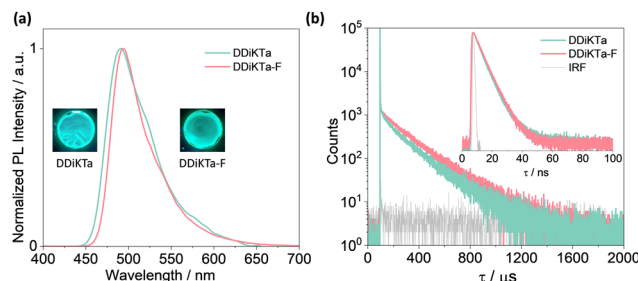


Fig. 4 (a) SS PL spectra ($\lambda_{\text{exc}} = 340$ nm); (b) time-resolved PL decays of **DDiKta** and **DDiKta-F** measured using MCS (inset: TRPL decays of the prompt component measured using TCSPC); $\lambda_{\text{exc}} = 375$ nm.

is similar to that measured for 2-MeTHF glass. Temperature-dependent transient PL decay analysis reveals the expected increase in the delayed emission with increasing temperature, which confirms the TADF in the 2 wt% doped film in mCP (Fig. S24, ESI[†]). The emission decays with the associated average prompt (τ_{p}) and delayed (τ_{d}) lifetimes are 5.6 ns and 188 μs (Table 1), respectively. These values are intermediate to those of **DDiKta** ($\tau_{\text{p}} = 5.9$ ns and $\tau_{\text{d}} = 159$ μs) and **DikTa** ($\tau_{\text{p}} = 4.8$ ns and $\tau_{\text{d}} = 242$ μs); in air, the delayed emission of **DDiKta-F** was not completely quenched (Fig. S25, ESI[†]). From these photophysical measurements, the RISC rate constant (k_{RISC}) of **DDiKta-F** was determined to be $2.16 \times 10^4 \text{ s}^{-1}$ (Table S2, ESI[†]),^{21,22} which is intermediate to those of **DDiKta** ($k_{\text{RISC}} = 1.77 \times 10^4 \text{ s}^{-1}$) and **DikTa** ($k_{\text{RISC}} = 2.52 \times 10^4 \text{ s}^{-1}$).

Having identified the potential of **DDiKta-F** as an emitter for OLEDs, we next fabricated vacuum-deposited devices. The devices have the following architecture: ITO/TAPC (35 nm)/TCTA (10 nm)/CzSi (10 nm)/x wt% emitter/mCP (20 nm)/TmPyPB (40 nm)/LiF (1 nm)/Al (100 nm), where indium tin oxide (ITO) is the anode and 4,4'-cyclohexylidenebis[N,N-bis(4-methylphenyl)benzenamine] (TAPC) acts as the hole-transport layer. 9-(4-tert-butylphenyl)-3,6-bis(triphenylsilyl)-9H-carbazole (CzSi) is the exciton blocking layer, 1,3,5-tri(m-pyridin-3-ylphenyl)benzene (TmPyPB) acts as the electron-transporting material, and LiF modifies the work function of the aluminium cathode. The chemical structures of the materials used in these devices are shown in Fig. S27 (ESI[†]). The device stacks and their related performance are shown in Fig. 5 and Fig. S28 and S29 (ESI[†]), respectively.

The electroluminescence peak of the OLED, λ_{EL} of 493 nm and FWHM of 46 nm match those of the PL spectrum of the 2 wt% films in mCP ($\lambda_{\text{PL}} = 494$ nm and FWHM = 49 nm). The EL is narrower compared to the previously reported device with

Table 1 Photophysical data of **DDiKta-F** and **DDiKta** in 2 wt% doped films in mCP

Emitter	Φ_{PL}^a / %	$\lambda_{\text{PL}}/\text{nm}$	FWHM/nm	S_1^b/T_1^c / eV	$\Delta E_{\text{ST}}/\text{eV}$	$\tau_{\text{p}}, \tau_{\text{d}}/\text{ns}, \mu\text{s}$
DDiKta-F	78	494	49	2.58, 2.40	0.18	5.6, 188
DDiKta	68	491	60	2.64, 2.45	0.19	5.9, 159
DikTa ¹⁷	46	467	46	2.75, 2.55	0.20 ¹¹	4.8, 242

^a Φ_{PL} was measured using an integrating sphere under nitrogen ($\lambda_{\text{exc}} = 340$ nm). ^b Obtained from the onset of the SS PL spectrum at 77 K. ^c Obtained from the onset of the delayed emission spectrum (1–10 ms) at 77 K ($\lambda_{\text{exc}} = 340$ nm).



DDiKta (9 wt% in DPEPO), which emitted at a λ_{EL} of 500 nm and had an FWHM of 59 nm.¹⁵ This small red-shifted emission compared to the SS PL in 2 wt% mCP film can be attributed to a combination of the use of the higher polarity DPEPO host and higher doping concentrations. By contrast, the EL is red-shifted compared to the device with **DiKta** (3.5 wt% in mCP), which emitted at a λ_{EL} of 465 nm and had a FWHM of 59 nm.¹¹ The corresponding Commission Internationale de l'Éclairage (CIE) coordinates are (0.16, 0.50) for the device with **DDiKta-F**, which are close to those of the device with **DDiKta** (0.18, 0.53), yet are red-shifted compared to the device with **DiKta** (0.14, 0.18). The device with **DDiKta-F** exhibited an EQE_{max} of 15.3%, which is similar to those of **DDiKta** (19.0%) and **DiKta** (14.7%). Gratifyingly, the efficiency roll-off was less severe, with an EQE of 100 cd m⁻² at 9.9% for the device with **DDiKta-F**, which was higher than those of **DDiKta** (EQE₁₀₀ = 8.1%) and **DiKta** (EQE₁₀₀ = 8.3%). This modestly improved efficiency roll-off can be explained by a higher figure of merit (FOM) that describes productive exciton utilization, $\text{FMO} = \frac{k_{\text{r}}k_{\text{RISC}}}{k_{\text{ISC}}}$,²³ of $4.75 \times 10^3 \text{ s}^{-1}$ for **DDiKta-F**, compared to those of 4.71×10^3 and $1.87 \times 10^3 \text{ s}^{-1}$ for **DDiKta** and **DiKta**, respectively.

a simple method to maintain narrowband emission in MR-TADF compounds while simultaneously enhancing the Φ_{PL} and k_{RISC} .

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There are no conflicts to declare.

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