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

 Sen Wu,[§] Ya-Nan Hu,[§] Dianming Sun,^{*a} Kai Wang,^{ib} Xiao-Hong Zhang^{ib} ^{*bc} and Eli Zysman-Colman^{ib} ^{*a}

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,

^a Organic Semiconductor Centre, EaStCHEM School of Chemistry, University of St Andrews, St Andrews, Fife KY16 9ST, UK.
E-mail: eli.zysman-colman@st-andrews.ac.uk, sd235@st-andrews.ac.uk;
Fax: +44-1334 463808; Tel: +44-1334 463826

^b Institute of Functional Nano & Soft Materials (FUNSOM), Joint International Research Laboratory of Carbon-Based Functional Materials and Devices, Soochow University, Suzhou, Jiangsu 215123, P. R. China.
E-mail: xiaohong_zhang@suda.edu.cn

^c Jiangsu Key Laboratory of Advanced Negative Carbon Technologies, Soochow University, Suzhou, Jiangsu, 215123, P. R. China

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§ 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** ($\Delta E_{\text{HOMO-LUMO}} = 3.70$ 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 $\lambda_{\text{PL}} = 428$ nm and a small FWHM = 14 nm, which closely aligns with the emission in hexane at $\lambda_{\text{PL}} = 436$ nm (FWHM = 21 nm). By contrast, the simulated emission spectrum of **DDiKta-F** is red-shifted at $\lambda_{\text{PL}} = 474$ 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 $\langle S_1 | \hat{H}_{\text{SOC}} | T_3 \rangle$ 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** ($\lambda_{\text{abs}} = 440$ nm and $\epsilon = 10.4 \times 10^3 \text{ M}^{-1} \text{ cm}^{-1}$) and **DikTa** ($\lambda_{\text{abs}} = 433$ 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

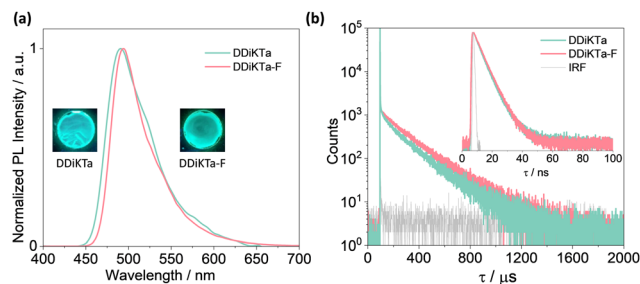


Fig. 4 (a) SS PL spectra ($\lambda_{\text{exc}} = 340$ nm); (b) time-resolved PL decays of **DDiKta** and **DDiKta-F** measured using MCS (inset: TRPL decays of the prompt component measured using TCSPC); $\lambda_{\text{exc}} = 375$ nm.

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)benzamine] (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	$S_1^b/T_1^c/\text{eV}$	$\Delta E_{\text{ST}}/\text{eV}$	$\tau_{\text{p}}, \tau_{\text{d}}/\text{ns}, \mu\text{s}$
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).



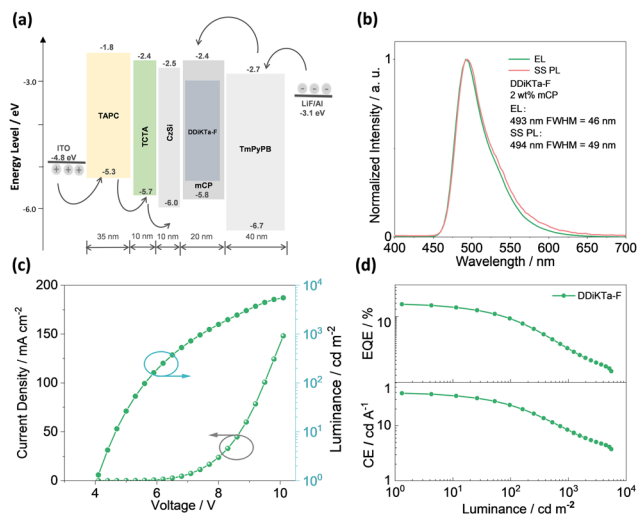


Fig. 5 (a) Device configuration and energy levels for each layer; (b) electroluminescence spectra for devices; (c) J - V - L characteristics; and (d) EQE and CE versus luminance characteristics.

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** ($\text{EQE}_{100} = 8.1\%$) and **DiKta** ($\text{EQE}_{100} = 8.3\%$). This modestly improved efficiency roll-off can be explained by a higher figure of merit (FOM) that describes productive exciton utilization, $\text{FOM} = \frac{k_{\text{r}}k_{\text{RISC}}}{k_{\text{ISC}}}$,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.

In conclusion, we demonstrated an easy-to-access synthetic route for constructing a p-extended dimeric MR-TADF emitter by fusing two **DiKta** units onto a fluorene bridge. Through this strategy, the structural motion was reduced compared to that of the parent dimeric emitter **DDiKta**. This led to an improved Φ_{PL} of 79% and a red-shifted and narrower emission at 494 nm (FWHM = 49 nm) in 2 wt% doped films in mCP. Moreover, the ΔE_{ST} decreased to 0.18 eV, which led to a modest improvement in k_{RISC} from $1.77 \times 10^4 \text{ s}^{-1}$ to $2.16 \times 10^4 \text{ s}^{-1}$. The device with **DDiKta-F** exhibited an EQE_{max} of 15.3% and emission at 493 nm. Owing to the faster k_{RISC} , the device exhibited a smaller efficiency roll-off of 35% at 100 cd m^{-2} than the devices with **DDiKta** (56%) and **DiKta** (44%). This emitter design, annelating multiple MR-TADF cores about a central fluorene, provides

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

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Conflicts of interest

There are no conflicts to declare.

References

- 1 C. W. Tang and S. A. VanSlyke, *Appl. Phys. Lett.*, 1987, **51**, 913.
- 2 M. A. Baldo, D. F. O'Brien, Y. You, A. Shoustikov, S. Sibley, M. E. Thompson and S. R. Forrester, *Nature*, 1998, **395**, 151–154.
- 3 A. Endo, K. Sato, K. Yoshimura, T. Kai, A. Kawada, H. Miyazaki and C. Adachi, *Appl. Phys. Lett.*, 2011, **98**, 083302.
- 4 Y. Tao, K. Yuan, T. Chen, P. Xu, H. Li, R. Chen, C. Zheng, L. Zhang and W. Huang, *Adv. Mater.*, 2014, **26**, 7931–7958.
- 5 H. Uoyama, K. Goushi, K. Shizu, H. Nomura and C. Adachi, *Nature*, 2012, **492**, 234–238.
- 6 Y. J. Cho, S. K. Jeon, S.-S. Lee, E. Yu and J. Y. Lee, *Chem. Mater.*, 2016, **28**, 5400–5405.
- 7 A. C. Arsenault, D. P. Puzzo, I. Manners and G. A. Ozin, *Nat. Photonics*, 2007, **1**, 468–472.
- 8 T. Hatakeyama, K. Shiren, K. Nakajima, S. Nomura, S. Nakatsuka, K. Kinoshita, J. Ni, Y. Ono and T. Ikuta, *Adv. Mater.*, 2016, **28**, 2777–2781.
- 9 H. Jiang, J. Jin and W. Y. Wong, *Adv. Funct. Mater.*, 2023, **33**, 2306880.
- 10 R. K. Konidena and K. R. Naveen, *Adv. Photonics Res.*, 2022, **3**, 2200201.
- 11 D. Hall, S. M. Suresh, P. L. dos Santos, E. Duda, S. Bagnich, A. Pershin, P. Rajamalli, D. B. Cordes, A. M. Z. Slawin, D. Beljonne, A. Köhler, I. D. W. Samuel, Y. Olivier and E. Zysman-Colman, *Adv. Opt. Mater.*, 2020, **8**, 1901627.
- 12 X. Li, Y.-Z. Shi, K. Wang, M. Zhang, C.-J. Zheng, D.-M. Sun, G.-L. Dai, X.-C. Fan, D.-Q. Wang, W. Liu, Y.-Q. Li, J. Yu, X.-M. Ou, C. Adachi and X.-H. Zhang, *ACS Appl. Mater. Interfaces*, 2019, **11**, 13472–13480.
- 13 Y. Yuan, X. Tang, X.-Y. Du, Y. Hu, Y.-J. Yu, Z.-Q. Jiang, L.-S. Liao and S.-T. Lee, *Adv. Opt. Mater.*, 2019, **7**, 1801536.
- 14 C. Zhou, A. Shatskiy, A. Z. Temerdashev, M. D. Kärkäs and P. Dinér, *Commun. Chem.*, 2022, **5**, 92.
- 15 D. Sun, S. M. Suresh, D. Hall, M. Zhang, C. Si, D. B. Cordes, A. M. Z. Slawin, Y. Olivier, X. Zhang and E. Zysman-Colman, *Mater. Chem. Front.*, 2020, **4**, 2018–2022.
- 16 D. Hall, J. C. Sancho-García, A. Pershin, G. Ricci, D. Beljonne, E. Zysman-Colman and Y. Olivier, *J. Chem. Theory Comput.*, 2022, **18**, 4903–4918.
- 17 S. Wu, L. Zhang, J. Wang, A. Kumar Gupta, I. D. W. Samuel and E. Zysman-Colman, *Angew. Chem., Int. Ed.*, 2023, **62**, e202305182.
- 18 T. J. Penfold, E. Gindensperger, C. Daniel and C. M. Marian, *Chem. Rev.*, 2018, **118**, 6975–7025.
- 19 Y. Kondo, K. Yoshiura, S. Kitera, H. Nishi, S. Oda, H. Gotoh, Y. Sasada, M. Yanai and T. Hatakeyama, *Nat. Photon.*, 2019, **13**, 678.
- 20 X. Qiu, G. Tian, C. Lin, Y. Pan, X. Ye, B. Wang, D. Ma, D. Hu, Y. Luo and Y. Ma, *Adv. Opt. Mater.*, 2020, **9**, 20200.
- 21 K. Masui, H. Nakanotani and C. Adachi, *Org. Electron.*, 2013, **14**, 2721–2726.
- 22 Y. Tsuchiya, S. Diesing, F. Bencheikh, Y. Wada, P. L. dos Santos, H. Kaji, E. Zysman-Colman, I. D. W. Samuel and C. Adachi, *J. Phys. Chem. A*, 2021, **125**, 8074–8089.
- 23 S. Diesing, L. Zhang, E. Zysman-Colman and I. Samuel, *ChemRxiv*, 2023, preprint, DOI: [10.26434/chemrxiv-2023-c0hgg](https://doi.org/10.26434/chemrxiv-2023-c0hgg).

