Supplementary Information

An efficient yellow thermally activated delayed fluorescence emitter with universal applications in both doped and non-doped organic light-emitting diodes

Xiaojie Chen, Zhan Yang, Zongliang Xie, Juan Zhao,* Zhiyong Yang, Yi Zhang,* Jiarui Xu, Zhenguo Chi* and Matthew. P. Aldred

PCFM Lab, GD HPPC Lab, Guangdong Engineering Technology Research Center for High-performance Organic and Polymer Photoelectric Functional Films, State Key Laboratory of Optoelectronic Material and Technologies, School of Chemistry, Sun Yat-sen University, Guangzhou 510275, PR China

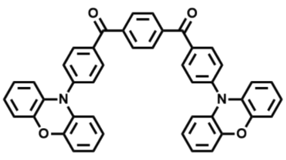
Corresponding Authors: chizhg@mail.sysu.edu.cn, ceszy@mail.sysu.edu.cn, zhaoj95@mail.sysu.edu.cn

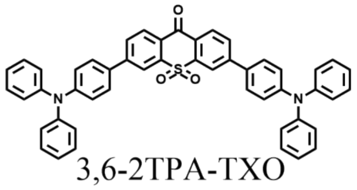
Table S1. Summary of device performance of yellow TADF-based OLEDs reported in the literature.

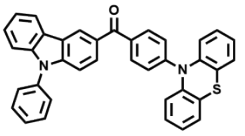
Yellow TADF emitter	λ_{EL} [a] (nm)	L [b] (cd m^{-2})	CE [b] (cd A^{-1})	PE [b] (lm W^{-1})	EQE [b] (%)	EQE [c] (%)	RO [d] (%)	Ref.
OPDPO	560	32590	73.1	38.2	26.7	21.8	18	This work
p-Px2BBP	548	57120	20.1	/	6.9	/	/	1
3,6-2TPA-TXO	551	20000	82.7	78.9	24.3	3.7	75	2
4CzPNPh	560	~30000	63.3	53.7	22.5	20.9	8	3
TXO-TPA	552	/	43.3	47.4	18.5	~ 6.0	68	4
DBT-BZ-PTZ	539	~ 10000	46.0	43.3	15.1	9.7	36	5
DBT-BZ-PTZ	563	~ 24000	26.5	29.1	9.7	8.5	13	5
CP-BP-PTZ	542	32250	62.4	57.3	19.6	13.6	31	6
CP-BP-PTZ	554	46820	46.1	55.7	15.3	12.7	17	6
Py56	562	~ 10000	96.3	105.5	29.2	20.6	30	7
CzSOXO	550	8466	43.1	/	13.6	8.8	35	8
PXZDSO2	560	17000	49.3	38.5	16.7	13.7	18	9
b3	574	~ 30000	/	/	9.0	~ 6.2	31	10
TPXZ-*as*-TAZ	560	11270	34.8	31.2	13.0	11.5	12	11
tri-PXZ-TRZ	550	/	/	/	13.3	/	/	12
TA-3Cz	546	23145	39.0	40.8	11.8	~ 6.0	50	13

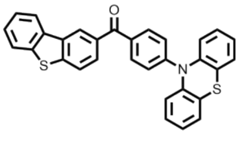
Abbreviations: L, Luminance; CE, current efficiency; PE, power efficiency; EQE, external quantum efficiency; RO, efficiency roll-off; Ref, reference.

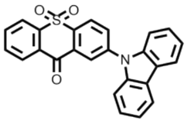
[a] EL peak wavelength. [b] Measured at maximum value. [c] Measured at a luminance of 1000 cd m^{-2}. [d] RO = EQE roll-off from maximum value to that at 1000 cd m^{-2}.

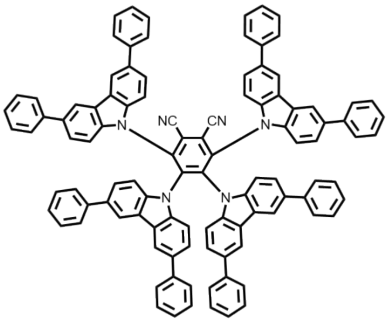

p-Px2BBP


3,6-2TPA-TXO

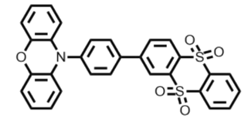

CP-BP-PTZ

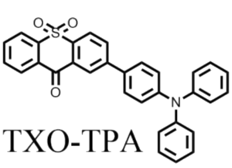

DBT-BZ-PTZ

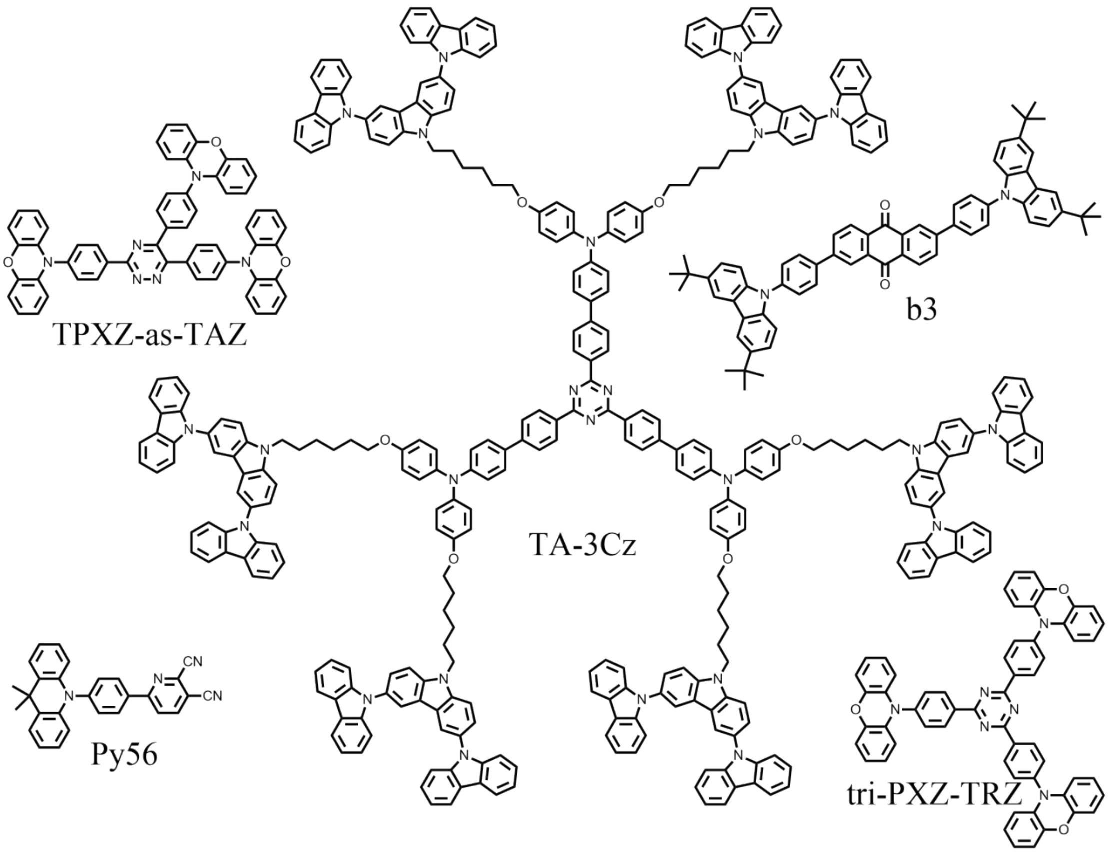

CzSOXO



4CzPNPh


PXZDSO2


TXO-TPA


TPXZ-as-TAZ

b3

TA-3Cz

Py56

tri-PXZ-TRZ

Figure S1. Chemical structures of previous yellow TADF emitter materials listed in Table S1.

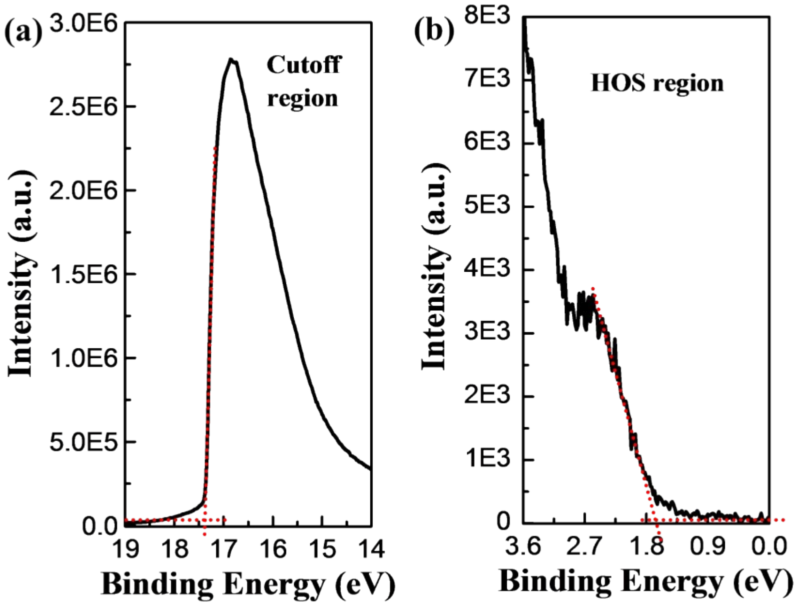


Figure S2. Ultraviolet photoelectron spectroscopy spectra of OPDPO in (a) the cutoff region and (b) the highest-occupied states (HOS) region. The dotted red lines in (a) and (b) determine two energy points of 17.37 eV and 1.65 eV for OPDPO, and thus the HOMO of OPDPO can be determined by subtracting the energy separation by 21.22 eV and calculated to be 21.22 − (17.37 − 1.65) = 5.5 (eV).

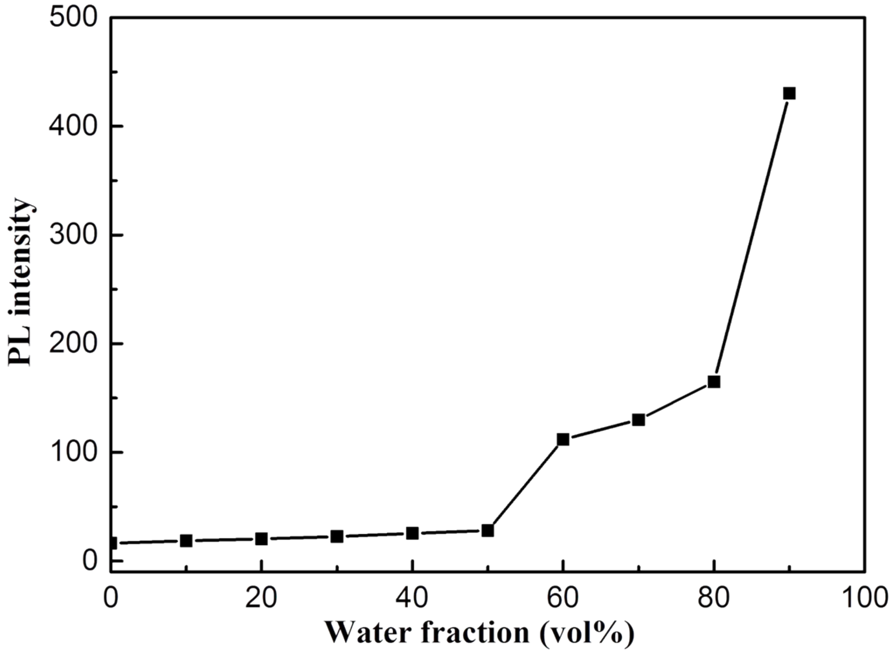


Figure S3. PL intensity of 2CzTPEPCz versus the water fraction in THF/water mixture.

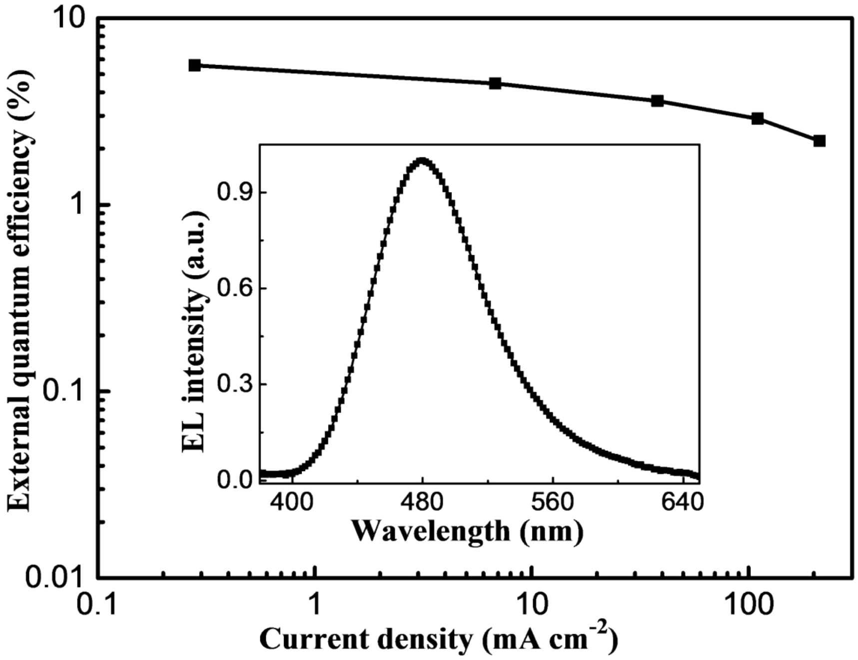
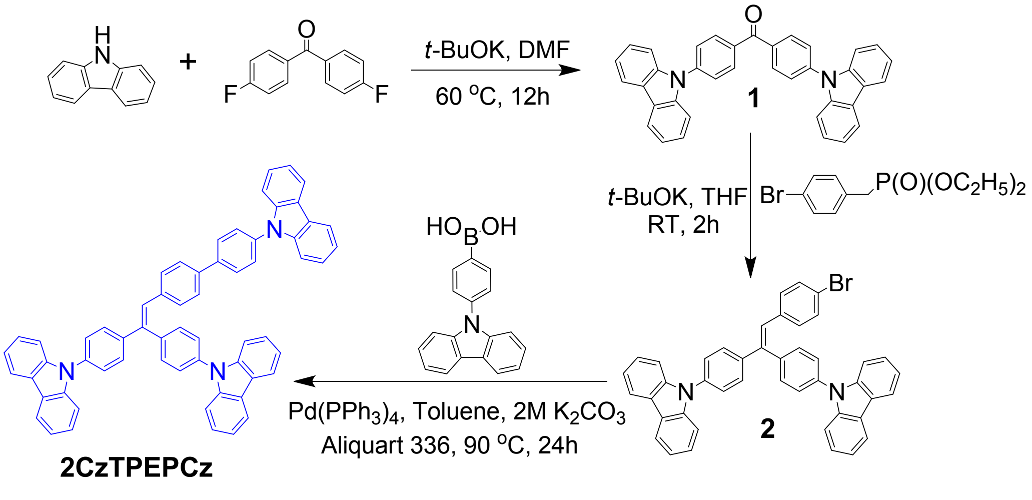


Figure S4. EQE–luminance curves of device B1 with a device configuration as: ITO/PEDOT:PSS(40 nm)/CBP(20 nm)/2CzTPEPCz (15 nm)/TPBI(40 nm)/Mg:Ag. Inset: the normalized EL intensity of device B1.

Synthesis of 2CzTPEPCz

Scheme S1 shows the synthetic route for **2CzTPEPCz**, wherein compound **1** and compound **2** were synthesized according to our previous procedures.[3]



Scheme S1. Synthetic route for 2CzTPEPCz.

A 2.0 M aqueous K_2CO_3 solution (3.0 mL) was added to a toluene solution (20 mL) containing compound **2** (1.33 g, 2.0 mmol) and [4-(9H-carbazol-9-yl)phenyl]boronic acid (0.58 g, 2.0 mmol) and stirred for 30 mins under an argon atmosphere. Then,

$Pd(PPh_3)_4$ catalyst (0.05 g) was added to the reaction mixture and stirred at 90 ℃ for 24 h. After cooling down to room temperature, the product was extracted with dichloromethane/water. The organic layers were collected, dried over Na_2SO_4, concentrated using a rotary evaporator and purified by silica gel column chromatography (dichloromethane/n-hexane, gradient elution from 1:5 to 1:1 v/v) to yield 1.39 g white powder (84% yield). ^{1}H NMR (500 MHz, DMSO-d_6) δ = 8.26 (dd, J = 12.4, 5.1, 6H), 7.97 (d, J = 8.3, 2H), 7.78 (t, J = 7.3, 4H), 7.71 (dd, J = 16.5, 8.1, 6H), 7.62 (d, J = 8.1, 2H), 7.56 – 7.40 (m, 13H), 7.37 – 7.26 (m, 8H). ^{13}C NMR (125 MHz, deuterated chloroform ($CDCl_3$)) δ = 141.87, 141.38, 140.86, 140.79, 140.76, 139.51, 139.21, 138.89, 137.37, 137.29, 137.05, 136.56, 132.09, 130.36, 129.04, 128.97, 128.29, 127.45, 127.40, 126.89, 126.83, 126.06, 123.60, 123.56, 123.50, 120.50, 120.43, 120.40, 120.19, 120.15, 120.07, 110.04, 109.91, 109.86, 109.83. HRMS, *m/z*: $[M]^+$ 827.3291; calcd. for $C_{62}H_{41}N_3$, 827.3295. Anal. Calcd. for $C_{62}H_{41}N_3$: C 89.93%, H 4.99%, N 5.07%; found: C 89.90%, H 5.01%, N 5.03%.

REFERENCES

(1) Lee, S. Y.; Yasuda, T.; Yang, Y. S.; Zhang, Q. S.; Adachi, C. Luminous Butterflies: Efficient Exciton Harvesting by Benzophenone Derivatives for Full-Color Delayed Fluorescence OLEDs. *Angew. Chem. Int. Ed.* **2014**, *53*, 6402–6406.

(2) Li, Y. C.; Li, X.-L.; Chen, D. J.; Cai, X. Y.; Xie, G. Z.; He, Z. Z.; Wu, Y.-C.; Lien, A.; Cao, Y.; Su, S.-J. Design Strategy of Blue and Yellow Thermally Activated Delayed Fluorescence Emitters and Their All-Fluorescence White OLEDs with External Quantum Efficiency beyond 20%. *Adv. Funct. Mater.* **2016**, *26*, 6904–6912.

(3) Li, J.; Ding, D. X.; Tao, Y. T.; Wei, Y. Y.; Chen, R. F.; Xie, L. H.; Huang, W.; Xu, H. A Significantly Twisted Spirocyclic Phosphine Oxide as a Universal Host for High-Efficiency Full-Color Thermally Activated Delayed Fluorescence Diodes. *Adv. Mater.* **2016**, *28*, 3122–3130.

(4) Wang, H.; Xie, L. S.; Peng, Q.; Meng, L. Q.; Wang, Y.; Yi, Y. P.; Wang, P. F. Novel Thermally Activated Delayed Fluorescence Materials-Thioxanthone Derivatives and Their Applications for Highly Efficient OLEDs. *Adv. Mater.* **2014**, *26*, 5198–5204.

(5) Guo, J. J.; Li, X.-L.; Nie, H.; Luo, W.; Hu, R.; Qin, A.; Zhao, Z.; Su, S.-J.; Tang, B. Z. Robust Luminescent Materials with Prominent Aggregation-Induced Emission and

Thermally Activated Delayed Fluorescence for High-Performance Organic Light-Emitting Diodes. *Chem. Mater*. **2017**, *29*, 3623–3631.

(6) Huang, J.; Nie, H.; Zeng, J. J.; Zhuang, Z. Y.; Gan, S. F.; Cai, Y. J.; Guo, J. J.; Su, S.-J.; Tang, B. Z. Highly Efficient Nondoped OLEDs with Negligible Efficiency Roll-Off Fabricated from Aggregation-Induced Delayed Fluorescence Luminogens. *Angew. Chem. Int. Ed*. **2017**, *56*, 12971–12976.

(7) Pan, K. C.; Li, S.-W.; Ho, Y.-Y.; Shiu, Y.-J.; Tsai, W.-L.; Jiao, M.; Lee, W.-K.; Wu, C.-C.; Chung, C.-L.; Chatterjee, T.; et al. Efficient and Tunable Thermally Activated Delayed Fluorescence Emitters Having Orientation-Adjustable CN-Substituted Pyridine and Pyrimidine Acceptor Units. *Adv. Funct. Mater*. **2016**, *26*, 7560–7571.

(8) Wang, Z. H.; Li, Y. C.; Cai, X. Y.; Chen, D. C.; Xie, G. Z.; Liu, K. K.; Wu, Y.-C.; Lo, C.-C.; Lien, A.; Cao, Y.; et al. Structure-Performance Investigation of Thioxanthone Derivatives for Developing Color Tunable Highly Efficient Thermally Activated Delayed Fluorescence Emitters. *ACS Appl. Mater. Interfaces*. **2016**, *8*, 8627–8636.

(9) Xie, G. Z.; Li, X. L.;, Chen, D. J.; Wang, Z. H.; Cai, X. Y.; Chen, D. C.; Li. C. Y.; Su, S.-J. Evaporation-and Solution-Process-Feasible Highly Efficient Thianthrene-9,9’,10,10’-Tetraoxide-Based Thermally Activated Delayed Fluorescence Emitters with Reduced Efficiency Roll-Off. *Adv. Mater*. **2016**, *28*, 181–187.

(10) Zhang, Q. S.; Kuwabara, H.; Potscavage Jr, W. J.; Huang, S. P.; Hatae, Y.; Shibata, T.; Adachi, C. Anthraquinone-Based Intramolecular Charge-Transfer Compounds: Computational Molecular Design, Thermally Activated Delayed Fluorescence, and Highly Efficient Red Electroluminescence. *J. Am. Chem. Soc*. **2014**, *136*, 18070–18081.

(11) Xiang, Y. P.; Gong, S. L.; Zhao, Y. B.; Yin, X. J.; Luo, J. J.; Wu, K. L.; Lu, Z.-H.; Yang, C. L. Asymmetric-triazine-cored Triads As Thermally Activated Delayed Fluorescence Emitters for High-Efficiency Yellow OLEDs with Slow Efficiency Roll-Off. *J. Mater. Chem. C*, **2016**, *4*, 9998–10004.

(12) Tanaka, H.; Shizu, K.; Nakanotani, H.; Adachi, C. Twisted Intramolecular Charge Transfer State for Long-Wavelength Thermally Activated Delayed Fluorescence. *Chem. Mater*. **2013**, *25*, 3766–3771.

(13) Sun, K. Y.; Sun, Y. B.; Huang, T. Y.; Luo, J. R.; Jiang, W.; Sun, Y. M. Design Strategy of Yellow Thermally Activated Delayed Fluorescent Dendrimers and Their Highly Efficient Non-doped Solution-Processed OLEDs with Low Driving Voltage. *Org. Electron*. **2017**, *42*, 123–130.

(14) Yang, Z.; Chi, Z.; Yu, T.; Zhang, X.; Chen, M.; Xu, B.; Liu, S.; Zhang, Y.; Xu, J. Triphenylethylene Carbazole Derivatives as a New Class of AIE Materials with Strong Blue Light Emission and High Glass Transition Temperature. *J. Mater. Chem*. **2009**, *19*, 5541-5546.