Support Information

Molecular dipole interfacial engineering for high-performance quantum-dot light-emitting diodes

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Keywords: Quantum dot light-emitting diodes; self-assembled monolayers; Dipole interlayer; Carrier injection; Molecular arrangement.

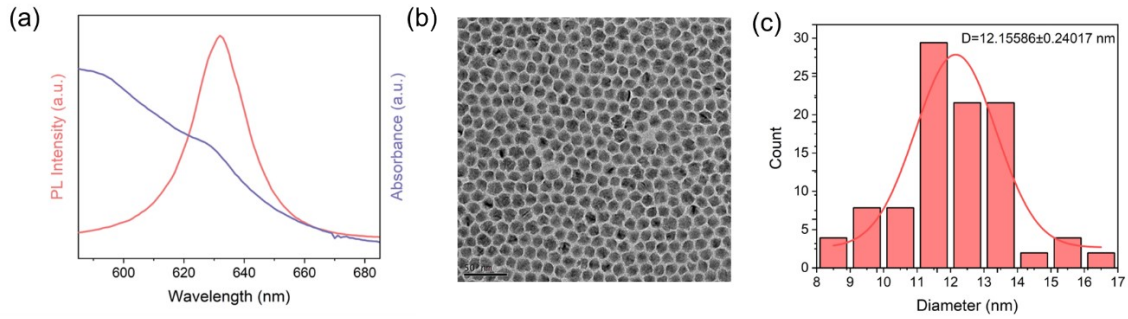

Figure S1 (a) PL and absorption spectra of red CdSe@CdS QDs. (b)TEM images and (c) particle diameter distribution of QDs.

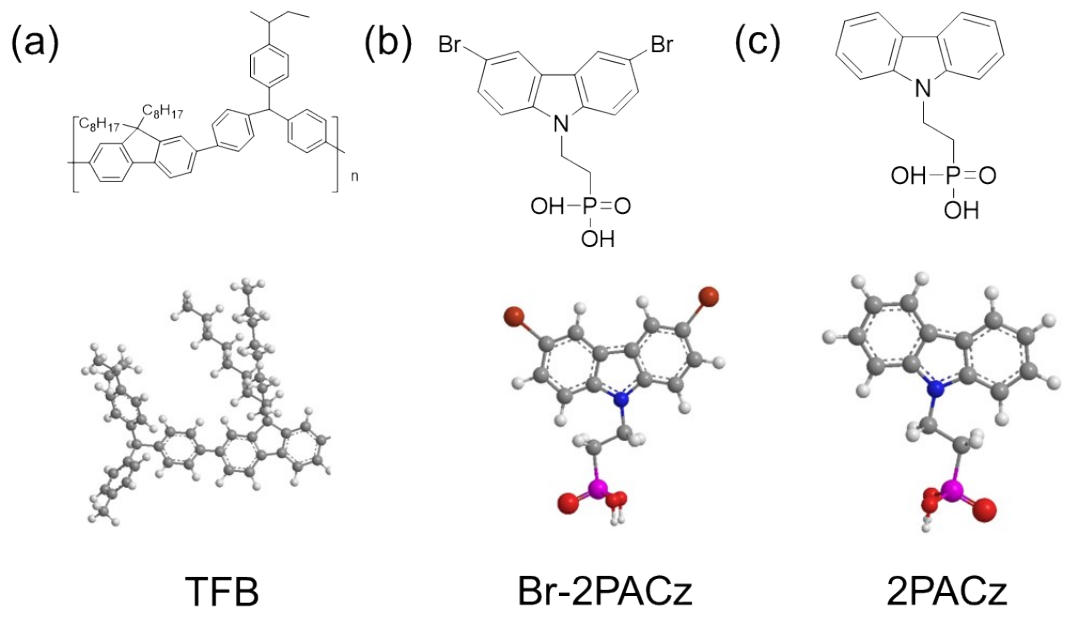

Figure S2 Chemical Structure and molecular model of (a) TFB, (b) Br-2PACz and (c) 2PACz.

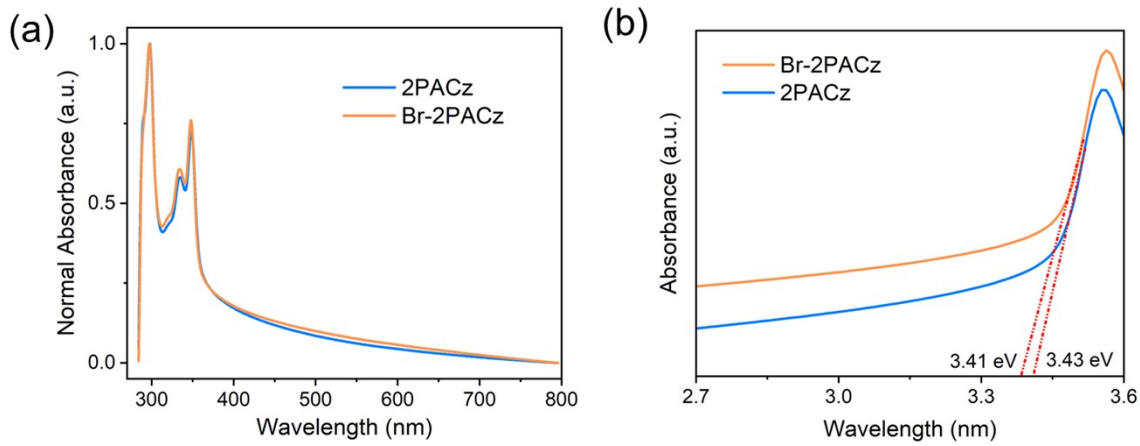

Figure S3 (a) Absorption spectra of the 2PACz and Br-2PACz films. (b) UPS results of 2PACz and Br-2PACz films.

Ultraviolet photoelectron spectroscopy (UPS) and optical bandgap were measured to calculate the highest occupied molecular orbitals (HOMO) level and the lowest unoccupied molecular orbital (LUMO) levels. The valence band region (E_{onset}) and the secondary photoelectron cutoff (E_{cutoff}) are obtained from the UPS results. The HOMO level is calculated by the following formula: HOMO=21.22-$|E_{cutoff}-E_{onset}|$. The LUMO is defined as the energy difference between the HOMO levels and the optical bandgap.

Calculated material HOMO and LUMO by UPS data.

For Br-2PACz:

VBM=21.22-$|E_{cutoff}-E_{onset}|$

=21.22-16.38+0.79

=5.63 eV

CBM=5.63-3.41=2.22 eV

For 2PACz:

VBM=21.22-$|E_{cutoff}-E_{onset}|$

=21.22-17.02+1.15

=5.35 eV

CBM=5.35-3.43=1.92 eV

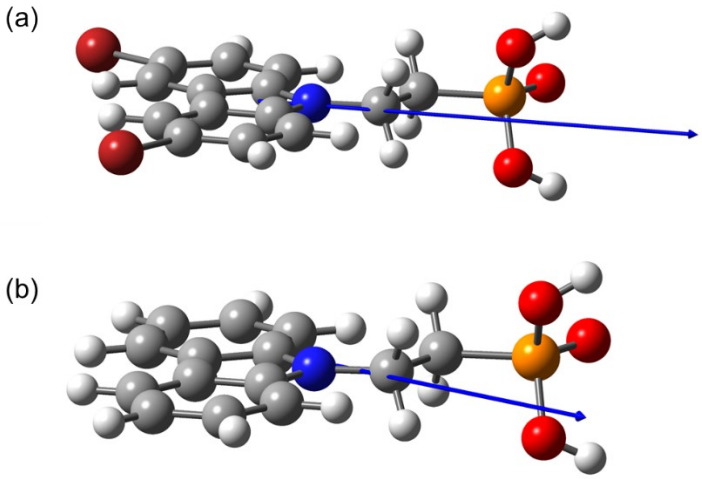

Figure S4 Br-2PACz and 2PACz dipole moment direction.

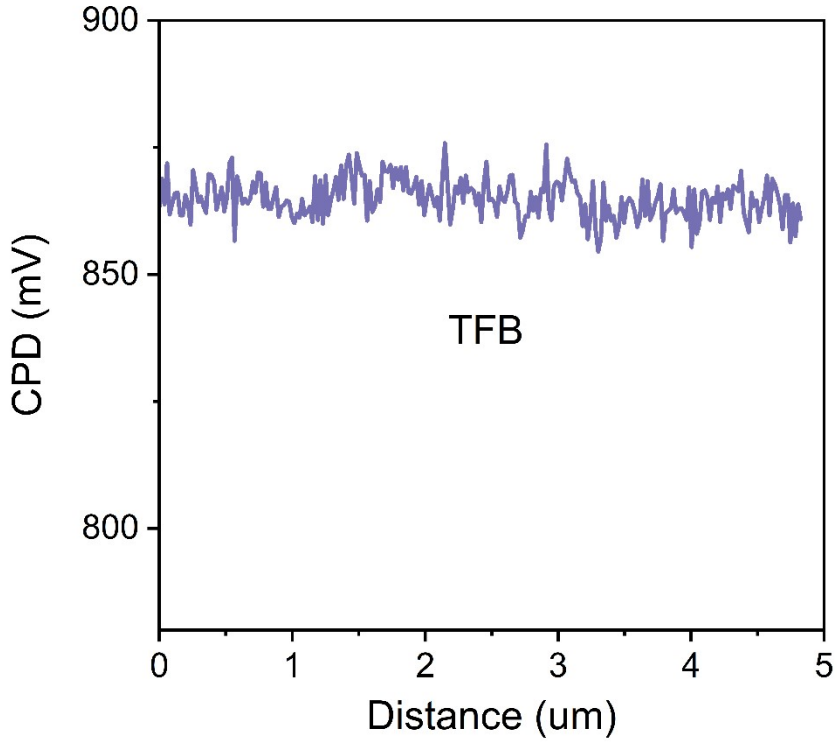

Figure S5 Contact potential differences (CPD) of TFB film

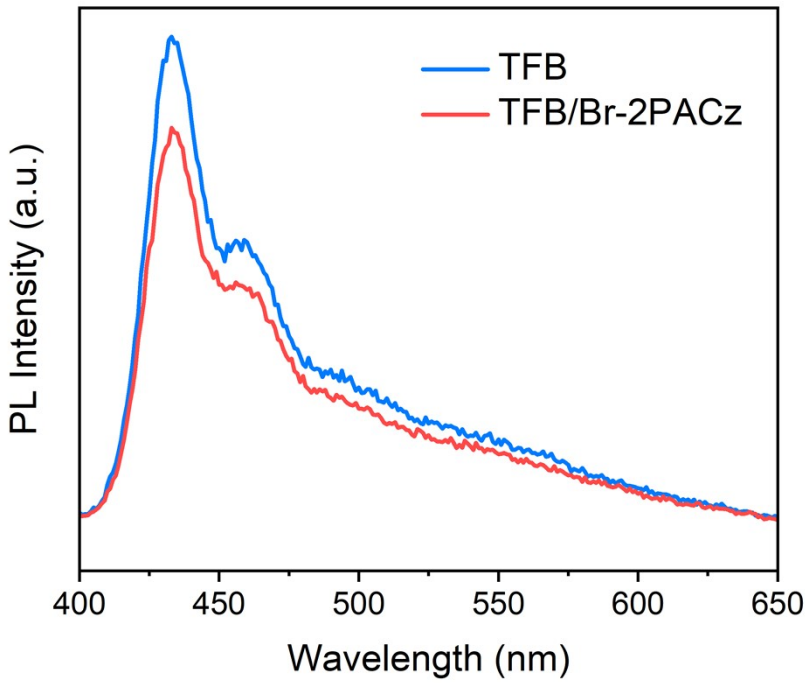

Figure S6 PL spectra of TFB and TFB/Br-2PACz films.

Table S1 Fitting results of PL decay curves.

sample	T_1(ns)	T_2(ns)	A_1	A_2	$\chi 2$	τ_{avg}(ns)
TFB	7.94	18.71	2794	2421	1.153	15.17
TFB/Br-2PACz	8.80	23.18	2826	1671	1.155	17.56

The PL decay curve can be fitted by the tri-exponential function:

$$decay\ (t) = \sum_{n=1}^{2} A_n e^{-t/T_n}$$

where t is time, A_1 and A_2 are constants, and T_1 and T_2 represent the interaction between excitons and phonons, the decay lifetimes corresponding to the intrinsic exciton relaxation, and the interaction between excitons and defects, respectively. The average lifetime (T_{ave}) can be calculated as:

$$T_{ave} = \frac{\sum_{n=1}^{2} A_n T_n^2}{\sum_{n=1}^{2} A_n T_n}$$

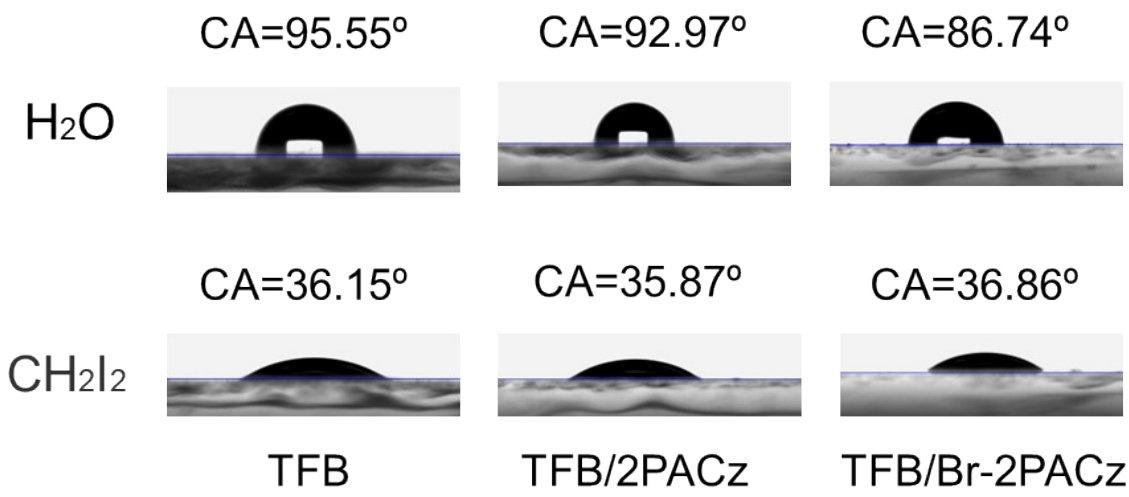

Figure S7 The contact angle of TFB, TFB/2PACz and TFB/Br-2PACz

The contact angle of the material is measured using water and diiodomethane as non-polar solvents. The following formula calculates the surface tension of different components:

Water: London dispersion (γ^d)=51, polar (γ^p)=21.8,γ_L=72.8.

Diiodomethane: London dispersion (γ^d)=0, polar (γ^p)=50.8, γ_L=50.8.

$$\gamma_{water}(1+cos\theta_{water}) = \frac{4\gamma_{water}^{d}\gamma^{d}}{\gamma_{water}^{d}+\gamma^{d}} + \frac{4\gamma_{water}^{p}\gamma^{p}}{\gamma_{water}^{p}+\gamma^{p}}$$

$$\gamma_{EG}(1+cos\theta_{EG}) = \frac{4\gamma_{Diiodomethane}^{d}\gamma^{d}}{\gamma_{Diiodomethane}^{d}+\gamma^{d}} + \frac{4\gamma_{Diiodomethane}^{p}\gamma^{p}}{\gamma_{Diiodomethane}^{p}+\gamma^{p}}$$

$$\gamma = \gamma^{d} + \gamma^{p}$$

Table S2 Detailed parameters of TFB, TFB/2PACz and TFB/Br-2PACz films

Surface	Contact angle θH_2O [º]	Contact angle θCH_2I_2 [º]	γ^d [mN m^{-1}]	γ^p [mN m^{-1}]	Surface tension [mN m^{-1}]
TFB	95.55	36.15	42.48	0.12	42.6
TFB/2PACz	92.97	35.87	41.89	0.36	42.25
TFB/Br-2PACz	86.74	36.86	39.53	1.63	41.16

The values in the table are the average values calculated for 5 samples

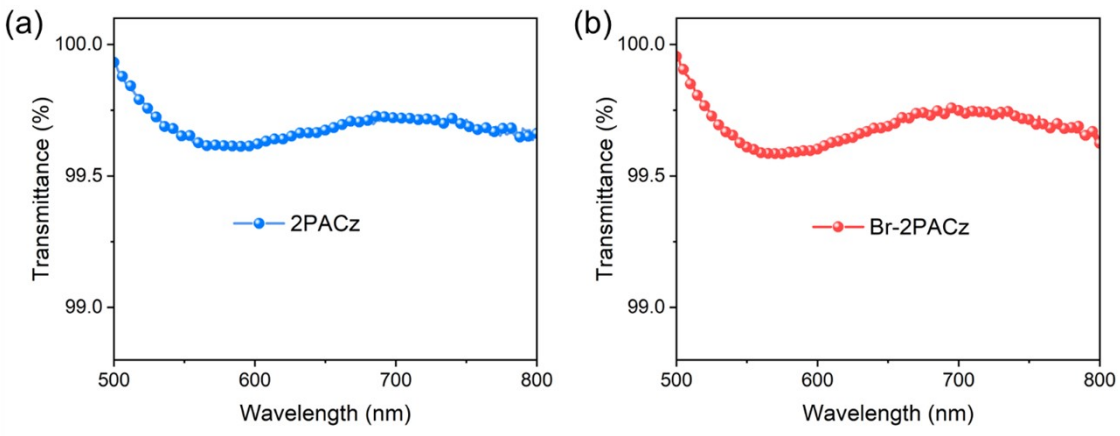

Figure S8 Transmittance spectra of (a) 2PACz and (b) Br-2PACz films.

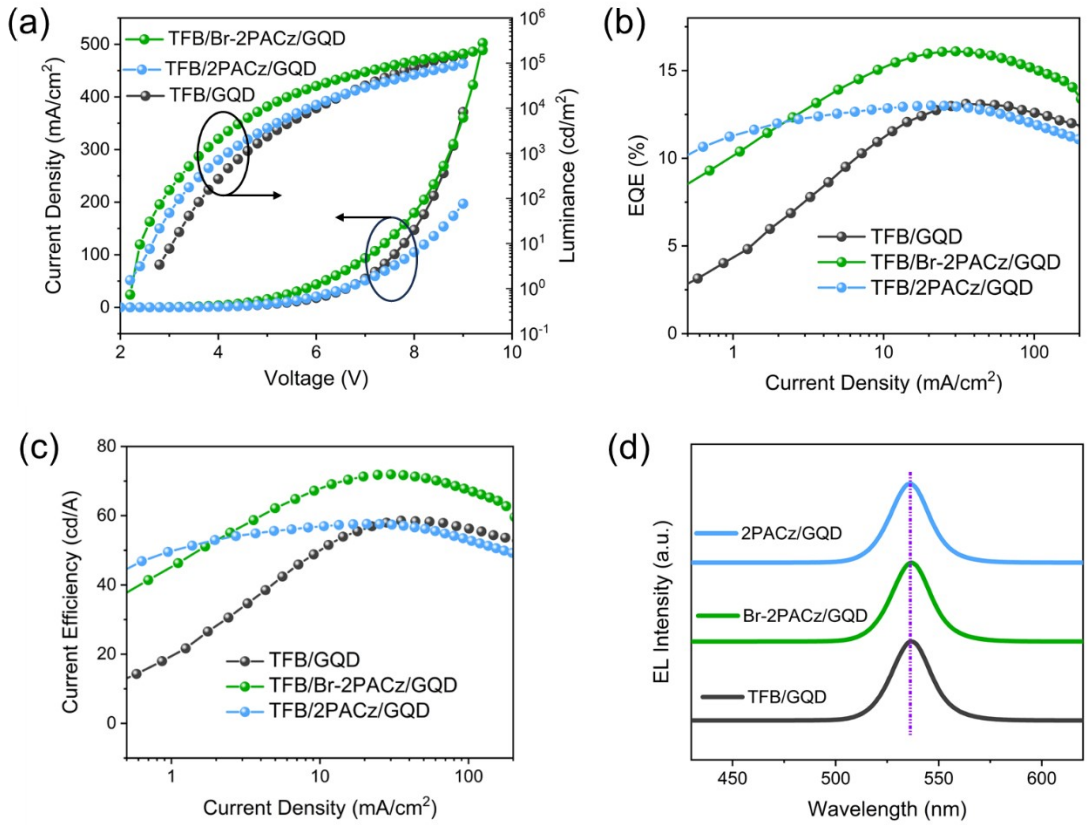

Figure S9 A series of device performance of (a-d) G-QLEDs.

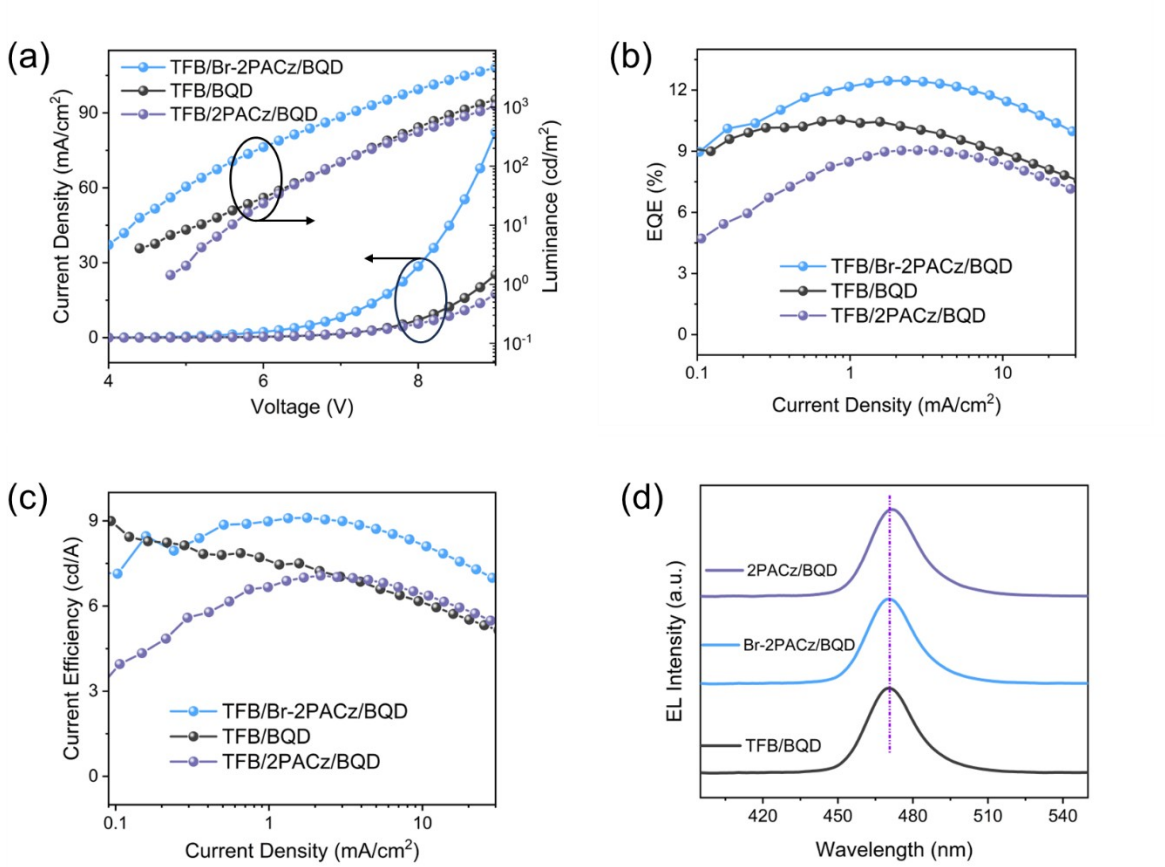

Figure S10 A series of device performance of (a-d) B-QLEDs.

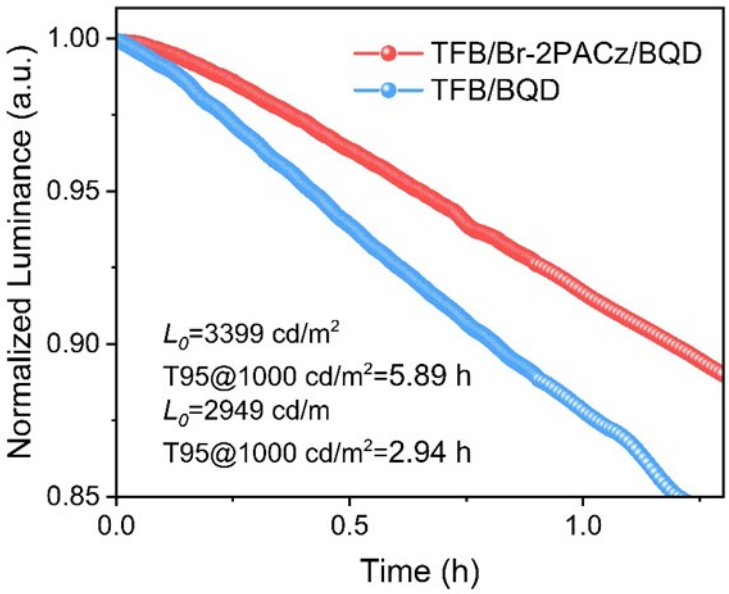

Figure S11 The lifetime of standard and optimized B-QLEDs.

Table S3 Relevant parameters of red/green/blue QLED

	HTL	EQE [%]	CE [cd A^{-1}]	Lmax [cd m^{-2}] @7V	Turn-on Voltage [V]
R-QLED	TFB	20.58	20.60	206001.50	2
	TFB/2PACz	20.52	18.29	237424.73	2
	TFB/Br-2PACz	25.03	24.66	274887.88	1.8
G-QLED	TFB	13.1	58.55	31823.658	2.6
	TFB/2PACz	13.0	57.64	28724.99	2.2
	TFB/Br-2PACz	16.11	71.91	63495.08	2.2
B-QLED	TFB	10.55	7.86	118.03	4.0
	TFB/2PACz	9.04	7.02	118.06	4.6
	TFB/Br-2PACz	12.46	9.1	687.68	3.6