

Fusing the acridine and benzofuran/benzothiophene as novel hybrid donor for high-performance and low efficiency roll-off TADF OLEDs

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Transient PL characteristics, fabrication and performance measurement for DPEPO-hosted devices were the same as the reports.¹⁻³ Apart from the above experiment, the computational details and measurement instruments so on were cited by our previous work.⁴⁻⁶

The evaluation of exciton dynamic rate constants was calculated by equation S1-S7:

$$k_{PF} = \frac{\phi_{PF}}{\tau_P} \quad \text{Equation S1}$$

$$k_{DF} = \frac{\phi_{DF}}{\tau_D} \quad \text{Equation S2}$$

$$k_{ISC} = \frac{\phi_{DF}}{\phi_{PF} + \phi_{DF}} k_{PF} \quad \text{Equation S3}$$

$$k_{RISC} = \frac{k_{DF} k_{PF} \phi_{DF}}{k_{ISC} \phi_{PF}} \quad \text{Equation S4}$$

$$k_{PF} = k_r^S + k_{nr}^S + k_{ISC} \quad \text{Equation S5}$$

$$\phi_{PF} = \frac{k_r^S}{k_r^S + k_{nr}^S + k_{ISC}} = \frac{k_r^S}{k_{PF}} \quad \text{Equation S6}$$

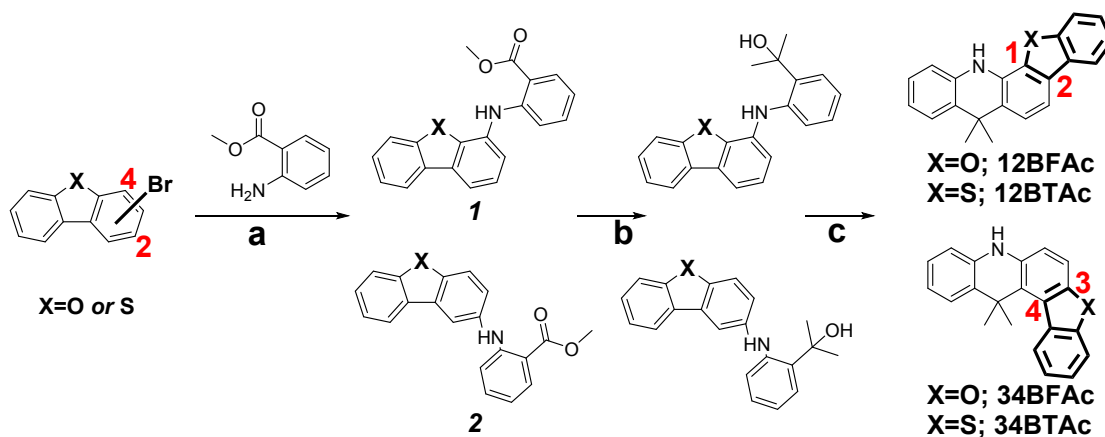
$$\phi_{ISC} = \frac{k_{ISC}}{k_r^S + k_{nr}^S + k_{ISC}} = \frac{k_{ISC}}{k_{PF}} \quad \text{Equation S7}$$

Table S1 The detail kinetic parameters

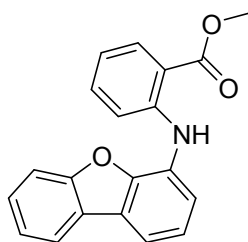
Emitters	ϕ_{PL}^a (%)	$\phi_{\text{P}}/\phi_{\text{D}}^b$ (%)	$\tau_{\text{p}}/\tau_{\text{d}}^c$ (ns)/(μs)	k_{PF}^d (10^7 s^{-1})	k_{DF}^d (10^5 s^{-1})	k_{ISC}^d (10^7 s^{-1})	k_{RISC}^d (10^5 s^{-1})	$k_{\text{r}}^{\text{S},d}$ (10^7 s^{-1})	$k_{\text{nr}}^{\text{S},d}$ (10^6 s^{-1})	Φ_{ISC}^d (%)
12BFAc-PM	65	53/16	11/6.4	4.8	0.3	1.1	0.3	2.5	11.3	24
12BTAc-PM	87	29/58	8/3.8	3.6	1.5	2.4	4.7	1.0	1.5	67
34BFAc-PM	95	55/40	21/3.5	2.6	1.1	1.1	1.9	1.5	0.8	42
34BTAc-PM	92	56/36	25/3.4	2.3	1.0	0.9	1.7	1.3	1.1	39

^a Absolute PL quantum yield measured with integrating spheres, ^b According to the prompt and delayed components in transient delay curves.; ^c Fitted transient PL curve of prompt and decay components; ^d Calculated using equations S1-S7; ^e Data from Figure 3b;

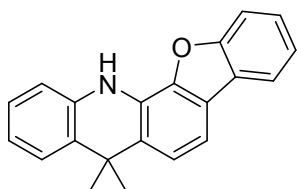
We selected the following routes. As shown in Scheme S1, the alcohol type intermediate **1** were prepared according to the reports.^{2, 7} Differently, the intermediate **2** were synthesized referencing from the other reports.⁸ Subsequently, according to our previous reports, alcohol type intermediates were synthesized using Grignard reaction and further were readily converted into novel Ac-benzofuran/benzothiophene hybrid donors (**12BFAc**, **12BTAc**, **34BFAc** and **34BTAc**) with the refluxed reaction of hydrochloric acid and glacial acetic acid.⁹



Scheme 1 (a) **1**: Pd(OAc)₂, Xantphos, Cs₂CO₃, N₂, refluxed 24 h; **2**: Pd(OAc)₂, P(t-Bu)₃, Cs₂CO₃, Toluene, N₂, refluxed, 24 h; (b) CH₃ClMg, dry tetrahydrofuran (THF), N₂, room temperature, overnight; (c) AcOH, HCl, refluxed 12 h;

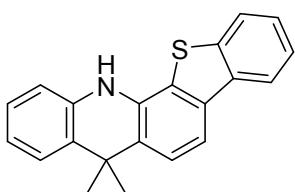


^1H NMR (600 MHz, DMSO- d_6) δ = 9.74 (s, 1H), 8.24 – 8.09 (m, 1H), 7.97 (dd, J =8.1, 1.7, 1H), 7.90 (d, J =7.6, 1H), 7.74 (d, J =8.2, 1H), 7.54 (td, J =8.1, 2.4, 2H), 7.47 – 7.37 (m, 3H), 7.17 (d, J =8.5, 1H), 6.92 – 6.82 (m, 1H), 3.91 (s, 3H).



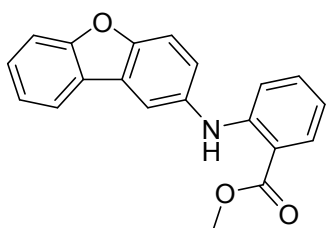
12BFac

^1H NMR (600 MHz, DMSO- d_6) δ = 9.28 (s, 1H), 8.11 – 8.02 (m, 1H), 7.72 (d, J =8.2, 1H), 7.56 – 7.47 (m, 2H), 7.40 (dd, J =8.0, 2.9, 3H), 7.20 (dd, J =8.0, 1.3, 1H), 7.10 (dd, J =8.2, 6.9, 1H), 6.87 (t, J =7.4, 1H), 1.59 (s, 6H).

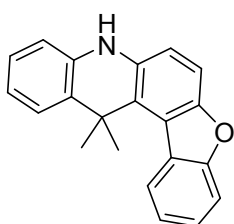


12BTac

^1H NMR (600 MHz, DMSO- d_6) δ = 8.71 (s, 1H), 8.30 – 8.24 (m, 1H), 8.10 – 8.04 (m, 1H), 7.85 – 7.79 (m, 1H), 7.56 (d, J =8.2, 1H), 7.51 (td, J =6.4, 5.6, 3.5, 2H), 7.43 (d, J =7.8, 1H), 7.23 (dd, J =8.0, 1.3, 1H), 7.15 – 7.09 (m, 1H), 6.89 (t, J =7.4, 1H), 1.61 (s, 6H).

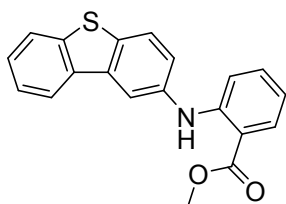


^1H NMR (600 MHz, DMSO- d_6) δ = 9.42 (s, 1H), 8.37 – 7.98 (m, 2H), 8.02 – 7.84 (m, 1H), 7.70 (t, J =8.7, 2H), 7.63 – 7.28 (m, 4H), 7.10 (d, J =8.9, 1H), 6.77 (t, J =7.7, 1H), 3.87 (s, 3H).

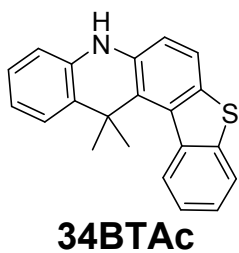


34BFac

^1H NMR (600 MHz, DMSO- d_6) δ 8.81 (s, 1H), 8.16 (dd, J = 8.1, 1.2 Hz, 1H), 7.69 (dd, J = 8.2, 1.1 Hz, 1H), 7.52 (t, J = 1.1 Hz, 1H), 7.46 (dd, J = 8.4, 6.7 Hz, 2H), 7.38 (dd, J = 7.8, 1.4 Hz, 1H), 7.02 (t, J = 1.1 Hz, 1H), 6.97 (d, J = 8.7 Hz, 1H), 6.77 (d, J = 1.3 Hz, 1H), 6.68 (dd, J = 8.0, 1.3 Hz, 1H), 1.95 (s, 6H).



^1H NMR (600 MHz, DMSO- d_6) δ = 9.46 (s, 1H), 8.37 – 8.26 (m, 1H), 8.22 (d, J =2.1, 1H), 7.97 (t, J =8.1, 2H), 7.89 (dd, J =8.0, 1.7, 1H), 7.53 – 7.33 (m, 4H), 7.24 – 7.17 (m, 1H), 6.85 – 6.72 (m, 1H), 3.85 (s, 3H).



^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 8.89 (s, 1H), 8.43 (d, $J = 8.5$ Hz, 1H), 8.03 (dd, $J = 7.9, 1.3$ Hz, 1H), 7.74 (d, $J = 8.5$ Hz, 1H), 7.55 (ddd, $J = 8.5, 6.6, 1.4$ Hz, 1H), 7.49 (t, $J = 7.4$ Hz, 1H), 7.37 (d, $J = 7.7$ Hz, 1H), 7.02 (dt, $J = 7.9, 3.3$ Hz, 2H), 6.81 – 6.74 (m, 1H), 6.69 (dd, $J = 7.9, 1.2$ Hz, 1H), 2.04 (s, 6H).

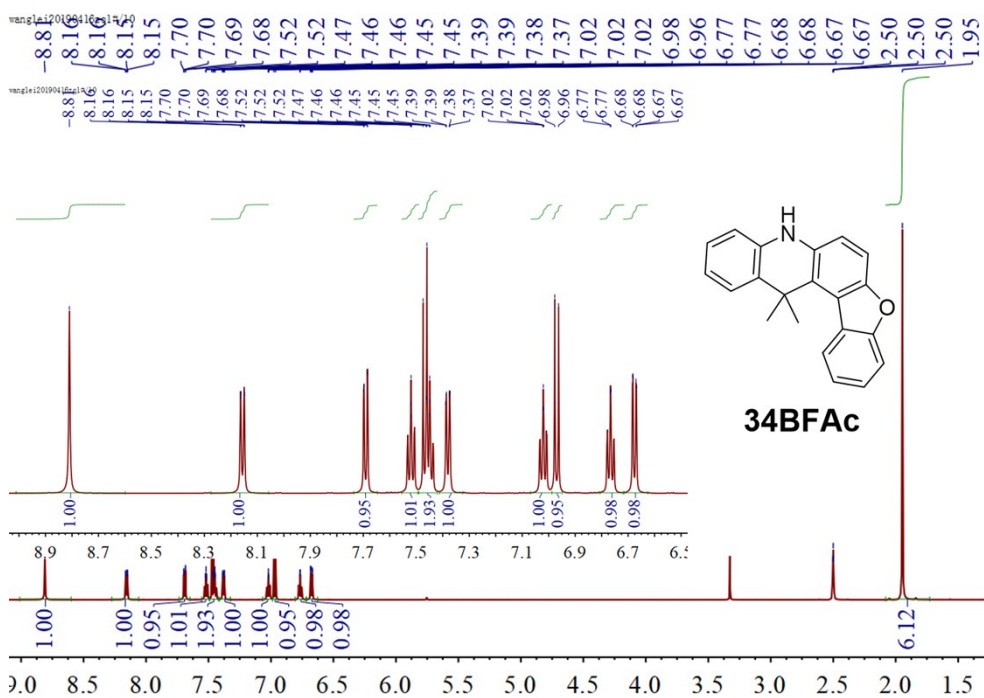


Fig. S1 ^1H NMR spectrum of 34BFAC

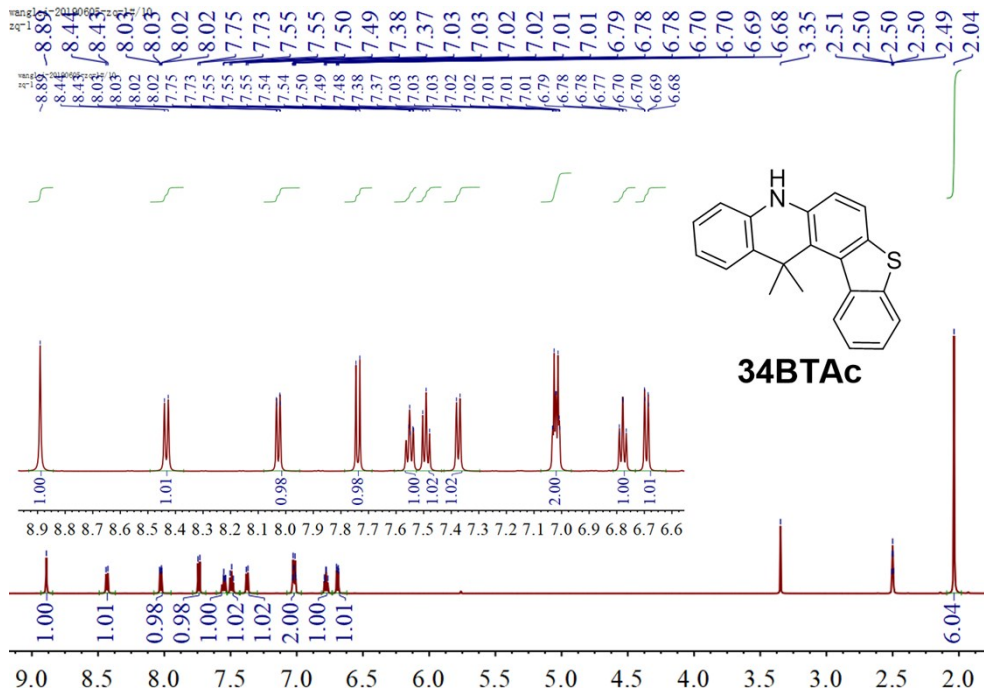
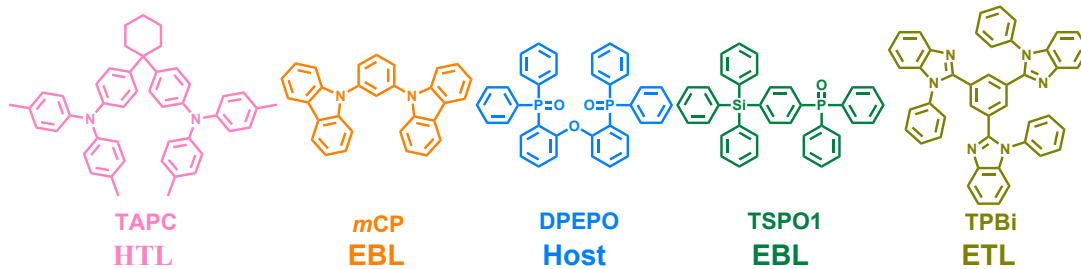


Fig. S2 ¹H NMR spectrum of 34BTAc

The description for the full name and function of the material in device fabrication was provided as follows:

TAPC: 1,1-bis[4-[*N,N*-di(*p*-tolyl)-amino]phenyl]-cyclohexane; TPBi: 1,3,5-tris(1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzene; *m*CP: 1,3-di(9*H*-carbazol-9-yl)benzene; TSP01: diphenyl(4-(triphenylsilyl)phenyl)phosphine oxide; DPEPO:(oxybis(2,1-phenylene))bis(diphenylphosphine oxide).

PEDOT: PSS and LiF acted as hole- and electron-injecting layers, respectively.



Scheme S2 The molecular structure and function of the material in device fabrication (HTL: hole-transporting layers; EBL: exciton blocking layer; ETL: electron-transporting layers.)

The TTA mode simulation can be described as follow:^{10, 11}

$$\frac{\eta_{ext}^{TT}(J)}{\eta_0} = \frac{J_0}{4J} \left(\sqrt{1 + 8\frac{J}{J_0}} - 1 \right)$$

where η , η_0 , and J_0 represent the EQE in the presence of TTA, initial EQE in the absence of TTA (at very low current densities, rendering the TTA quenching negligible), and the current density at the half-maximum of the EQE, respectively.

Moreover, the SPA model, which can be expressed by Equation:^{10, 11}

$$\frac{\eta_{ext}^{SP}(J)}{\eta_0} = \frac{1}{1 + \left(\frac{J}{J_0}\right)^{l+1}}$$

Where η_{ext}^{SP} is the EQE in the presence of SPA and l is the fitting parameter.

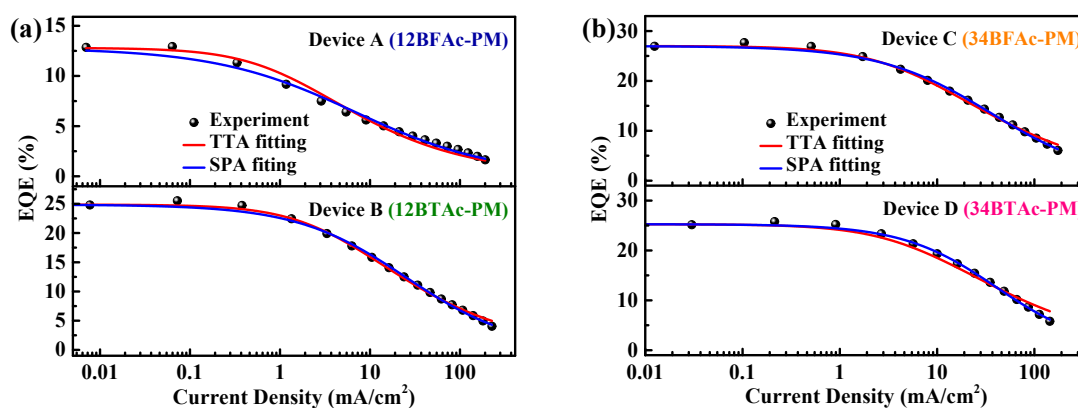


Fig. S3 The external quantum efficiency (EQE) as a function of current density and the fitting results according to TTA and SPA.

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