

Electronic Supplementary Information

Tert-butyl-substituted bicarbazole as bipolar host material for efficient green and yellow PhOLEDs

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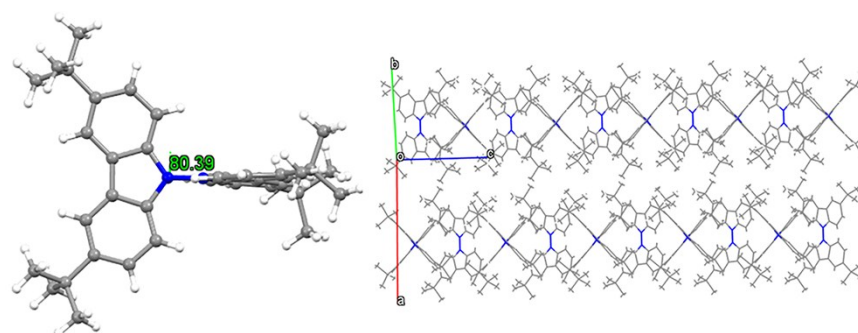
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Table S1 Crystal data of compound **tcaz-tcaz**

| Identification code | tcaz-tcaz |
|--|---|
| Empirical formula | C ₄₀ H ₄₈ N ₂ |
| Formula weight | 556.80 |
| Temperature/K | 128.15 |
| Crystal system | orthorhombic |
| Space group | Pccn |
| a/Å | 21.0420(9) |
| b/Å | 15.9328(7) |
| c/Å | 10.1429(5) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90 |
| Volume/Å ³ | 3400.5(3) |
| Z | 4 |
| ρ _{calc} g/cm ³ | 1.088 |
| μ/mm ⁻¹ | 0.062 |
| F(000) | 1208.0 |
| Crystal size/mm ³ | 0.22 × 0.18 × 0.16 |
| Radiation | MoKα (λ = 0.71073) |
| Index ranges | -26 ≤ h ≤ 26, -19 ≤ k ≤ 19, -12 ≤ l ≤ 12 |
| Reflections collected | 28676 |
| Independent reflections | 3486 [R _{int} = 0.0616, R _{sigma} = 0.0338] |
| Data/restraints/parameters | 3486/57/228 |
| Goodness-of-fit on F ² | 1.038 |
| Final R indexes [I >= 2σ (I)] | R ₁ = 0.0516, wR ₂ = 0.1242 |
| Final R indexes [all data] | R ₁ = 0.0673, wR ₂ = 0.1343 |
| Largest diff. peak/hole/eÅ ⁻³ | 0.22/-0.18 |

**Fig. S1.** Crystal structure and molecular packing of **tcaz-tcaz**.

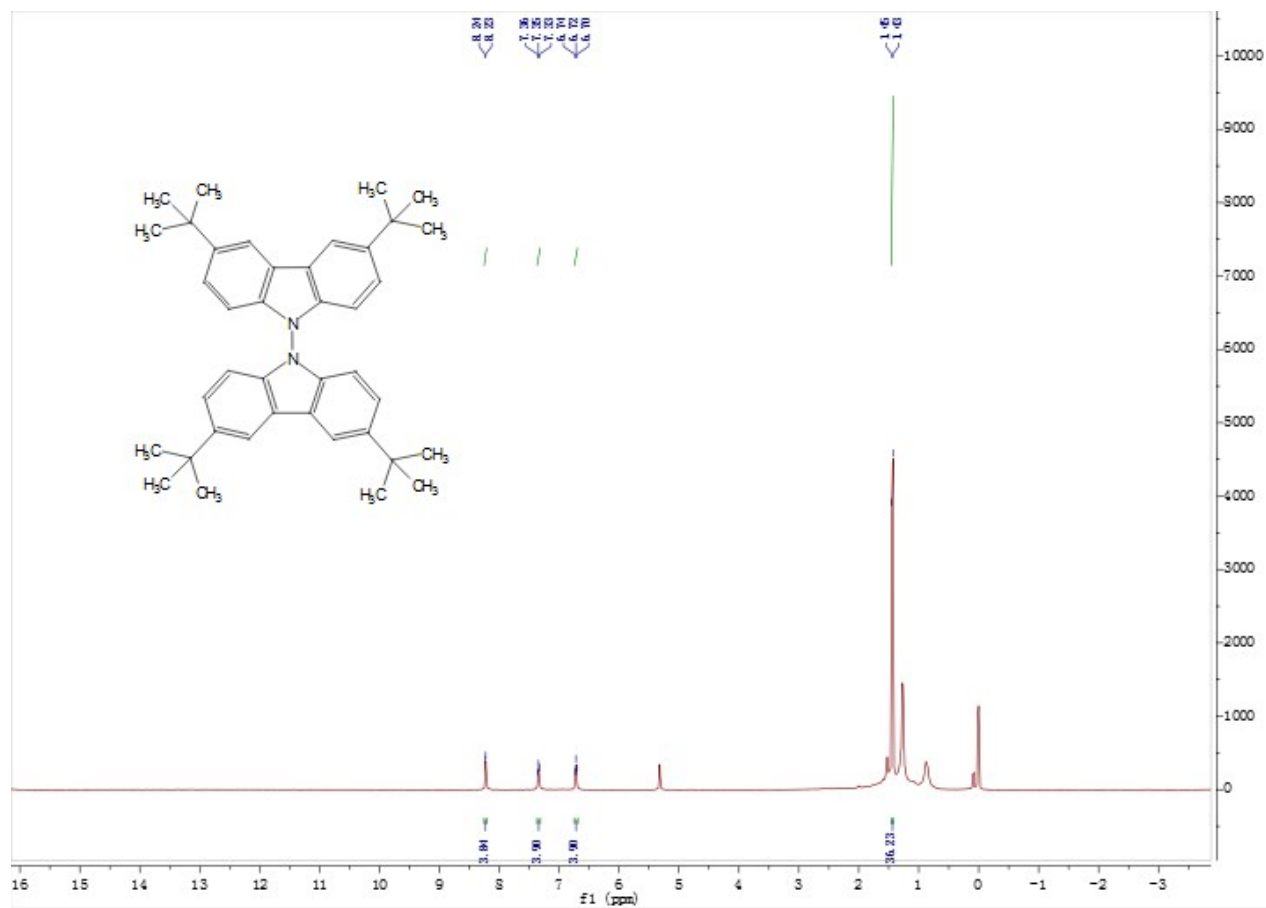


Fig. S2. ^1H NMR spectrum for tcaz-tcaz (400 MHz, dichloromethane- d_2).

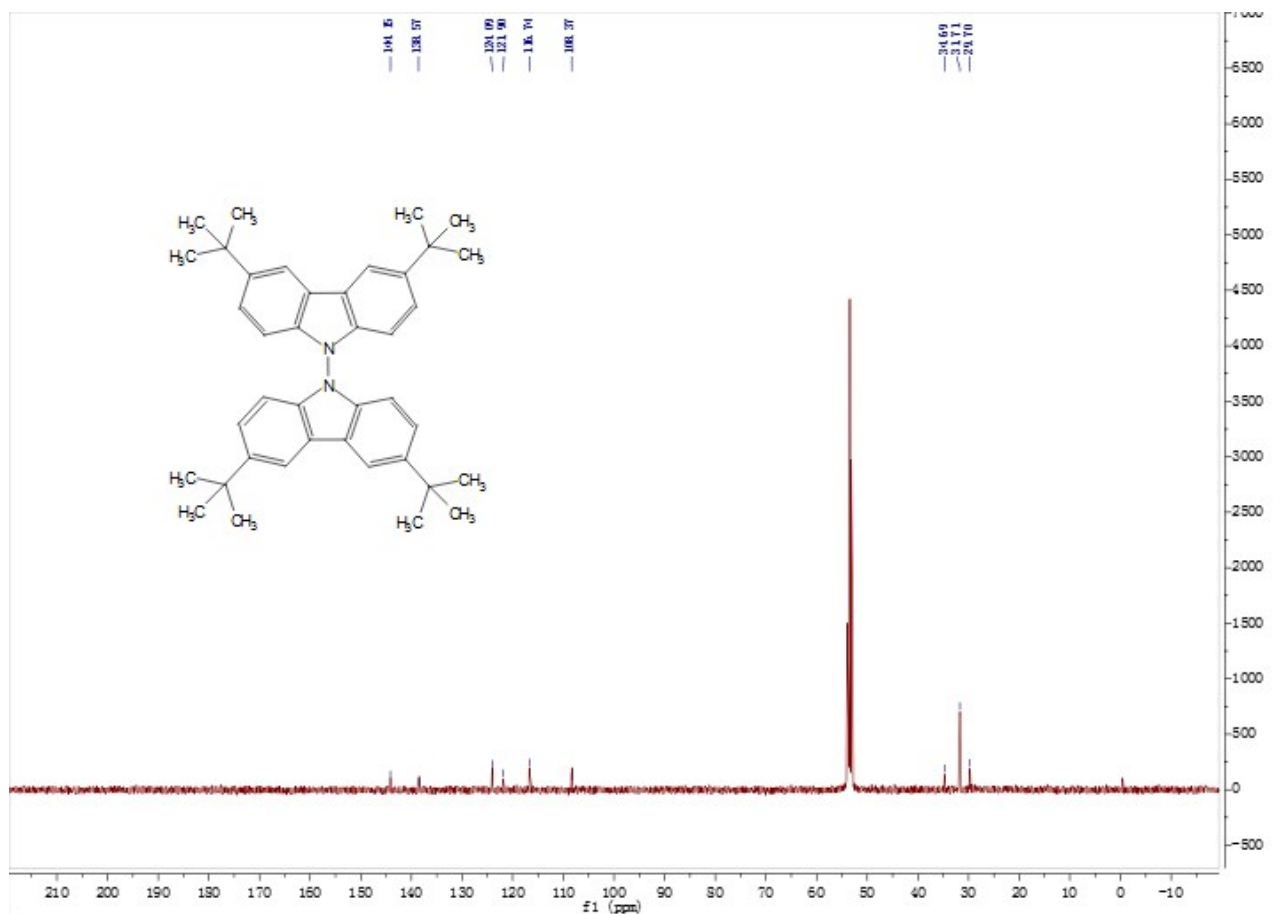


Fig. S3. ¹³C NMR spectrum for tcaz-tcaz (400 MHz, dichloromethane-d₂).

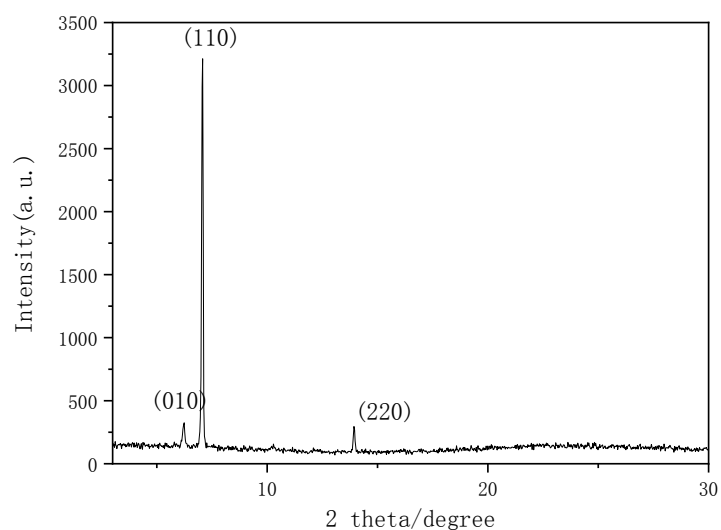


Fig. S4. XRD data of **tcaz-tcaz** crystal.

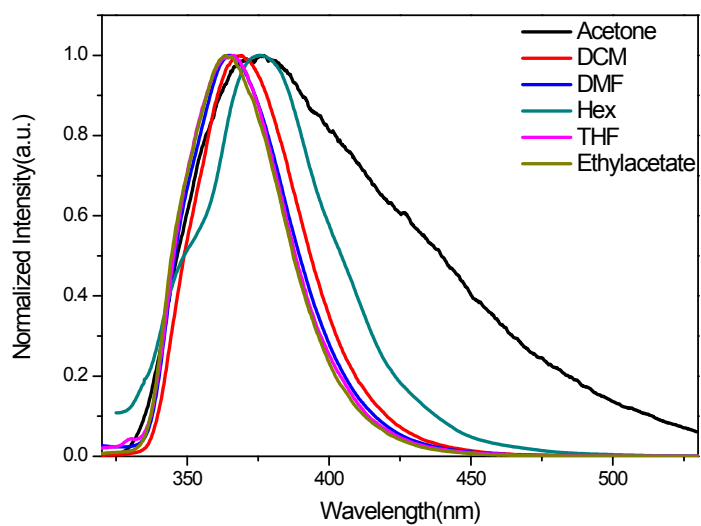


Fig. S5. PL Spectra of **tcaz-tcaz** in different solvents.

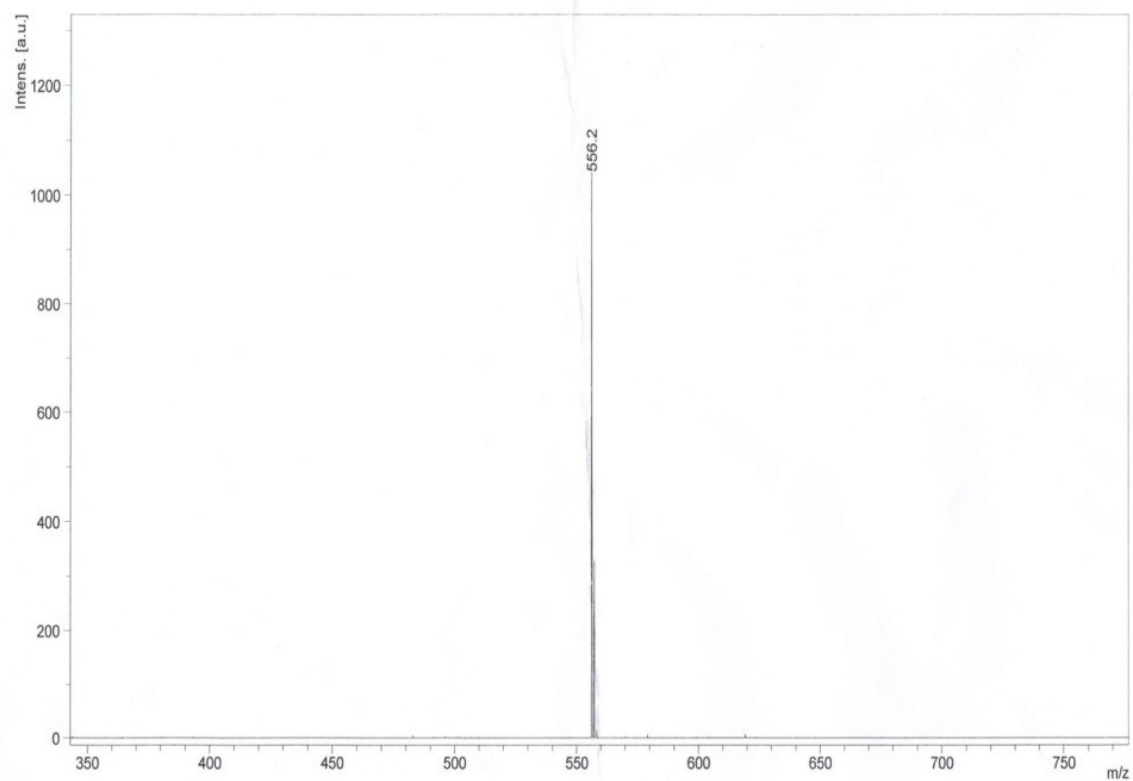


Fig. S6. MALDI-MS spectrum of **tcaz-tcaz**.

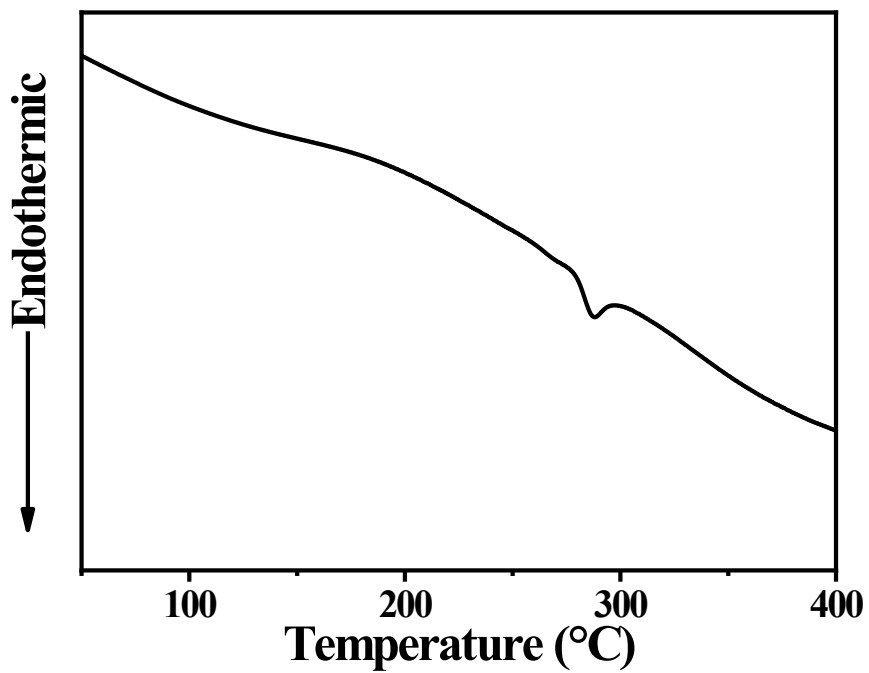


Fig. S7. The DSC curve of tcaz-tcaz.

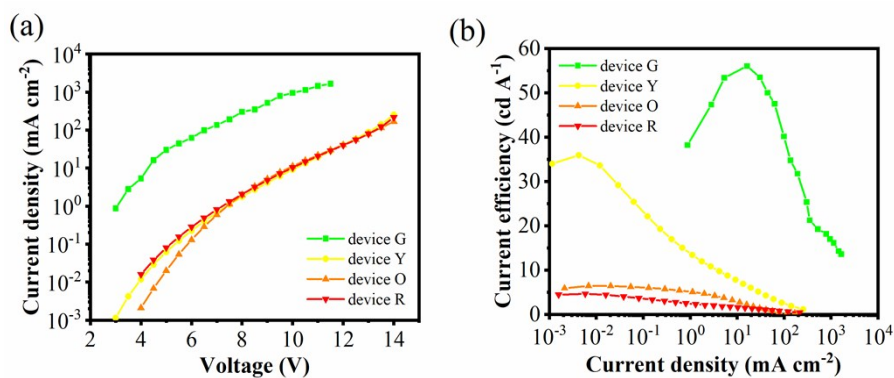


Fig. S8. (a) Current density *versus* voltage and (b) current efficiency *versus* current density characteristics of the devices.

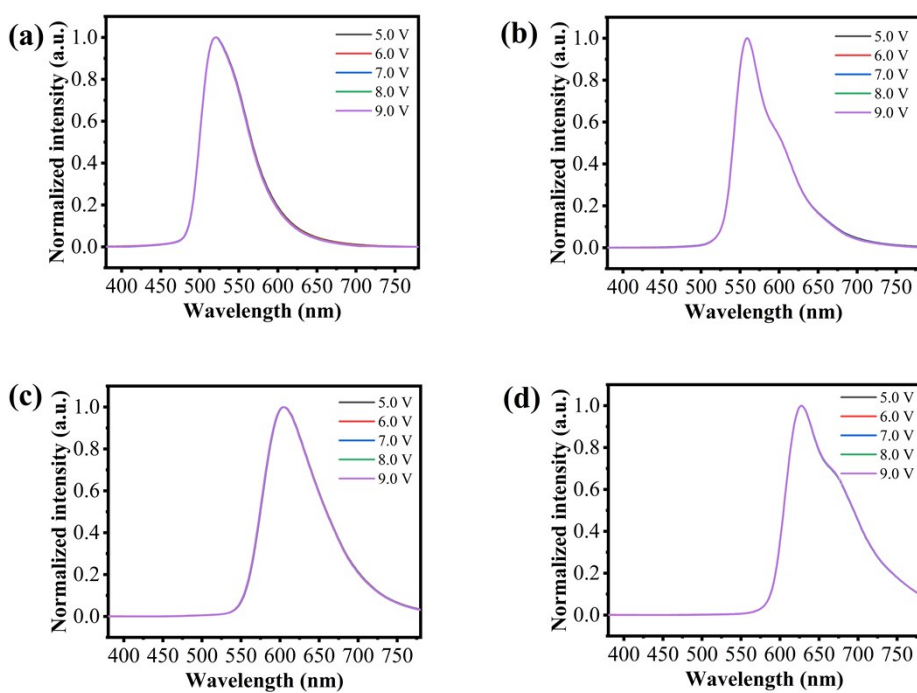


Fig. S9. EL spectra for the PhOLEDs with (a) green, (b) yellow, (c) orange and (d) red dopants at different driving voltages.

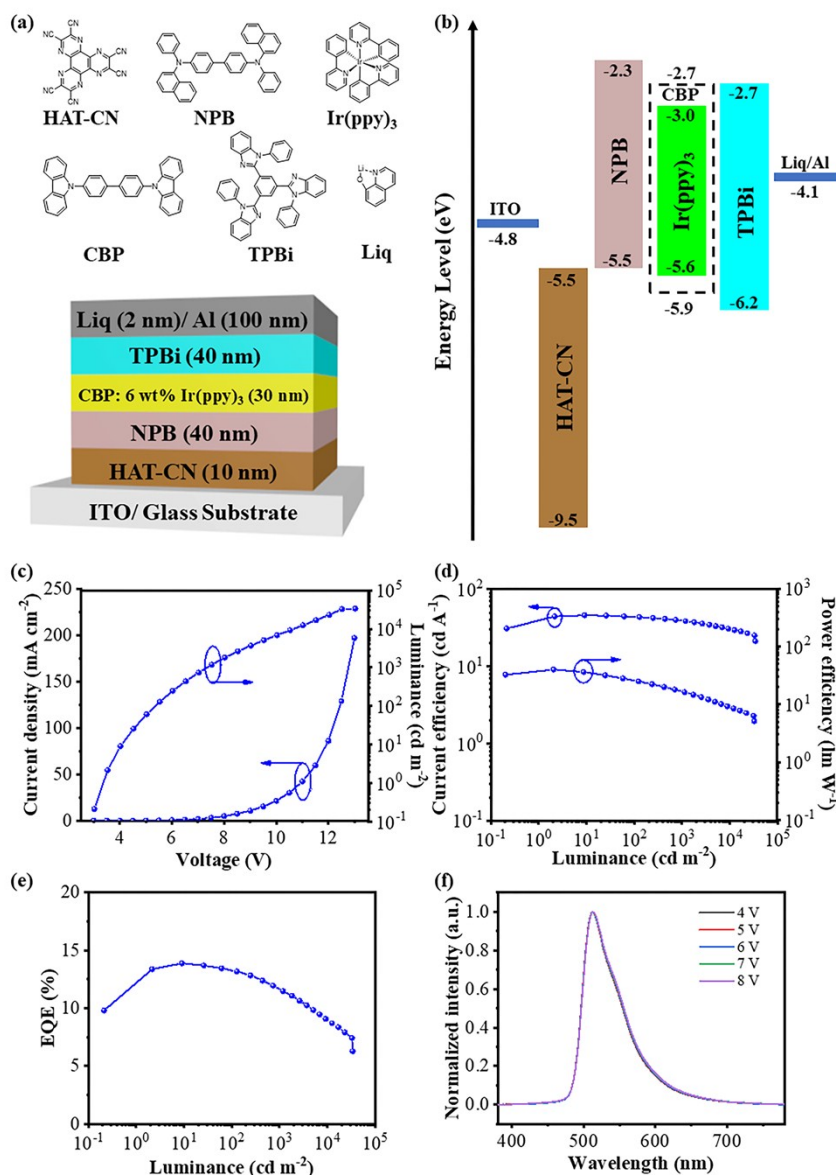


Fig. S10 (a-b) Schematic structure and chemical structures of the compounds used in the devices and energy level diagrams of the fabricated PhOLEDs. (c-e) Voltage *versus* luminance, power efficiency *versus* current density, and external quantum efficiency *versus* voltage characteristics and (f) EL spectra of the devices at different driving voltages.

Table S2 Summarised EL performance of the **CBP**-hosted device, compared with the **tcz-tcaz**-hosted device.

| Host | Dopant | V_{on}^a (V) | L_{max}^b (cd m ⁻²) | CE ^c (cd A ⁻¹) | PE ^d (lm W ⁻¹) | EQE _{max} ^e (%) | λ^f (nm) | CIE colour ^g |
|----------|----------------------|-------------------|--------------------------------------|--|--|--|---------------------|-------------------------|
| CBP | Ir(ppy) ₃ | 3.5 | 33880 | 45.4 | 36.2 | 13.7 | 512 | (0.28, 0.62) |
| tcz-tcaz | | 2.4 | 22460 | 56.1 | 40.0 | 15.5 | 522 | (0.30, 0.63) |

^a Turn-on voltage recorded at 1 cd m⁻². ^b Maximum luminance. ^c Maximum current efficiency. ^d Maximum power efficiency. ^e Maximum external quantum efficiency. ^f EL peak wavelength. ^g CIE refers to Commission International de l'Éclairage coordinates at 8 V.

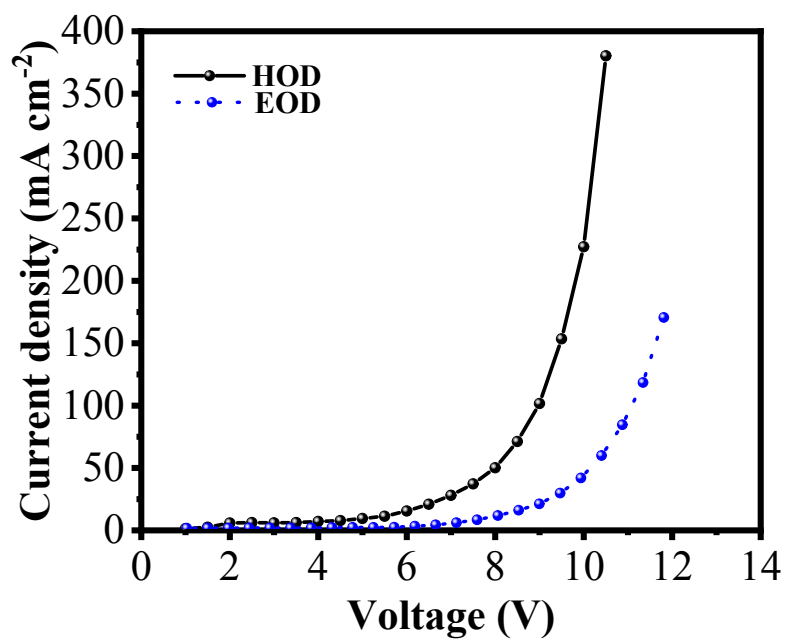


Fig. S11 Current density *versus* voltage characteristics of the HOD and EOD of **CBP**.