Supporting Information for:

Color-Tunable Delayed Fluorescence and Efficient Spin Orbit Charge Transfer Intersystem Crossing (SOCT-ISC) in Compact Carbazole-Anthracene-Bodipy Triads Employing Sequential Electron Transfer Approach

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1. General information

All the chemicals used in synthesis are analytical pure and were used as received. Solvents were dried and distilled before used for synthesis. $^1$H and $^{13}$C chemical shifts are reported in parts per million (ppm) relative to TMS, with the residual solvent peak used as an internal reference. $^1$H NMR spectra were recorded on a 400 MHz and 500 MHz Varian Unity Inova spectrometer (TMS as the standard of the chemical shifts). The mass spectra were measured by TOF MS MALDI and ESI spectrometer.

Triplet-Triplet Annihilation Upconversion

A continuous cw-laser (510 nm) was used as the excitation source for the upconversion. The upconversion quantum yield was determined using prompt fluorescence of IBDP (structure is shown in synthesis chart) ($\Phi_F = 2.7\%$ in MeCN) as standard.$^{[1,2]}$ The upconversion quantum yield was calculated with following equation (Eq 1), where $\Phi_{UC}$, $A_{sam}$, $I_{sam}$ and $\eta_{sam}$ represents the quantum yield, absorbance, integrated photoluminescence intensity and refractive index of samples. The equation is multiplied by a factor of 2 so as to set the maximum quantum yield to unity.

$$\Phi_{UC} = 2\Phi_{Std} \left(1 - 10^{-A_{sam}}\right) \left(\frac{I_{unk}}{I_{Std}}\right) \left(\frac{\eta_{unk}}{\eta_{Std}}\right)^2$$  
(Eq 1)
2. Synthesis and Molecular structure characterization data

Compounds 2 and 3 were prepared according to literature method.\(^3\) Compound 2: \(^1\)H NMR (CDCl\(_3, 400\) MHz); \(\delta\) 11.48 (s, 1H), 8.87 (d, 2H, \(J = 8.0\) Hz), 8.65 (d, 2H, \(J = 12.0\) Hz), 7.71–7.64 (m, 4H). TOF El-MS (\([\text{C}_{13}\text{H}_9\text{BrO}]^+\)) Calcd: \(m/z = 283.9837\). Found: \(m/z = 283.9844\).

Compound 3: \(^1\)H NMR (CDCl\(_3, 400\) MHz); \(\delta\) 11.59 (s, 1H), 9.01 (d, 2H, \(J = 8.0\) Hz), 7.72–7.57 (m, 7H), 7.43–7.39 (m, 4H). TOF El-MS (\([\text{C}_2\text{H}_{14}\text{O}]^+\)) Calcd: \(m/z = 282.1045\). Found: \(m/z = 282.1053\).

Compounds 4, BDP-AN, and BDP-AN-PH were prepared following literature method.\(^4\)

Compound 4: \(^1\)H NMR (CDCl\(_3, 400\) MHz); \(\delta\) 8.60 (d, 2H, \(J = 8.0\) Hz), 7.96 (d, 2H, \(J = 8.0\) Hz), 7.65–7.61 (m, 2H), 7.49–7.45 (m, 2H), 5.90 (s, 2H), 2.63 (s, 6H), 0.65 (s, 6H). MALDI– HRMS (\([\text{C}_{27}\text{H}_{22}\text{BrF}_2\text{N}_2]^+\)) Calcd: \(m/z = 502.1027\). Found: \(m/z = 502.1049\). BDP-AN: \(^1\)H NMR (CDCl\(_3, 400\) MHz); \(\delta\) 8.58 (s, 1H), 8.04 (d, 2H, \(J = 8.0\) Hz), 7.91 (d, 2H, \(J = 8.0\) Hz), 7.51–7.41 (m, 4H), 5.90 (s, 2H), 2.63 (s, 6H), 0.65 (s, 6H). \(^1^3\)C NMR (100 MHz, CDCl\(_3\)); \(\delta\)155.8, 142.9, 138.9, 132.4, 131.3, 129.7, 128.3, 128.2, 126.9, 125.7, 121.1, 14.7, 13.3. MALDI– HRMS (\([\text{C}_{27}\text{H}_{22}\text{BF}_2\text{N}_2]^+\)) Calcd: \(m/z = 424.1922\). Found: \(m/z = 424.1948\). BDP-AN-PH: \(^1\)H NMR (CDCl\(_3, 400\) MHz); \(\delta\) 7.76 (d, 2H, \(J = 8.0\) Hz), 7.69–7.57 (m, 5H), 7.47–7.35 (m, 6H), 5.93 (s, 2H), 2.64 (s, 6H), 0.75 (s, 6H). MALDI– HRMS (\([\text{C}_{33}\text{H}_{27}\text{BF}_2\text{N}_2]^+\)) Calcd: \(m/z = 500.2235\). Found: \(m/z = 500.2217\).

Synthesis of Compound AN-C-CZ: Under N\(_2\) atmosphere, 9-bromoanthracene (52 mg, 0.20 mmol), 9-phenyl-9H-carbazol-3-ylboronic acid (92 mg, 0.32 mmol) and K\(_2\)CO\(_3\) (100 mg, 0.72
mmol) were dissolved in 25 mL mixture of PhCH₃/EtOH/H₂O (4/2/1, v/v). Then Pd(PPh₃)₄ (20 mg, 5 mol%) was added after complete deoxygenation of above reaction mixture with N₂ bubbling for 20 minutes and reaction mixture was allowed to reflux for 8 h under nitrogen atmosphere. After completion of reaction, the reaction mixture was cooled to room temperature, extracted with CH₂Cl₂ (30 mL), washed with water (2 × 100 mL) and dried over anhydrous sodium sulfate. After evaporation of solvent under reduced pressure, the crude product was further purified with column chromatography (Silica gel, CH₂Cl₂/petroleum ether, 1/1, v/v) to give white solid (65 mg, yield: 78 %). ¹H NMR (CDCl₃, 400 MHz); δ 8.53 (s, 1H), 8.21 (s, 1H), 8.10–8.06 (m, 3H), 7.76 (d, 2H, J = 12.0 Hz), 7.72–7.65 (m, 4H), 7.61 (d, 1H, J = 8.0 Hz) 7.53–7.43 (m, 6H), 7.35–7.29 (m, 3H). MALDI– HRMS ([C₃₂H₂₁N]⁺) Calcd: m/z = 419.1674. Found: m/z = 419.1695.
Figure S1. $^1$H NMR of compound 2 (400 MHz, CDCl$_3$), 25°C

Figure S2. TOF EI mass spectrum of compound 2
Figure S3. $^1$H NMR of compound 3 (400 MHz, CDCl$_3$), 25°C

Figure S4. TOF EI mass spectrum of compound 3
Figure S5. $^1$H NMR of compound 4 (400 MHz, CDCl$_3$), 25°C

Figure S6. MALDI HR mass spectrum of compound 4
Figure S7. $^1$H NMR of compound AN-C-CZ (400 MHz, CDCl$_3$), 25°C

Figure S8. MALDI HR mass spectrum of compound AN-C-CZ
Figure S9. $^1$H NMR of compound BDP-AN-PH (400 MHz, CDCl$_3$), 25°C

Figure S10. MALDI HR mass spectrum of compound BDP-AN-PH
Figure S11. $^1$H NMR of compound **BDP-AN** (400 MHz, CDCl$_3$), 25°C

Figure S12. $^{13}$C NMR of compound **BDP-AN** (100 MHz, CDCl$_3$), 25°C
Figure S13. MALDI HR mass spectrum of compound BDP-AN

Figure S14. $^1$H NMR of compound BDP-AN-N-CZ (400 MHz, CDCl$_3$), 25°C
Figure S15. $^{13}$C NMR of compound BDP-AN-N-CZ (100 MHz, CDCl$_3$), 25°C

Figure S16. MALDI HR mass spectrum of compound BDP-AN-N-CZ
Figure S17. $^1$H NMR of compound BDP-AN-C-CZ (400 MHz, CDCl$_3$), 25°C

Figure S18. MALDI HR mass spectrum of compound BDP-AN-C-CZ
Figure S19. $^{13}$C NMR of compound BDP-AN-C-CZ (100 MHz, CDCl$_3$), 25°C
3. Crystal data of Compounds

Table S1. Crystallographic data for BDP-AN-C-CZ, BDP-AN-N-CZ and BDP-AN

<table>
<thead>
<tr>
<th>Compound</th>
<th>BDP-AN-C-CZ</th>
<th>BDP-AN-N-CZ</th>
<th>BDP-AN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical formula</td>
<td>C$<em>{92}$H$</em>{74}$B$_2$Cl$_4$F$_4$N$_6$O</td>
<td>C$<em>{45}$H$</em>{34}$BF$_2$N$_3$</td>
<td>C$<em>{27}$H$</em>{23}$BF$_2$N$_2$</td>
</tr>
<tr>
<td>$M$ (g mol$^{-1}$)</td>
<td>1518.99</td>
<td>665.56</td>
<td>424.28</td>
</tr>
<tr>
<td>Crystal system</td>
<td>Triclinic</td>
<td>Triclinic</td>
<td>Monoclinic</td>
</tr>
<tr>
<td>Space group</td>
<td>$P-1$</td>
<td>$P-1$</td>
<td>$C2/c$</td>
</tr>
<tr>
<td>a (Å)</td>
<td>14.2619(8)</td>
<td>12.309(4)</td>
<td>14.7132(19)</td>
</tr>
<tr>
<td>b (Å)</td>
<td>14.8156(8)</td>
<td>12.652(4)</td>
<td>20.895(3)</td>
</tr>
<tr>
<td>c (Å)</td>
<td>18.7795(10)</td>
<td>12.944(5)</td>
<td>7.2659(9)</td>
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<tr>
<td>α (deg)</td>
<td>84.9880(10)</td>
<td>106.387(6)</td>
<td>90</td>
</tr>
<tr>
<td>β (deg)</td>
<td>86.2700(10)</td>
<td>109.432(6)</td>
<td>97.143(2)</td>
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<tr>
<td>γ (deg)</td>
<td>80.9230(10)</td>
<td>104.590(6)</td>
<td>90</td>
</tr>
<tr>
<td>V (Å$^3$)</td>
<td>3898.1(4)</td>
<td>1685.3(10)</td>
<td>2216.4(5)</td>
</tr>
<tr>
<td>Z</td>
<td>2</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>$D_{\text{calc}}$ (g·cm$^{-3}$)</td>
<td>1.294</td>
<td>1.312</td>
<td>1.271</td>
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<tr>
<td>F(000)</td>
<td>1580</td>
<td>696</td>
<td>888</td>
</tr>
<tr>
<td>$\mu$ (Mo–Kα) (mm$^{-1}$)</td>
<td>0.215</td>
<td>0.084</td>
<td>0.085</td>
</tr>
<tr>
<td>$\theta$ (deg)</td>
<td>2.16–27.53</td>
<td>1.82–25.00</td>
<td>1.70–28.34</td>
</tr>
<tr>
<td>Reflections collected</td>
<td>81347</td>
<td>8649</td>
<td>7034</td>
</tr>
<tr>
<td>Independent reflections</td>
<td>16233(8671)</td>
<td>5901(3376)</td>
<td>2710(1516)</td>
</tr>
<tr>
<td>Parameters</td>
<td>983</td>
<td>465</td>
<td>150</td>
</tr>
<tr>
<td>$R_{\text{int}}$</td>
<td>0.1803</td>
<td>0.0370</td>
<td>0.0219</td>
</tr>
<tr>
<td>Δ(ρ) (e Å$^{-3}$)</td>
<td>1.797 and -1.080</td>
<td>0.404 and -0.218</td>
<td>0.177 and -0.264</td>
</tr>
<tr>
<td>Goodness of fit</td>
<td>1.289</td>
<td>1.027</td>
<td>1.028</td>
</tr>
<tr>
<td>$R^a$</td>
<td>0.1185 (0.1995)$^b$</td>
<td>0.0740 (0.1307)$^b$</td>
<td>0.0524 (0.0946)$^b$</td>
</tr>
<tr>
<td>$wR_2^a$</td>
<td>0.3481 (0.3961)$^b$</td>
<td>0.2114 (0.2341)$^b$</td>
<td>0.1416 (0.1704)$^b$</td>
</tr>
</tbody>
</table>

* $R = \sum |F_o| - |F_c| / \sum |F_o|$, $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)]^{1/2}$; $|F_o| > 4\sigma (|F_o|)$. $^b$ Based on all data.
4. UV/Vis absorption spectra

Solvent-dependency UV Vis absorption of compounds

Figure S20. UV/Vis absorption spectra in different solvents of (a) BDP-AN-N-CZ; (b) BDP-AN-C-CZ; (c) BDP-AN-PH; and (d) BDP-AN. \( c = 1.0 \times 10^{-5} \) M; 20 °C.
5. Fluorescence emission spectra

Solvent-dependent fluorescence emission of compounds

Figure S21. Fluorescence emission spectra of compounds; (a) BDP-AN-N-CZ; (b) BDP-AN-C-CZ; (c) BDP-AN-PH; and (d) BDP-AN. $\lambda_{ex} = 465$ nm ($A = 0.11$). Optically matched solution were used (All the compounds have same absorbance at the excitation wavelength); 20 $^\circ$C.
6. Fluorescence emission decay curves

**Figure S22.** Fluorescence emission decay traces of triads along with their reference compounds, \( \lambda_{ex} = 510 \) nm, monitored at 520 nm. \( c = 1.0 \times 10^{-5} \) M in toluene, 20 °C.

**Figure S23.** Comparison of fluorescence emission decay traces of compounds at LE emission and CT emission band, (a) BDP-AN; (b) BDP-AN-C-CZ; and (c) BDP-AN-N-CZ, \( \lambda_{ex} = 510 \) nm, \( c = 1.0 \times 10^{-5} \) M in acetonitrile, 20 °C.
7. Redox properties of compounds.

Figure S24. Cyclic voltammogram of compound AN-C-CZ in deaerated acetonitrile, containing 0.10 M Bu₄NPF₆ as supporting electrolyte, Ferrocene (Fc) was used as the internal reference. Scan rates: 50 mV/s. \( c = 1 \times 10^{-3} \) M, 20 °C.

For AN-C-CZ, one reversible reduction potential wave at ~2.36 V and two irreversible oxidation potential wave at +0.67 V and +0.88 V were recorded, which can be assigned to CZ and AN moiety respectively. The thermodynamically feasibility for PET, between donor units (CZ) and acceptor unit (BDP) in dyads and triads are calculated employing Rehm–Weller analysis.

\[
\Delta G^0_{CS} = e[ E_{OX} - E_{RED} ] - E_{00} + \Delta G_s
\]  
(Eq. 1)

\[
\Delta G_s = -\frac{e^2}{4\pi\varepsilon_s\varepsilon_0 R_{cc}} - \frac{e^2}{8\pi\varepsilon_0} \left( \frac{1}{R_D} + \frac{1}{R_A} \right) \left( \frac{1}{\varepsilon_{REF}} - \frac{1}{\varepsilon_s} \right)
\]  
(Eq. 2)
Where $\Delta G_S$ is the static Coulombic energy, which is described by eq. 3. $e = \text{electronic charge,}$ $E_{\text{OX}} = \text{half-wave potential for one-electron oxidation of the electron-donor unit,}$ $E_{\text{RED}} = \text{half-wave potential for one-electron reduction of the electron-acceptor unit;}$ $E_{00} = \text{energy level approximated with the fluorescence emission (for the singlet excited state)},$ $\varepsilon_S = \text{static dielectric constant of the solvent,}$ $R_{CC} = \text{center-to-center separation distance between the electron donor (carbazole) and electron acceptor (BDP), determined by DFT optimization of the geometry,}$ $R_D$ is the radius of the electron donor, $R_A$ is the radius of the electron acceptor, $\varepsilon_{\text{REF}} = \text{the static dielectric constant of the solvent used for the electrochemical studies,}$ $\varepsilon_0 = \text{permittivity of free space.}$ The solvents used in the calculation of free energy of the electron transfer is toluene ($\varepsilon_S = 2.38$), CH$_2$Cl$_2$ ($\varepsilon_S = 8.93$) and acetonitrile ($\varepsilon_S = 37.5$).

\[
E_{CS} = e[E_{\text{OX}} - E_{\text{RED}}] + \Delta G_S
\]  
(Eq. 3)

\[
\Delta G_{\text{CR}} = - (\Delta G_{CS} + E_{00})
\]  
(Eq. 4)

**Table S2. Driving Forces of Charge Recombination ($\Delta G^0_{\text{CR}}$) and Charge Separation ($\Delta G^0_{\text{CS}}$) and the Energy of Charge Separated State ($E_{CSS}$) for Dyads/Triads in Different Solvents $^a$**

<table>
<thead>
<tr>
<th></th>
<th>$\Delta G^0_{CS}$ (eV)</th>
<th>$\Delta G^0_{CR}$ (eV)</th>
<th>$E_{CSS}$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>TOL</td>
<td>DCM</td>
<td>ACN</td>
</tr>
<tr>
<td>BDP-AN-C-CZ$^a$</td>
<td>-0.26</td>
<td>-0.47</td>
<td>-0.53</td>
</tr>
<tr>
<td>BDP-AN-N-CZ$^a$</td>
<td>0.15</td>
<td>-0.37</td>
<td>-0.52</td>
</tr>
<tr>
<td>AN-C-CZ$^b$</td>
<td>-0.03</td>
<td>-0.38</td>
<td>-0.48</td>
</tr>
</tbody>
</table>

$^a$ $E_{00} = 2.43$ eV, $^b$ $E_{00} = 3.10$ eV. $E_{00}$ is the approximated energy level with the cross point of UV–Vis absorption and fluorescence emission after normalization at the singlet excited state.
8. Nanosecond Time-resolved Difference Absorption Spectra

Figure S25. Nanosecond transient absorption spectra of compound; (a) BDP-AN-N-CZ and (c) BDP-AN-PH, upon ns pulsed laser excitation (\(\lambda_{\text{ex}} = 502\) nm). Fig (b) and (d) are their respective decay curves at 505 nm, \(c = 1.0 \times 10^{-5}\) M in dichloromethane, 20 °C.
Figure S26. Nanosecond transient absorption spectra of compound; (a) BDP-AN-C-CZ and (c) BDP-AN, upon ns pulsed laser excitation ($\lambda_{\text{ex}} = 502$ nm). Fig (b) and (d) are their respective decay curves at 505 nm, $c = 1.0 \times 10^{-5}$ M in acetonitrile, 20 °C.
Figure S27. Nanosecond transient absorption spectra of compound; (a) BDP-AN-N-CZ and (c) BDP-AN-PH, upon ns pulsed laser excitation ($\lambda_{\text{ex}} = 502$ nm). Fig (b) and (d) are their respective decay curves at 505 nm, $c = 1.0 \times 10^{-5}$ M in acetonitrile, 20 °C.
Figure S28. Nanosecond transient absorption spectra of compound; (a) BDP-AN-C-CZ and (c) BDP-AN, upon ns pulsed laser excitation (λ_{ex} = 502 nm). Fig (b) and (d) are their respective decay curves at 505 nm, c = 1.0 × 10^{-5} M in toluene, 20 °C.
Figure S29. Nanosecond transient absorption spectra of compound; (a) BDP-AN-N-CZ and (c) BDP-AN-PH, upon ns pulsed laser excitation (λ<sub>ex</sub> = 502 nm). Fig (b) and (d) are their respective decay curves at 505 nm, c = 1.0 × 10⁻⁵ M in toluene, 20 °C.
9. Femtosecond Transient Absorption Spectra

Figure S30. (a) Transient absorption spectra of BDP-AN in deareated toluene with the excitation of 400 nm; (b) Evolution Associated Difference spectra. Respective kinetics traces at three different wavelengths, (c) 480 nm and 601 nm; (d) 513 nm, 20 °C.
Figure S31. (a) Transient absorption spectra of BDP-AN in deaerated dichloromethane with the excitation of 400 nm; (b) Evolution Associated Difference spectra. Respective kinetics traces at two different wavelengths, (c) 507 nm and (d) 571 nm, 20 °C.
Figure S32. (a) Transient absorption spectra of BDP-AN-C-CZ in deareated toluene with the excitation of 400 nm. Respective kinetics traces at three different wavelengths, (b) 479 nm and 580 nm; (c) 508 nm, 20 °C.

Figure S33. (a) Transient absorption spectra of BDP-AN-C-CZ in deareated dichloromethane with the excitation of 400 nm. Respective kinetics traces at two different wavelengths, (b) 575 nm and (c) 508 nm, 20 °C.
**Figure S34.** (a) Transient absorption spectra of BDP-AN-N-CZ in deareated toluene with the excitation of 400 nm. Respective kinetics traces at three different wavelengths, (b) 480 nm; (c) 560nm and 600 nm, 20 °C.

**Figure S35.** (a) Transient absorption spectra of BDP-AN-N-CZ in deareated dichloromethane with the excitation of 400 nm. Respective kinetics traces at three different wavelengths, (b) 480 nm and 574 nm; (c) 510nm, 20 °C.
Figure S36. (a) Transient absorption spectra of BDP-AN-PH in deoxygenated toluene with the excitation of 400 nm; (b) Evolution Associated Difference spectra. Respective kinetics traces at two different wavelengths, (c) 480 nm and (d) 510 nm, 20 °C.
Figure S37. (a) Transient absorption spectra of BDP-AN-PH in deaerated dichloromethane with the excitation of 400 nm; (b) Evolution Associated Difference spectra. Respective kinetics traces at two different wavelengths, (c) 477 nm and (d) 575 nm, 20 °C.
Figure S38. (a) Transient absorption spectra of AN-C-CZ in deareated toluene with the excitation of 400 nm; (b) Evolution Associated Difference spectra. Respective kinetics traces at two different wavelengths, (c) 440 nm and (d) 571 nm, 20 °C.
Figure S39. (a) Transient absorption spectra of AN-C-CZ in deareated dichloromethane with the excitation of 400 nm; (b) Evolution Associated Difference spectra. Respective kinetics traces at three different wavelengths, (c) 440 nm and 461 nm; (d) 560 nm, 20 °C.
Figure S40. (a) Transient absorption spectra of BDP-AN-C-CZ in deaerated toluene with the excitation of 500 nm; (b) Evolution Associated Difference spectra. Respective kinetics traces at two different wavelengths, (c) 511 nm; and (d) 575 nm, 20 °C.
Figure S41. (a) Transient absorption spectra of BDP-AN-C-CZ in deaerated dichloromethane with the excitation of 500 nm; (b) Evolution Associated Difference spectra. Respective kinetics traces at two different wavelengths, (c) 571 nm; and (d) 507 nm, 20 °C.
**Figure S42.** (a) Transient absorption spectra of BDP-AN-N-CZ in deareated toluene with the excitation of 500 nm; (b) Evolution Associated Difference spectra. Respective kinetics traces at two different wavelengths, (c) 480 nm; and (d) 513 nm, 20 °C.
Figure S43. (a) Transient absorption spectra of BDP-AN-N-CZ in deaerated dichloromethane with the excitation of 500 nm; (b) Evolution Associated Difference spectra. Respective kinetics traces at two different wavelengths, (c) 510 nm; and (d) 569 nm, 20 °C.
10. Triplet-Triplet Annihilation Upconversion

Figure S44 (a) TTA Upconversions with BDP-AN-N-CZ as the photosensitizer and perylene (Pery) as the acceptor. Excited with 510 nm cw-laser (50 mW cm$^{-2}$). $c[\text{perylene}] = 2.0 \times 10^{-5}$ M, in deaerated dichloromethane, 20 °C. (b) CIE diagram.

Figure S45 (a) TTA Upconversions with BDP-AN-PH as the photosensitizer and perylene (Pery) as the acceptor. Excited with 510 nm cw-laser (50 mW cm$^{-2}$). $c[\text{perylene}] = 2.0 \times 10^{-5}$ M, in deaerated dichloromethane, 20 °C. (b) CIE diagram.
Figure S46 (a) TTA Upconversions with BDP-AN-C-CZ as the photosensitizer and perylene (Pery) as the acceptor. Excited with 510 nm cw-laser (50 mW cm$^{-2}$). \( c[\text{perylene}] = 2.0 \times 10^{-5} \text{ M} \), in deaerated toluene, 20 °C.
11. Delayed Fluorescence

**Figure S47** (a) Delayed fluorescence of BDP-AN-C-CZ upon nanosecond pulsed laser excitation ($\lambda_{ex} = 505$ nm, 1.8 mJ/pulse. Pulse duration: 5 ns). (a) Nanosecond transient emission spectra of BDP-AN-C-CZ in deaerated dichloromethane; (b) Decay traces at 525 nm in deaerated dichloromethane, 20 °C
12. Photophysical process of compounds

The overall photophysical process involved in BDP-AN-N-Cz can be depicted by the following Jablonski diagram. C stands for the carbazole unit, A stands for Anthracene and BDP stands for the bodipy unit. The number of the superscript designates the spin multiplicity. Similar photophysical process was observed in polar solvents acetonitrile with only change in CSS energy levels, but in case of non-polar solvent, toluene, the PET is not thermodynamically feasible process as the both CSS energy level lies higher than singlet excited state.

Scheme 1: Jablonski Diagram Demonstrating the Photophysical Processes Involved in BDP-AN-N-CZ upon Photoexcitation

- The energy levels of the excited singlet states are derived from the spectroscopic data; the energy level of charge transfer state are obtained from electrochemical data, also confirmed by the CT emission band. The triplet energy levels are estimated by TD-DFT method. The numbers in the superscripts indicates the spin multiplicity.
The overall photophysical process involved in BDP-AN dyad can be depicted by the following jablonski diagram. AN stands for Anthracene and BDP stands for the bodipy unit. The number of the superscript designates the spin multiplicity. Similar photophysical process was observed in another reference dyad BDP-AN-PH with slight variation in CSS energy levels.

Scheme 2: Jablonski Diagram Demonstrating the Photophysical Processes Involved in (a) BDP-AN and (b) BDP-AN-PH upon Photoexcitation

\[ \text{Scheme 2: Jablonski Diagram Demonstrating the Photophysical Processes Involved in (a) BDP-AN and (b) BDP-AN-PH upon Photoexcitation}^{\text{a}} \]

\[ \text{The energy levels of the excited state are derived from the spectroscopic and electrochemical data. The triplet energy levels are estimated by TD-DFT method. The numbers in superscripts indicates the spin multiplicity}^{\text{a}} \]

13. Theoretical Computations
**Figure S48** Selected frontier molecular orbitals and the energy levels (eV) of compounds calculated by TDDFT at B3LYP/631-G(d) level with Gaussian 09W, based on optimized ground state. **BDP-C-CZ** and **BDP-N-CZ** stands for **BDP-AN-C-CZ** and **BDP-AN-N-CZ** respectively.
References


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