Supporting Information for:
Aggregation-induced emission and reversible mechanochromic luminescence of carbazole-based triphenylacrylonitrile derivatives

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Fig. S1 $^1$H-NMR (400 MHz, DMSO-d$_6$) spectra of compound Cz1-TPAN.

Fig. S2 $^{13}$C-NMR (100 MHz, DMSO-d$_6$) spectrum of compound Cz1-TPAN.
Fig. S3 The MALDI/TOF MS spectrum of compound Cz1-TPAN.

Fig. S4 $^1$H-NMR (400 MHz, DMSO-$d_6$) spectra of compound Cz2-TPAN.
Fig. S5 $^{13}$C-NMR (100 MHz, DMSO-d$_6$) spectrum of compound Cz2-TPAN.

Fig. S6 The MALDI/TOF MS spectrum of compound Cz2-TPAN.
Fig. S7  The optimized molecular configurations of Cz1-TPAN (a, b) and Cz2-TPAN (c, d) in two different views calculated by the DFT method (B3LYP/6-31G level) on Gaussian 09 software.
Fig. S8 Normalized UV-vis absorption (a) and fluorescence emission (b, $\lambda_{ex} = 400$ nm) spectra of Cz1-TPAN in different solvents ($2.0 \times 10^{-5}$ M).

Fig. S9 Normalized UV-vis absorption (a) and fluorescence emission (b, $\lambda_{ex} = 420$ nm) spectra of Cz2-TPAN in different solvents ($2.0 \times 10^{-5}$ M).
Fig. S10 Cyclic voltammetry diagrams of Cz1-TPAN and Cz2-TPAN in anhydrous CH$_2$Cl$_2$ with 0.1 M Bu$_4$NPF$_6$ as electrolyte at a scan rate of 50 mV/s.

Fig. S11 Maximum fluorescent emission of Cz1-TPAN upon repeating treatment of grinding and fuming with DCM.
**Fig. S12** XRD patterns of Cz2-TPAN in as-synthesized solid states. Inset is photographs in as-synthesized solid states under UV illumination.

**Fig. S13** The structure of Cz1-TPAN in single crystal.
Table S1: Electrochemical data and HOMO/LUMO energy levels of Cz1-TPAN and Cz2-TPAN.

<table>
<thead>
<tr>
<th>Compounds</th>
<th>( E_{1/2}^{ox} ) ((V))</th>
<th>HOMO (^b) ((eV))</th>
<th>LUMO (^b) ((eV))</th>
<th>( E_g ) ((eV))</th>
<th>HOMO (^d) ((eV))</th>
<th>LUMO (^d) ((eV))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cz1-TPAN</td>
<td>0.88</td>
<td>-5.29</td>
<td>-2.51</td>
<td>2.78</td>
<td>-5.02</td>
<td>-1.94</td>
</tr>
<tr>
<td>Cz2-TPAN</td>
<td>0.68</td>
<td>-5.09</td>
<td>-2.35</td>
<td>2.74</td>
<td>-4.71</td>
<td>-1.94</td>
</tr>
</tbody>
</table>

\(^a\) \(E_{1/2}^{ox}\) = first half-wave potential; Fc/\(\text{Fc}^+\) was used as the external reference. \(^b\) calculated using the empirical equation: \(E_{\text{HOMO}} = -(E_{1/2}^{ox} + 4.41)\) and \(E_{\text{LUMO}} = E_{\text{HOMO}} + E_g\). \(^c\) Estimated from the onset of the absorption spectra \((E_g = 1240/\lambda_{\text{onset}})\). \(^d\) Obtained from quantum chemical calculation using TDDFT/B3LYP/6-31G(d).