Supporting Information

Theoretical Study on the Light-emitting Mechanism of Circularly Polarized Luminescence Molecules with both Thermally Activated Delayed Fluorescence and Aggregation Induced Emission

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Fig. S1 Visible geometry changes between S$_1$ (black) and two triplet excited states (red) in toluene and solid phase for S-BN-AF respectively.

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Fig. S2 Visible geometry changes between $S_1$ (black) and five triplet excited states.
(red) in toluene and solid phase for R-BN-CF respectively.
Fig. S3 ECD spectra for R-BN-AF (black) and S-BN-AF (red) (a) as well as R-BN-CF (black) and S-BN-CF (red) (b) in toluene. The rotatory strength is also illustrated.
Fig. S4 Transition characteristics for $S_1$, $T_1$, $T_2$, $T_3$, $T_4$ and $T_5$ states of R-BN-CF in toluene. The value above every arrow represents the ratio of depicted NTOs in the
corresponding transition.

Table S1. The local excitation (LE) ratio for each singlet and triplet excited state for S-BN-AF respectively.

<table>
<thead>
<tr>
<th></th>
<th>$S_1$</th>
<th>$T_1$</th>
<th>$T_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>toluene</td>
<td>16.31%</td>
<td>40.70%</td>
<td>19.32%</td>
</tr>
<tr>
<td>solid</td>
<td>20.56%</td>
<td>39.06%</td>
<td>38.90%</td>
</tr>
</tbody>
</table>

Table S2. The local excitation (LE) ratio for each singlet and triplet excited state for R-BN-CF respectively.

<table>
<thead>
<tr>
<th></th>
<th>$S_1$</th>
<th>$T_1$</th>
<th>$T_2$</th>
<th>$T_3$</th>
<th>$T_4$</th>
<th>$T_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>toluene</td>
<td>21.33%</td>
<td>90.53%</td>
<td>86.06%</td>
<td>59.80%</td>
<td>80.98%</td>
<td>32.98%</td>
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<tr>
<td>solid</td>
<td>34.69%</td>
<td>90.23%</td>
<td>85.78%</td>
<td>65.16%</td>
<td>82.27%</td>
<td>74.55%</td>
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</table>