Self-reversible thermofluorochromism of D-A-D triphenylamine derivatives and effect of molecular conformation and packing

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Figure S1. Absorption spectra of 1, 2 and 3 in CH$_3$CN.

Figure S2. Heating and cooling cycle studies of 1 and 2.
Figure S3. Excitation spectra of (a) 1 and (b) 2 before and after heating.
Figure S4. ABAB pattern of 2 in the crystal lattice. C (grey), N (blue), O (red), H (white).

Figure S5. Inclusion of toluene in the crystal lattice of 2 and different intermolecular interactions involved in the crystal lattice.
Figure S6. PXRD pattern of experimental and simulated (a) 1, (b) 2 and (c) 3.
Figure S7. DSC of (a) 1 and (b) 2.
Figure S8. PXRD pattern of 1 and 2 before and after heating.

Table S1. HOMO-LUMO energy level of 1-3.

<table>
<thead>
<tr>
<th></th>
<th>HOMO (eV)</th>
<th>LUMO (eV)</th>
<th>Band gap (eV)</th>
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<tbody>
<tr>
<td>1</td>
<td>-5.336</td>
<td>-2.498</td>
<td>2.838</td>
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<tr>
<td>2</td>
<td>-5.173</td>
<td>-2.302</td>
<td>2.871</td>
</tr>
<tr>
<td>3</td>
<td>-5.172</td>
<td>-2.340</td>
<td>2.832</td>
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