Supporting Information

A Novel Photo-Responsive Azobenzene-Containing Nano-Ring Host for Fullerene Guest Facile Encapsulating and Releasing

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Table S1. The \( \theta_p \) (\(^\circ\)) of some selected C atom (see Figure S2) of the azobenzene, [10]CPP and [4]AB nanoring

Figure S3. Simulated UV-visible-NIR absorption spectrum compare for the trans-[4]AB, [4]AB\( \supseteq C_{60} \) and [4]AB\( \supseteq C_{70} \) host-guest complexes

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Figure S1. π-orbital axis vector (POAV) shown for a nonplanar conjugated carbon atom bonded to atoms 1, 2, 3, through the schematized σ bonds $\sigma_1$, $\sigma_2$, $\sigma_3$, and definition of the angles $\theta_{\sigma\pi}$ made by the π-orbital to each of the σ bonds.

Figure S2. Atom label of the [10]CPP, azobenzene and [4]AB for POVA listed in Table S1.
Table S1 the \( \theta_p (\circ) \) of some selected C atom (see Figure S2) of the azobenzene, [10]CPP and [4]AB nanoring

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<th>Atom label</th>
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<th>7</th>
<th>8</th>
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</table>

Equation S1

\[
\text{Strain} = E_0 - E_A - (E_B - 2E_C) \quad \text{Eq}(S1)
\]

Where \( E_0 \) is the energy of the free [4]AB nanoring, \( E_A \) is the energy of the open-ring structure (A) of the [4]AB, \( E_B \) is the energy of the open-ring structure (B) of the [2]AB, \( E_C \) is the energy of the azobenzene (C). For clarity, the structures of A, B and C are given below.