Supporting Information

Revealing the way of self-complementary dimerization for a shape-persistent macrocycle using DFT calculations

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Figure S1. Total energy as a function of (a) rotational angle and (b) intermolecular distance. Counterpoise (CP) corrected and uncorrected total energies are denoted as ▲ and ▼. In (a), the total energies are calculated at intermolecular distance of 3.70 Å (dotted lines) and 3.91 Å (solid lines). In (b), both the CP-corrected and uncorrected total energies are calculated with the off-set angle θ = 51.5°. The two energy profiles would merge at d = ~7 Å, indicating that the BSSE for the non-bonded interactions has a long range effect.

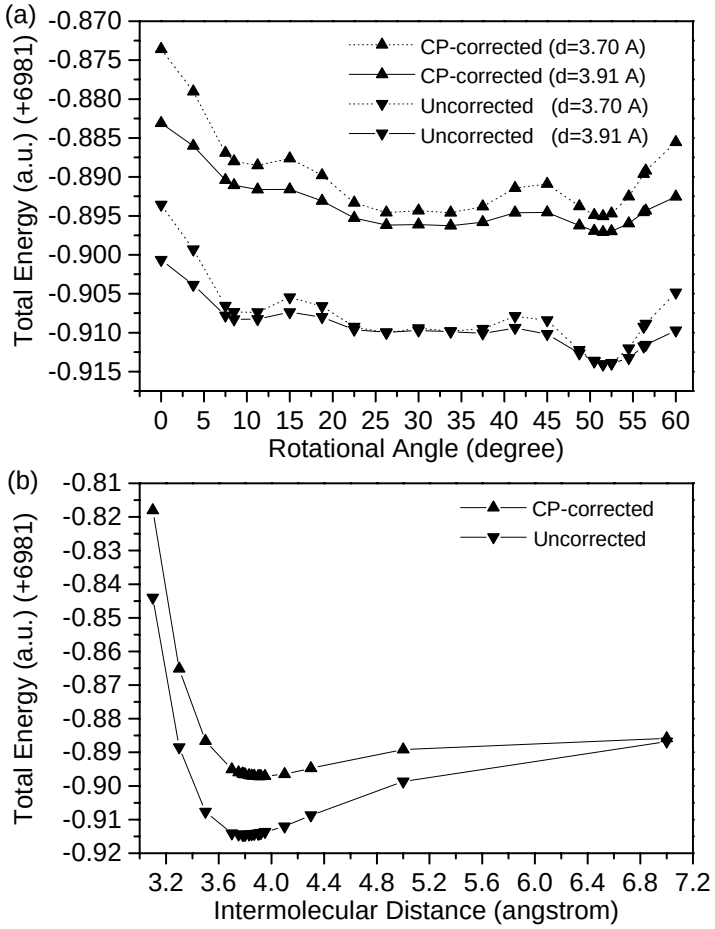

Figure S2. Basis set superposition error (BSSE) as a function of (a) rotational angle and (b) intermolecular distance. In (a), the intermolecular distance is 3.91 Å. In (b), the off-set angle is 51.5°.