Supporting Information

Theoretical Simulation of Structural Transformation and Chirality Switch in Host-Guest Self-Assembly

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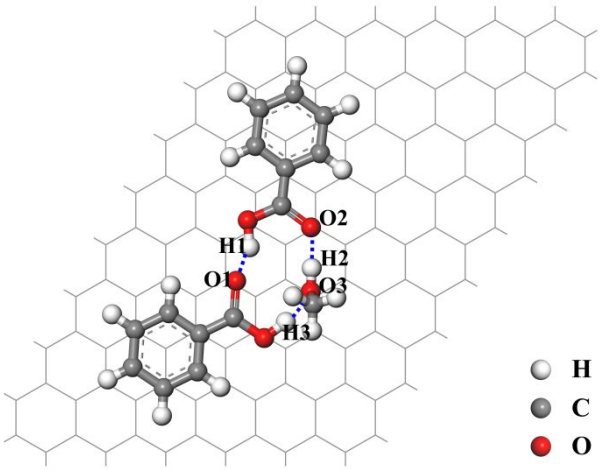

Figure S1. Simplified fragment with key atoms forming hydrogen bonds labeled. The white, gray, and red atoms represent H, C, and O atoms, respectively. The blue dashed lines represent O-H…O hydrogen bonds.

Table S1. The bond lengths of simplified fragment using DFT and MM calculations with different force fields (corresponding atomic labels are shown in Figure S1.)

	H3-O3	H2-O2	H1-O1
DFT	**1.695**	**1.540**	**1.692**
cvff	**1.631**	**1.646**	**1.632**
Dreiding	2.055	2.052	2.052
pcff	1.786	1.880	1.681

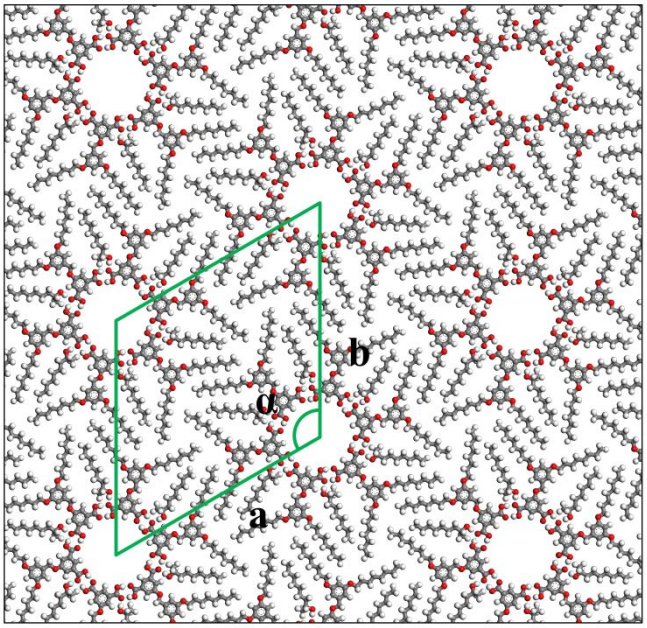

Figure S2. The imaginary CCW starfish model which does not contain the guest COR. The green solid line represents the unit cell.

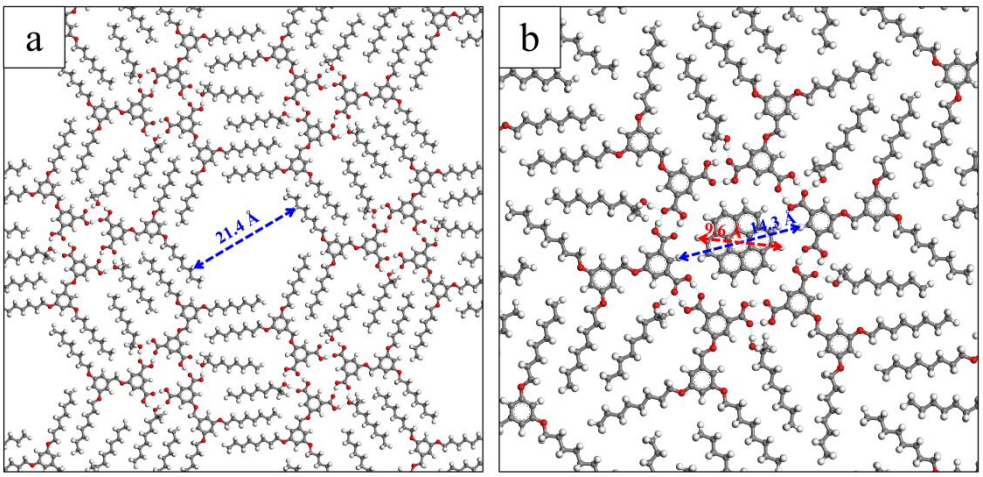

Figure S3. The MM-optimized configuration with pore sizes. (a) CCW honeycomb structure I composed of BIC-C8 and S-nonanol. (b) CCW starfish structure I composed of BIC-C8, S-nonanol and COR. The blue dotted lines indicate the diameter of pores and the red dotted line indicates the diameter of COR.

Table S2. Surface density (nm^{-2}) of BIC-Cn (n=8, 16)/S-nonanol in the absence and the presence of COR

	In the absence of COR	In the presence of COR
BIC-C8	13.7	16.4
BIC-C16	10.8	12.5

Table S3. Adsorption energy and hydrogen bond characteristic parameters of BIC-C16/S-nonanol

	E_{ad} (kcal/mol)	Average bond length (Å)	Average bond angle (°)
CCW	-1032.5	1.78	164.0
CW	-983.7	1.81	161.0

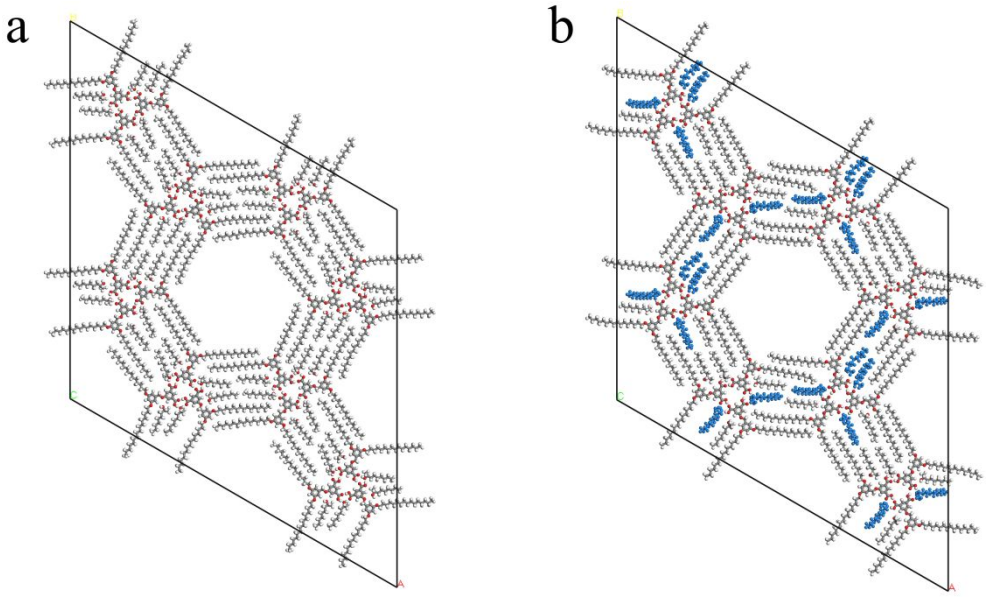

Figure S4. 2×2 supercell snapshots of BIC-C16/S-nonanol at 100ps. (a) CCW and (b) CW configuration. The distorted solvent molecules are shown in blue.

Table S4. Adsorption energy and hydrogen bond characteristic parameters of BIC-C16/S-nonanol in the presence of COR

	E_{ad} (kcal/mol)	Average bond length (Å)	Average bond angle (°)
CCW	-655.4	1.732	165.849
CW	-652.8	1.730	165.753

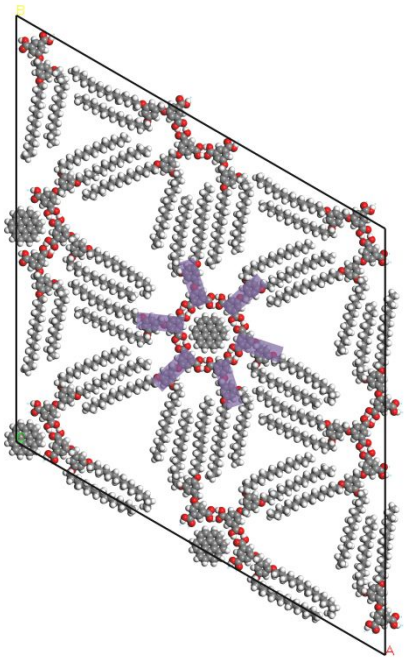

Figure S5. 2×2 CW supercell snapshot of BIC-C16/S-nonanol in the presence of COR at 100 ps. The axes of six BIC molecules are indicated by purple rectangles.

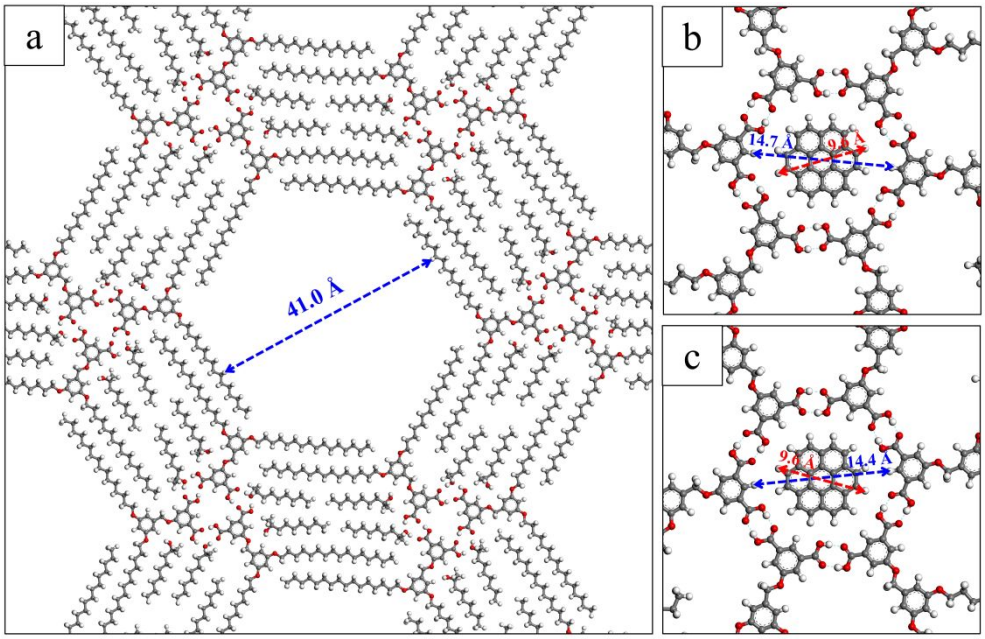

Figure S6. The MM-optimized configuration with pore sizes. (a) CCW honeycomb structure II composed of BIC-C16 and S-nonanol. (b) CCW and (c) CW starfish structure II composed of BIC-C8, S-nonanol and COR. The blue dotted lines indicate the diameter of pores and the red dotted lines indicate the diameter of COR.