Figure S1 shows the mean square displacement (MSD) curves of the surfactant species with different carbon-chain lengths. Linear fitting was performed over the 200–600 ps interval, and the corresponding diffusion coefficients were estimated using Einstein's relation:

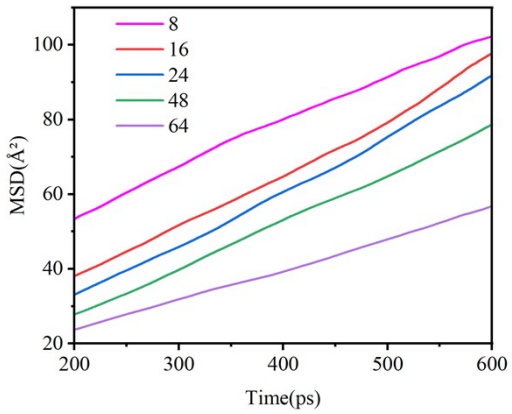

Fig.S1 Mean Square Displacement (MSD) plots for templates with varying carbon chain lengths

$$D = \frac{1}{6N_\alpha} \lim_{t\to\infty} \frac{d}{dt} \sum_{i=1}^{N_\alpha} \left\langle [r_i(t) - r_i(0)] \right\rangle^2$$

where $r_i(t)$ and $r_i(0)$ represent the atomic coordinates of moleculeat i time t and the initial time, respectively. The calculated diffusion coefficients are summarized in Table S1. A decreasing trend in the diffusion coefficient is observed with increasing carbon-chain length, indicating lower relative molecular mobility for longer-chain surfactants under the present simulation conditions. Owing to the limited simulation timescale, these results are discussed only as supplementary qualitative information.

Table S1: Self-diffusion coefficients of template agents with different carbon chain lengths

/	8C	16C	24C	48C	64C
MSD slope	0.1454	0.1216	0.1021	0.0816	0.0652
Self-diffusion coefficient(Å²/ps)	0.0242	0.0202	0.0170	0.0136	0.0109