Supplementary Information

Monte Carlo simulation of temperature-induced reversible morphological changes between sphere and vesicle formed by AB diblock copolymers

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- **S1.** The simulation results obtained in larger simulation box, L=50.
- **S2.** The repeated simulation results with different initial states.

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S1: The simulation results obtained in larger simulation box, L=50.

Directly heating process

Figure S1. Snapshots at different stages showing the pathway of morphological change between sphere and vesicle under rapid temperature change rate (a)-(e) quenching process; (f)-(j) directly heating process. (a) 1.0×10^{5} MCS, (b) 8.0×10^{5} MCS, (c) 2.5×10⁶MCS, (d) 3.7×10⁶MCS, (e) 4.8×10⁶MCS, (f) 250MCS, (g) 1000MCS, (h) 3000MCS, (i) 2.5×10^4 MCS, (j) 4.0×10^5 MCS. For clarity, the cross sections of the vesicles are given in (e') and (e'').





Directly heating process

Figure S2. The pathways of morphological transition evolving from initial state 2 under rapid temperature change rate. (a)-(e) quenching process; (f)-(j) directly heating process. For clarity, the cross sections of the micelles are given in (e)', (f), (g).



Figure S3. The pathways of morphological transition evolving from initial state 3 under rapid temperature change rate. (a)-(e) quenching process; (f)-(j) directly heating process. For clarity, the cross sections of the micelles are given in (e)', (f), (g).



Figure S4. The pathways of morphological transition evolving from initial state 2 under slow temperature change rate. (a') and (h') are the cross sections of the corresponding vesicles.



Figure S5. The pathways of morphological transition evolving from initial state 3 under slow temperature change rate. (a') and (h') are the cross sections of the corresponding vesicles.