

## Electronic Supplementary Information

### Monte Carlo study of the micelles constructed by ABCA tetrablock copolymers and their formation in A-selective solvents

Jiani Ma,<sup>ab</sup> Jie Cui,<sup>b</sup> Yuanyuan Han,<sup>\*b</sup> Wei Jiang<sup>b</sup> and Yingchun Sun<sup>\*a</sup>

<sup>a</sup>*Northeast Normal University, School of Physics, Changchun 130024, P. R. China*

<sup>b</sup>*State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China*

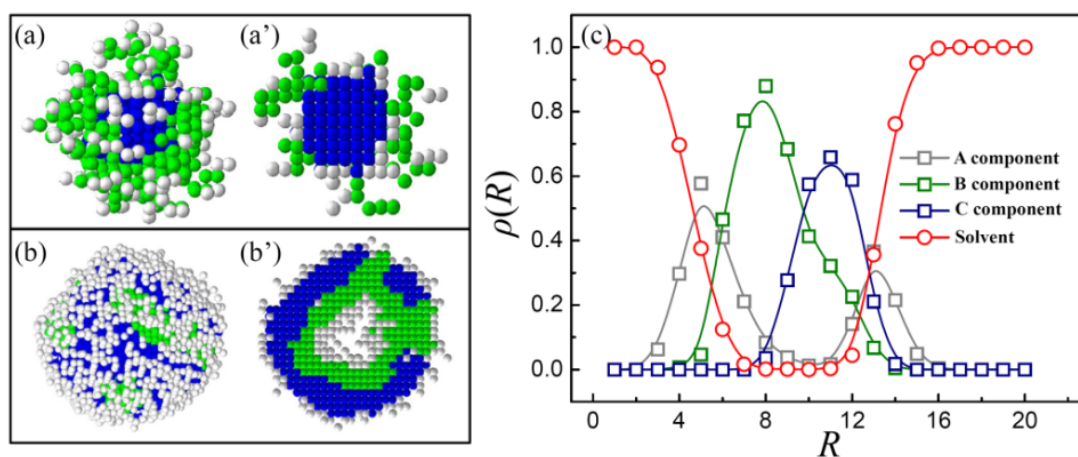
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\*Corresponding authors: E-mail: [yyhan@ciac.ac.cn](mailto:yyhan@ciac.ac.cn); [sunyc149@nenu.edu.cn](mailto:sunyc149@nenu.edu.cn).

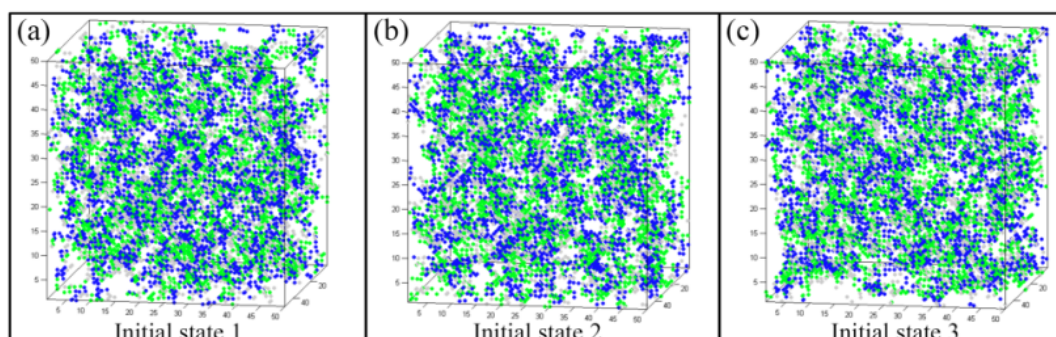
Telephone: +86-431-85262642. Fax: +86-431-85262126.

**S1. Illustration showing the distribution of solvophilic blocks A in the micelles and density variations of segments A, B, C and solvent with  $R$  ( $R$  is the radii around the mass center of the vesicle).**



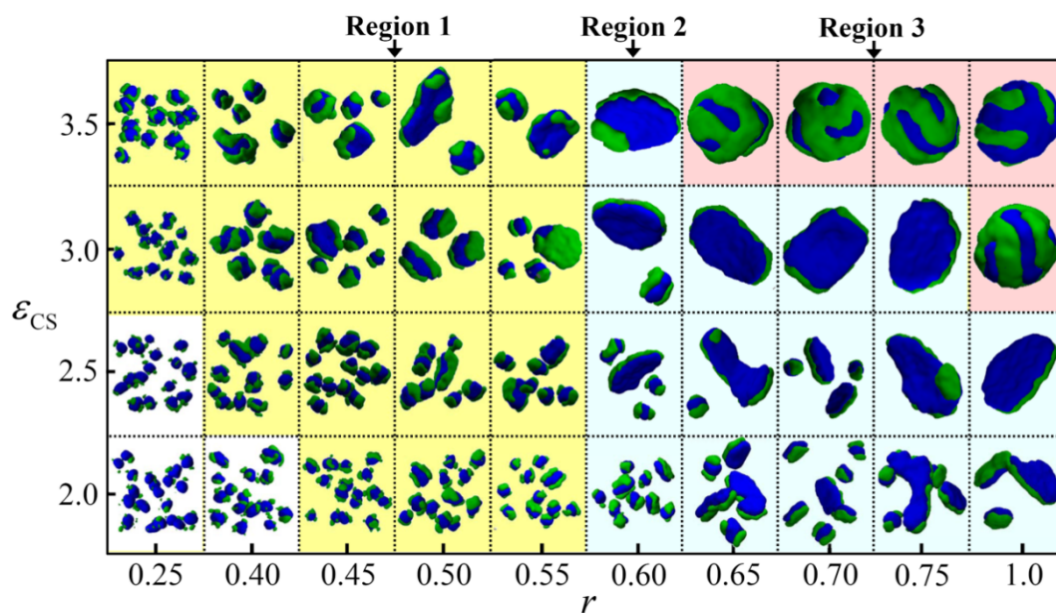
**Figure S1.** One of the spherical micelles (a) and vesicle (b) formed by  $A_2B_6C_6A_2$  tetrablock copolymers with  $\epsilon_{CS} = 2.0$ ,  $r = 0.25$  and  $\epsilon_{CS} = 3.5$ ,  $r = 1.0$ . (a') and (b') are the cross-sections of (a) and (b). The insoluble blocks B and C are drawn in green and blue, and the soluble blocks A are drawn in light gray. (c) is the density variations of segments A, B, C, and solvent with  $R$  ( $R$  is the radii around the mass center of the vesicle) of the vesicle shown in (b).

**S2. Different initial states used in this paper, and additional simulation results obtained from different initial states.**

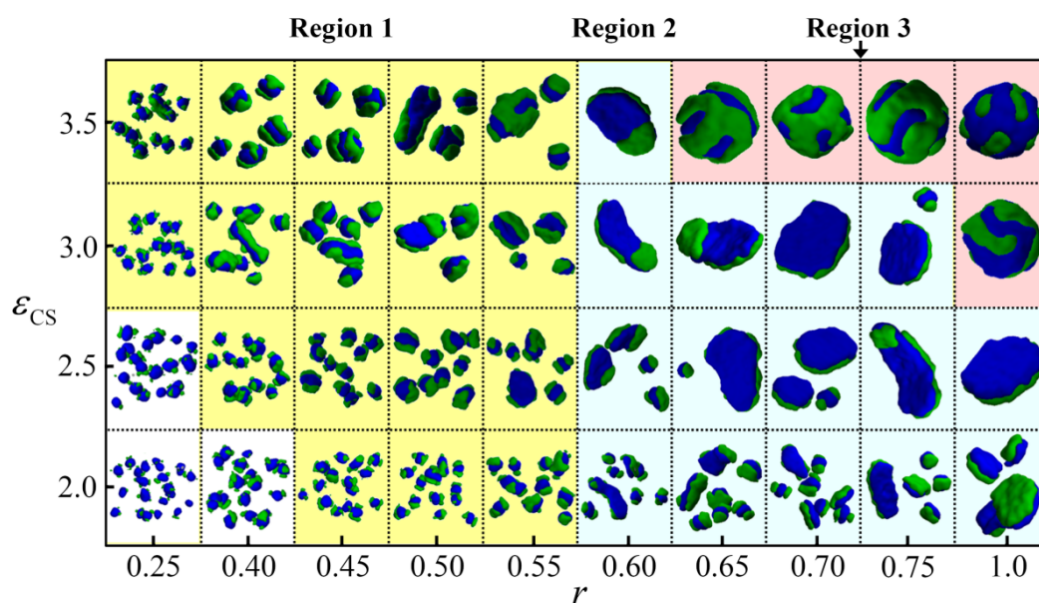


**Figure S2.** Different initial states (the athermal state of  $T = \infty$ ). (a) Initial state for the micelles shown in Figures 1, 4 and 5 in the manuscript; (b) Initial state for the

micelles shown in Figures S3, S5 and S7; (c) Initial state for the micelles shown in Figures S4, S6 and S8. The blocks A, B and C are drawn in light gray, green and blue, respectively.

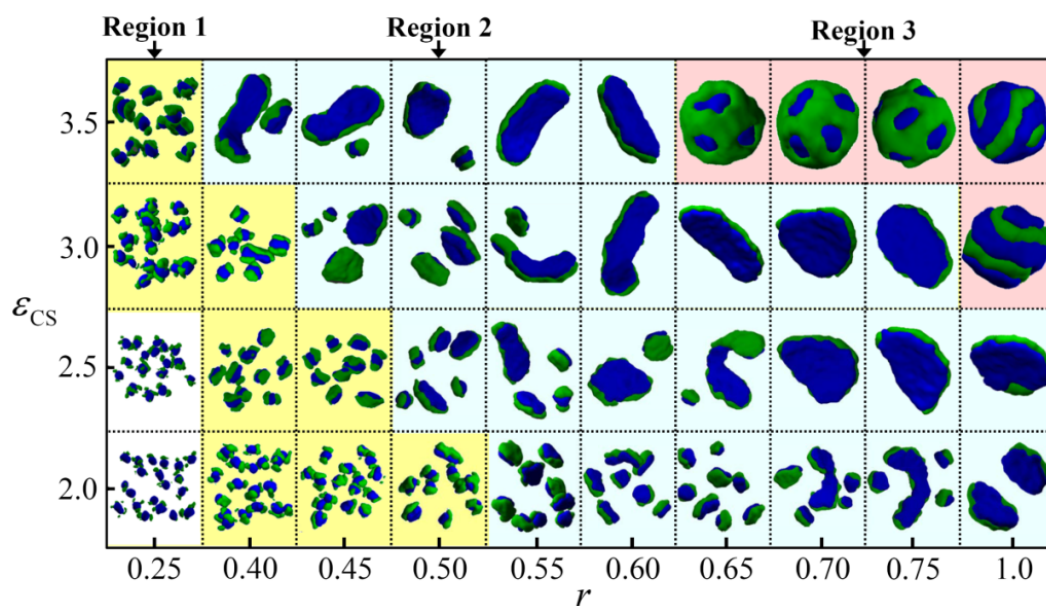


**Figure S3.** Morphological phase diagram of  $A_2B_6C_6A_2$  tetrablock copolymers as a function of  $\varepsilon_{CS}$  and  $r$  from **initial state 2**. The insoluble blocks B and C are drawn in green and blue, and the soluble blocks A are not shown in the images.

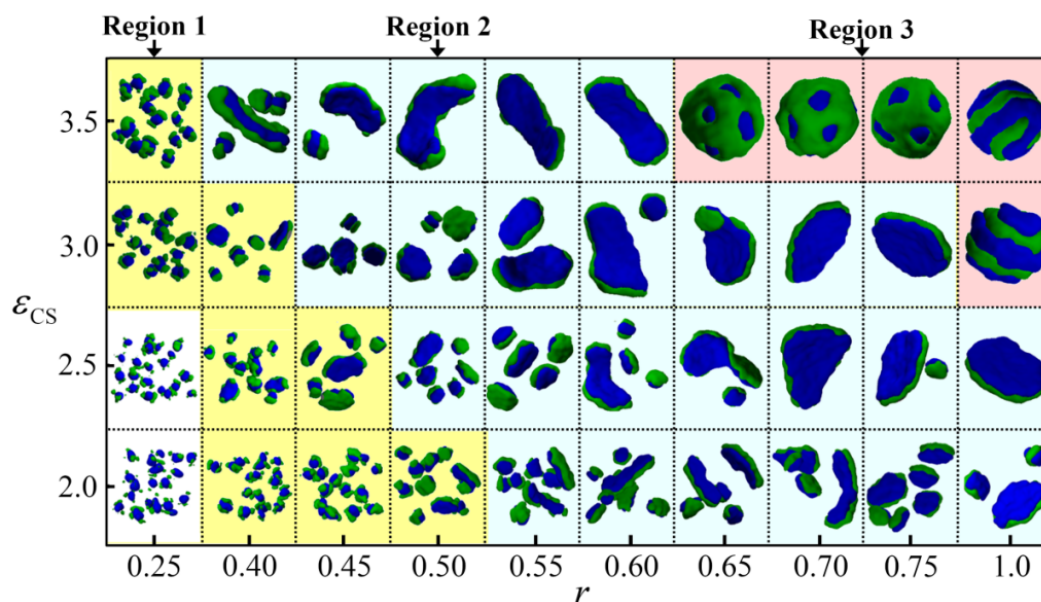


**Figure S4.** Morphological phase diagram of  $A_2B_6C_6A_2$  tetrablock copolymers as a

function of  $\varepsilon_{CS}$  and  $r$  from **initial state 3**. The insoluble blocks B and C are drawn in green and blue, and the soluble blocks A are not shown in the images.

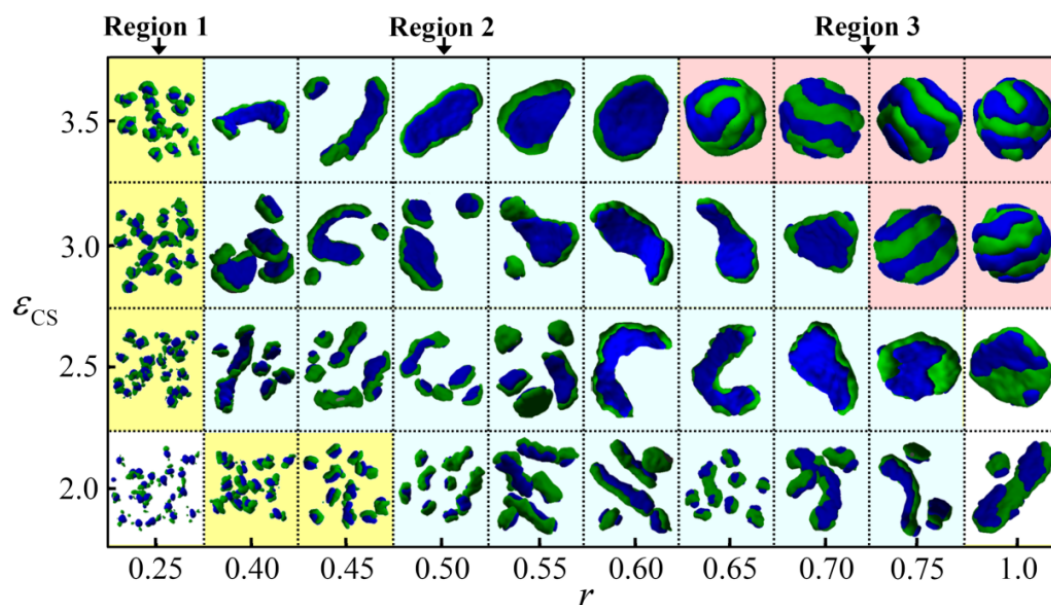


**Figure S5.** Morphological phase diagram of  $A_2B_7C_5A_2$  tetrablock copolymers as a function of  $\varepsilon_{CS}$  and  $r$  from **initial state 2**. The insoluble blocks B and C are drawn in green and blue, and the soluble blocks A are not shown in the images.

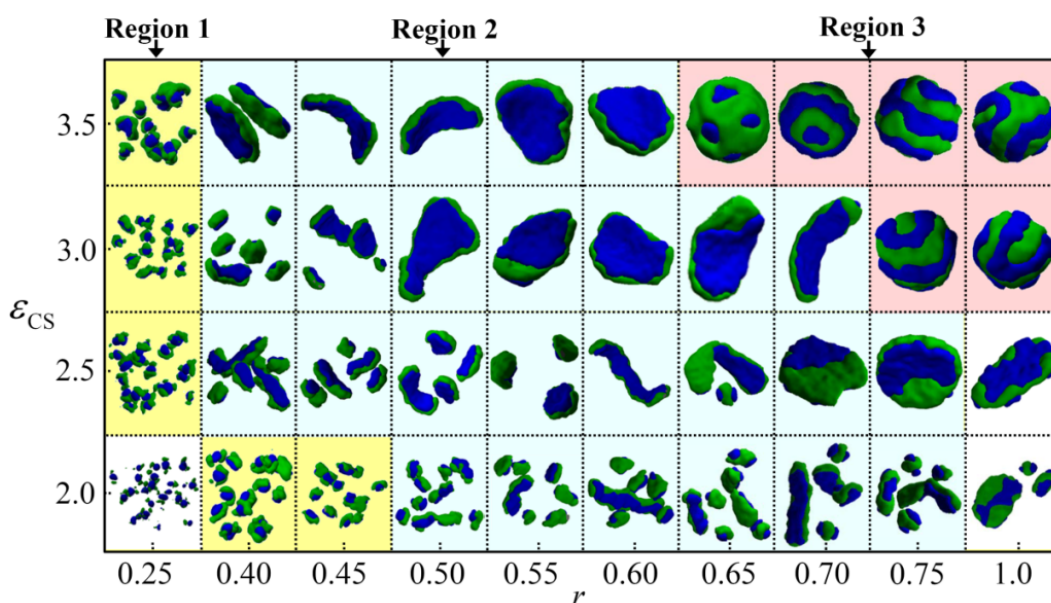


**Figure S6.** Morphological phase diagram of  $A_2B_7C_5A_2$  tetrablock copolymers as a function of  $\varepsilon_{CS}$  and  $r$  from **initial state 3**. The insoluble blocks B and C are drawn in

green and blue, and the soluble blocks A are not shown in the images.

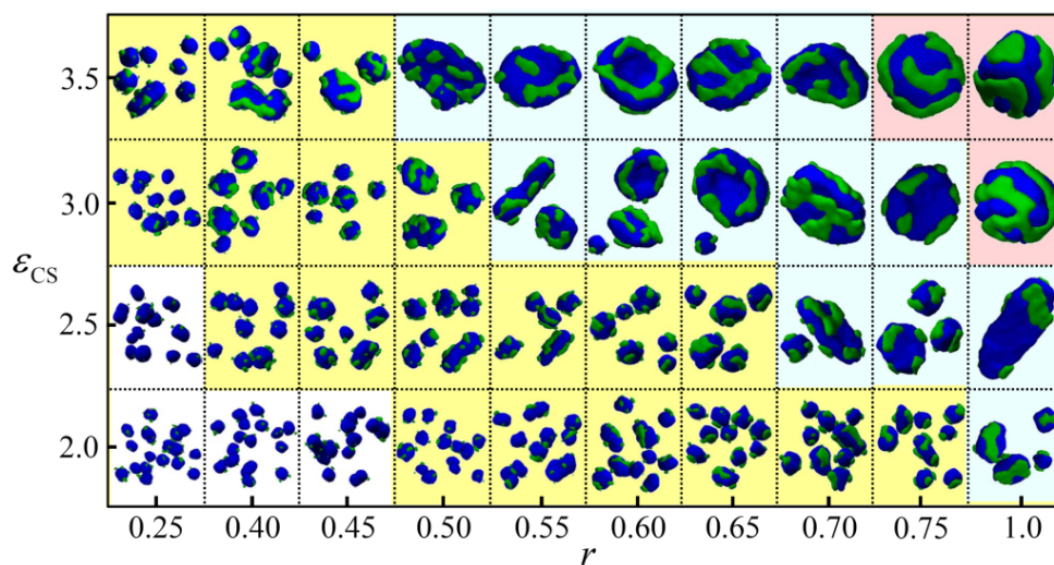


**Figure S7.** Morphological phase diagram of  $A_2B_8C_4A_2$  tetrablock copolymers as a function of  $\varepsilon_{CS}$  and  $r$  from **initial state 2**. The insoluble blocks B and C are drawn in green and blue, and the soluble blocks A are not shown in the images.

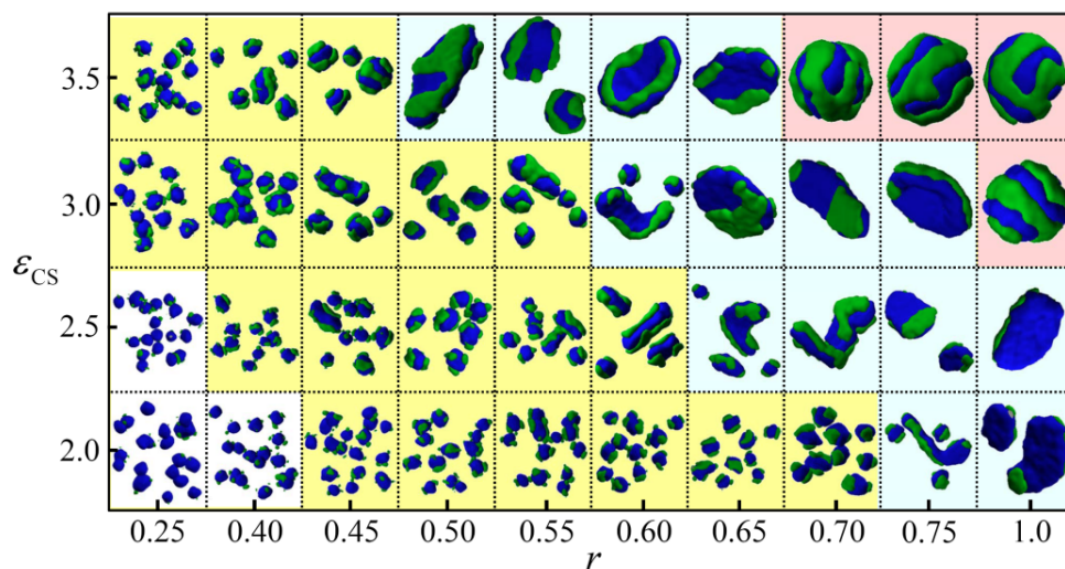


**Figure S8.** Morphological phase diagram of  $A_2B_8C_4A_2$  tetrablock copolymers as a function of  $\varepsilon_{CS}$  and  $r$  from **initial state 3**. The insoluble blocks B and C are drawn in green and blue, and the soluble blocks A are not shown in the images.

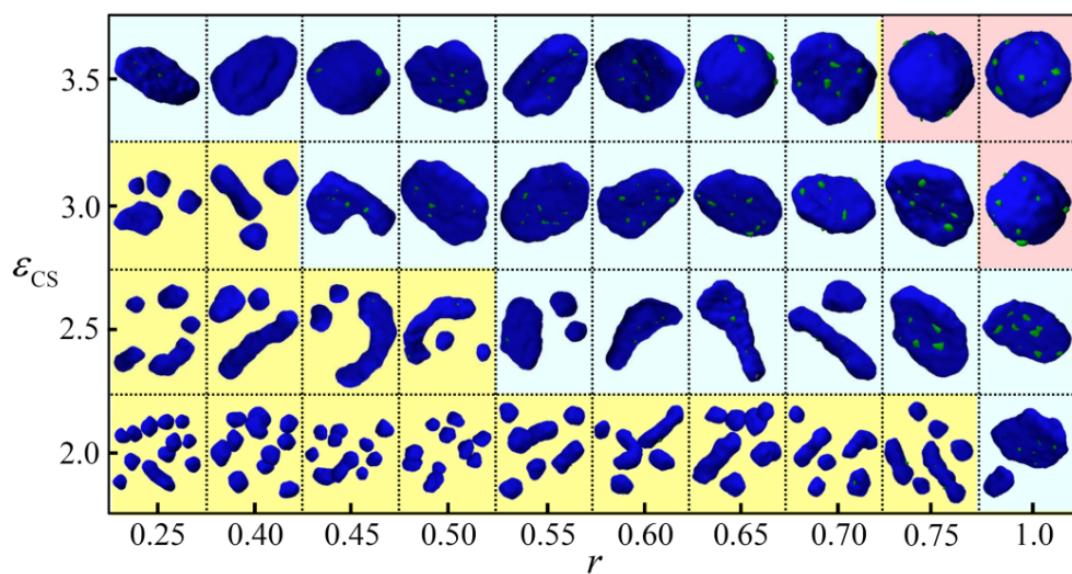
**S3. Simulation results of the ABCA tetrablock copolymer systems with other chain length ratios of blocks B to C.**



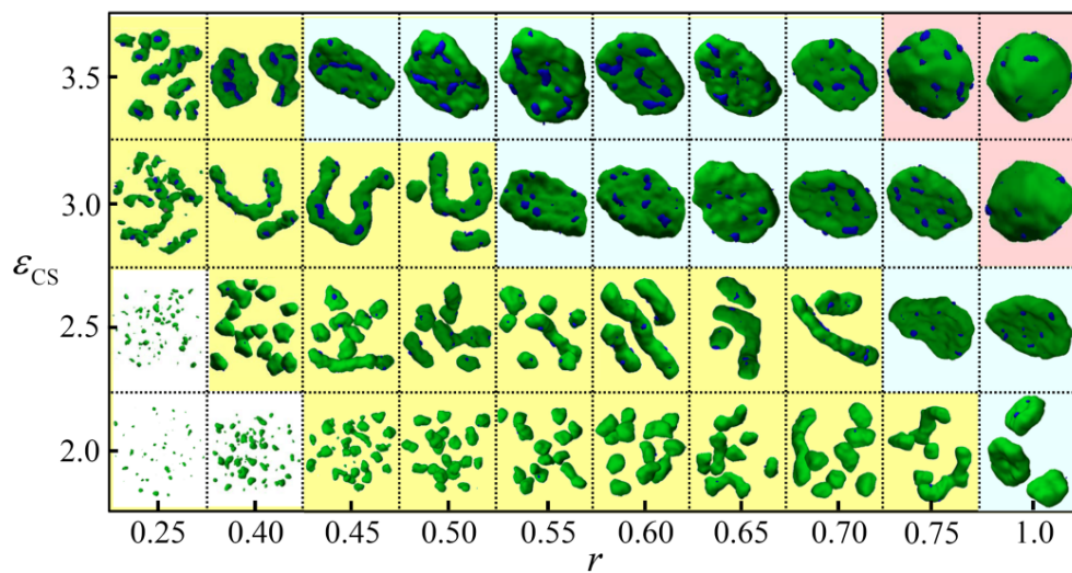
**Figure S9.** Morphological phase diagram of  $A_2B_4C_8A_2$  tetrablock copolymers as a function of  $\varepsilon_{CS}$  and  $r$ . The insoluble blocks B and C are drawn in green and blue, and the soluble blocks A are not shown in the images.



**Figure S10.** Morphological phase diagram of  $A_2B_5C_7A_2$  tetrablock copolymers as a function of  $\varepsilon_{CS}$  and  $r$ . The insoluble blocks B and C are drawn in green and blue, and the soluble blocks A are not shown in the images.

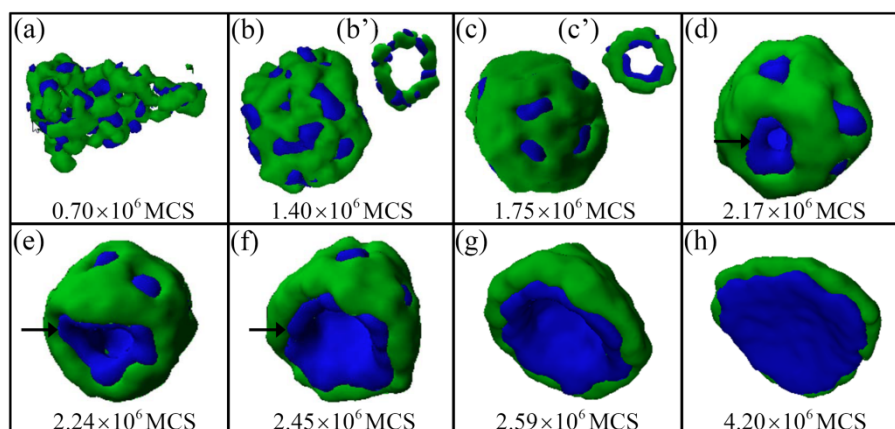


**Figure S11.** Morphological phase diagram of  $A_2B_2C_{10}A_2$  tetrablock copolymers as a function of  $\varepsilon_{CS}$  and  $r$ . The insoluble blocks B and C are drawn in green and blue, and the soluble blocks A are not shown in the images.



**Figure S12.** Morphological phase diagram of  $A_2B_{10}C_2A_2$  tetrablock copolymers as a function of  $\varepsilon_{CS}$  and  $r$ . The insoluble blocks B and C are drawn in green and blue, and the soluble blocks A are not shown in the images.

**S4. The formation pathway of the Janus lamella in Figure 8a in the manuscript.**



**Figure S13.** Morphological pathway (a)-(h) for Janus lamella formed by  $A_2B_8C_4A_2$  tetrablock copolymers with  $\varepsilon_{CS} = 3.5$  and  $r = 0.55$  (Figure 8a in the manuscript). For clarity, the cross-section of the vesicle is given in (b') and (c'). The pores in the vesicles are marked by black arrows. The insoluble blocks B and C are drawn in green and blue, and the soluble blocks A are not shown in the images.