Electronic Supplementary Material (ESI) for Soft Matter

Supporting Information:

Dissipative Particle Dynamics Simulation Study on the Mechanisms of Self-Assembly of Large Multimolecular Micelles from Amphiphilic Dendritic Multiarm Copolymers

Yuling Wang[1], *Bin Li*[2], *Yongfeng Zhou*[1]*, *Zhongyuan Lu*[2]*, *Deyue Yan*[1]

[1]School of Chemistry and Chemical Engineering, State Key Laboratory of Metal Matrix Composites, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai 200240, P. R. China and

[2]Institute of Theoretical Chemistry, State Key Laboratory of Theoretical and Computational Chemistry, Jilin University, Changchun 130023, China

Email: yfzhou@sjtu.edu.cn (Yongfeng Zhou); luzhy@jlu.edu.cn (Zhongyuan Lu)

S1. The UM structures based on models b, c and d

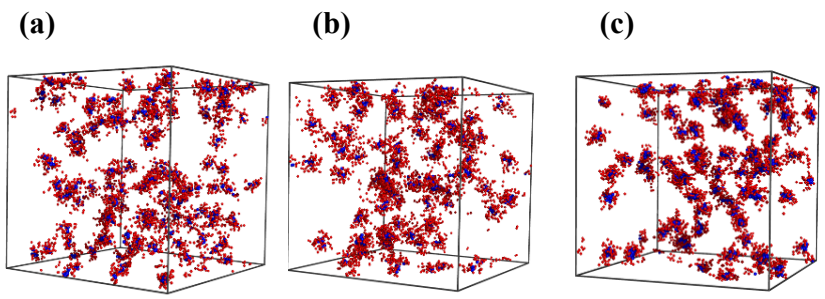

Figure S1. The morphologies of unimolecular micelles formed after 500000-step DPD simulations from dendritic multiarm copolymers based on model **b** (a), model **c** (b) and model **d** (c). The concentration is 1%, a_{BC}=20, and water beads are omitted for clarity. Hydrophobic dendritic core: blue beads; hydrophilic linear arms: red beads.

S2. The UMA structures based on models a and c

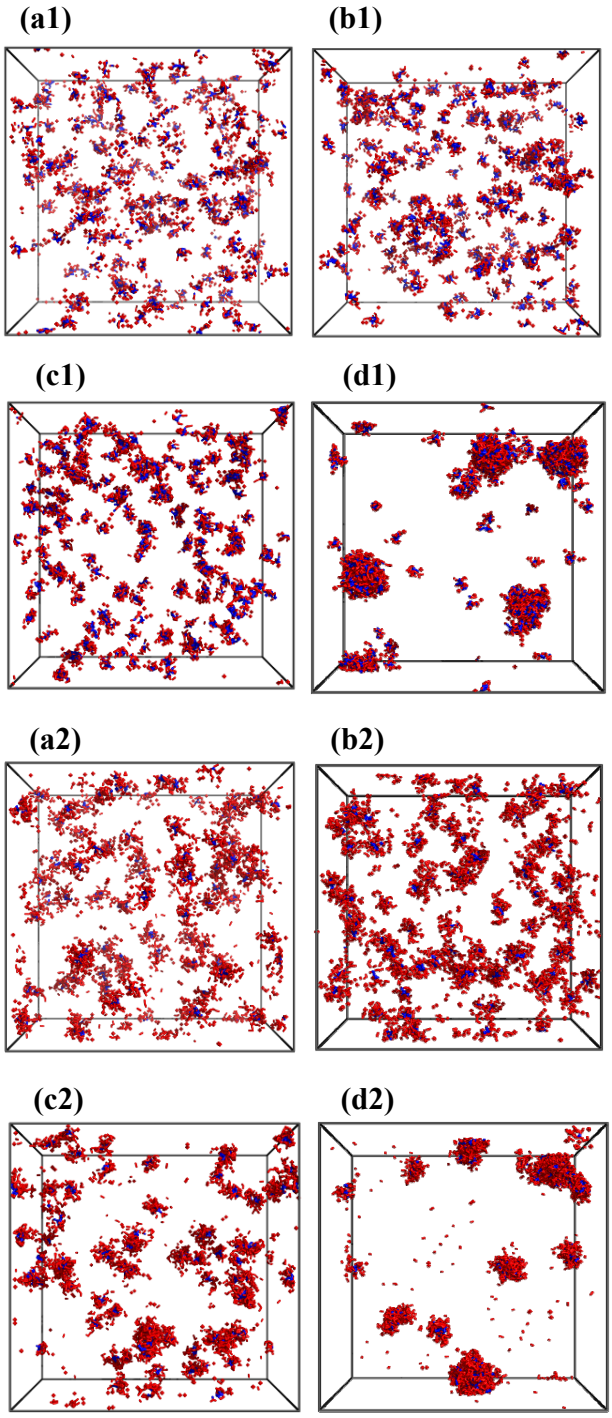

Figure S2. The morphologies of the micelles formed after 500000-step DPD simulations from dendritic multiarm copolymers, the concentration is 1%, a_{AC}=40 and a_{AB}=35: (a1-d1) is for model **a**, (a2-d2) is for model **c**; (a1-a2) a_{BC}=24, (b1-b2) a_{BC}=26, (c1-c2) a_{BC}=28, and (d1-d2) a_{BC}=30. Water beads are omitted for clarity. The color codes are the same as those in Figure S1.

S3. The ms-SM structures based on models a and c

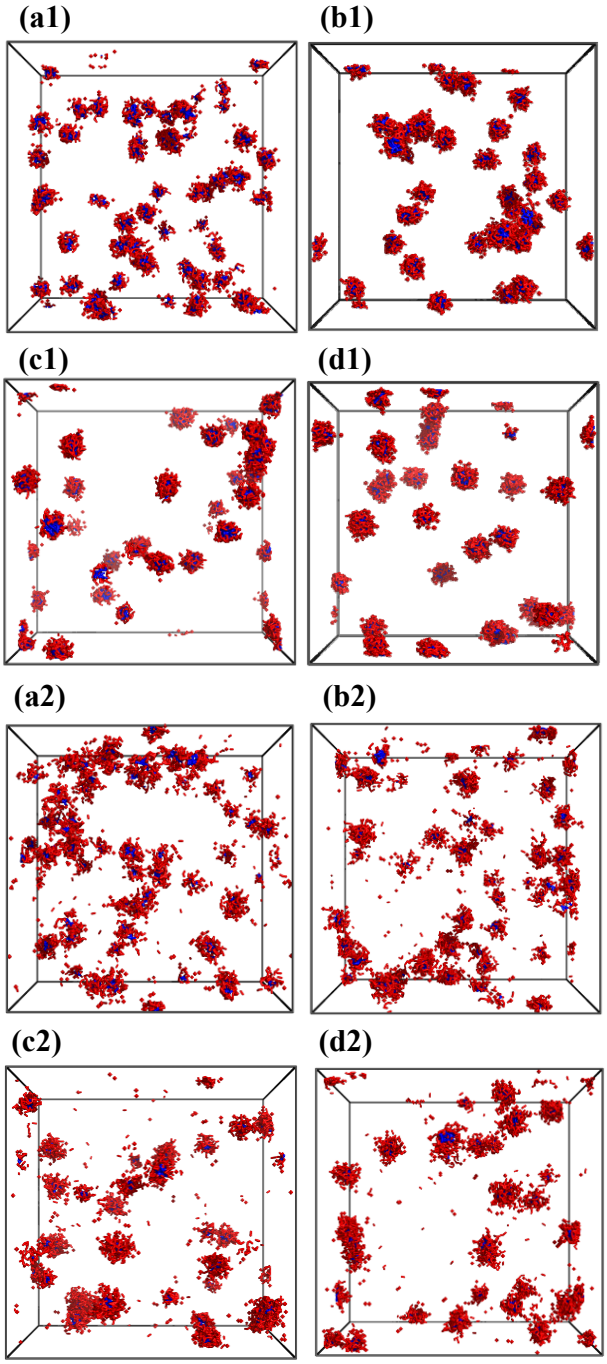

Figure S3. The morphologies of the micelles formed after 500000-step DPD simulations from dendritic multiarm copolymers, the concentration is 1%, a_{BC}=27 and a_{AB}=45: (a1-d1) is for model **a**, (a2-d2) is for model **c**. (a1-a2) a_{AC}=60, (b1-b2) a_{AC}=90, (c1-c2) a_{AC}=150, (d1-d2) a_{AC}=200. Water beads are omitted for clarity. The color codes are the same as those in Figure S1.