Abstract Submitted
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Effect of Hydrophobic Block Length on Vesicle Formation of Block Copolymers[1] RONG WANG, Nanjing University, Department of Polymer Science and Engineering, State Key Laboratory of Coordination Chemistry, MENGYING XIAO, DAIQIAN XIE, Nanjing University, Insistute of Theoretical and Computational Chemistry, Key Laboratory of Mesoscopic Chemistry — Self-assembly of amphiphilic block copolymers result in a wide range of aggregates in aqueous solution, including spheres, rods, lamellae, vesicles, and large compound vesicles with an inverted core-shell structure surrounded by hydrophilic surface. In the work, we carried out a systematic investigation of A1BnA1 triblock copolymers with different hydrophobic block length by using the dissipative particle dynamics (DPD). As the B/A ratio increase further, no well-defined disk-like micelles (bilayer structures) are seen. Spherical micelles rearrange internally and swell the hydrophilic group in the center until vesicles are formed. Because the longer chains appear to drift slowly, it is clear that the rearrangement process becomes slower in the system with longer hydrophobic block, which needs more time to form vesicles. The segregation of A segments (hydrophilic group) leaves in the internal layer when the two small spherical micelles merge into a larger one. We observe that the existence of the two pathways of vesicles formation based on the hydrophobic block length using DPD particle models.

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