Self-assembly of Giant Molecular Shape Amphiphiles in Solution
RONG WANG, SHIYING MA, Nanjing University — The self-assembly of giant molecular shape amphiphiles consisting of a hydrophilic head and one or more hydrophobic tails is investigated by dissipative particle dynamics. The morphology can transform from vesicles to worm-like cylinders and further to spheres by increasing the interaction parameter between the hydrophilic heads. The results are in agreement with the experimental observations. Through changing the interaction parameter between hydrophilic head and solvents, the length of hydrophobic tail and the size of hydrophilic head, the self-assembled aggregates exhibit a rich variety of morphological structures, such as, spheres, vesicles, worm-like cylinders, disk-like micelles and layered-rod-like micelles. Vesicles form for short hydrophobic tail, while disk-like micelles are taken shape for longer hydrophobic tail. As further increasing the diameter of hydrophilic head, large compound micelles are obtained for short hydrophobic tail, however layered-rod-like micelles form for longer tail. The simulation findings might be valuable for guiding the experimental studies and fascinating new possibility and applications in material science. This work was financially supported by NNSFC (21474051 and 21074053), NBRPC (2010CB923303) and PCSIRT.

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