

Abstract Submitted
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Self-assembly of Giant Molecular Shape Amphiphiles Studied by Dissipative Particle Dynamics¹ SHIYING MA, RONG WANG, Nanjing University — The self-assembly of giant molecular shape amphiphiles is investigated by dissipative particle dynamics. Depending on the hydrophobic block length, molecular concentration, and the size of hydrophilic head, the aggregate exhibits a rich variety of morphological conformations, including vesicles, spherical micelles, tower-type disk-like micelles, onion micelles and cylinder micelles. And the morphological phase diagram is also obtained. At a fixed hydrophobic block length the aggregates change the morphology from spheres to cylinders further to vesicles with increasing molecular concentration. In the lower molecular concentration, the shape amphiphiles with different length of hydrophobic block always adopt spherical micelles. However, in the high molecular concentration, the micellar morphological formation of spheres, vesicles, and multi-layers is dependent on both the molecular concentration and the hydrophobic block length. These simulation findings are consistent with experimental observations.

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