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Dissipative Particle Dynamics Simulation of Structure Properties of Lipid Micelles JINSUO ZHANG, YI JIANG, MSK-575, Los Alamos National Lab — We chose dissipative particle dynamics (DPD) simulation to study the micelle structure properties. The self-assembly lipid is modeled by a flexible chain with head and tail particles. By changing interaction parameters between the solution particles and the lipid particles, three types of solution are considered: water, oil and water-oil mixture. It is found that the tail/head chains forming the micelle core have a very disorder distribution. The relation between the core radius with the aggregation number as well as the number of oil particles inside is obtained based on the simulation results and the molecular packing parameter. The mean density of particles in the core is higher than that in the simulation box. For micelles without oils inside, the density depends on the number of head particles in a lipid molecule, and the dependence becomes weaker as more oil particles are captured. At the core surface, head particles form clusters with water particles incorporated between the clusters. Comparisons with results from other simulation method such as MD show that DPD achieves high performance in simulating micelle formation and structure properties.

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