Simulation on Coarse-grained Models of Amphiphiles

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(April 16, 1999)

Abstract

Studies of amphiphiles and other soft condensed matter systems, *e.g.* polymers, membranes *etc.*, have become an important area of research in recent years. Not only they show promises for prospective technological applications, but the physical phenomena occurring in these systems are often very different than that of small molecular systems. An amphiphlic molecule consists of two parts with opposite characters: a water loving (hydrophilic) "head" and a water avoiding (hydrophobic) "tail". Because of this duality in one unit, they can arrange themselves in a variety of structures in water, ranging from globular and cylindrical clusters (called spherical and cylindrical micelles), to bilayers, vesicular structures *etc.*. Surfactants, which occur in soap that we use everyday, phospolipid molecules, that occur in biological systems are examples of such amphiphiles. The self-assembling properties of these amphiphilic systems are quite complex. Naturally, computer simulations have been quite successful and extremely useful in providing insights into the various mechanisms of self-assembly. We will introduce coarse-grained models for the amphiphiles, both on lattices and in continuum and present simulation results for a variety of systems. We will also address the effect of the intermicellar interactions on the structural properties of self-assembled micelles.