

Coarse-Grained Model of PEG Surfactants

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We present a systematic approach to build a new coarse-grained (CG) molecular model for polyethylene glycol (PEG) surfactants in the presence of water. The intramolecular bond potentials are determined to reproduce the bond and angle distributions based on the all-atom molecular dynamics (AA-MD) simulation data. A careful choice of the potential function for non-bonded interactions is essential for better structural properties. We adopt two Lennard-Jone (LJ) functions, namely LJ12-4 and LJ9-6. In most cases, the density and surface/interfacial tension are used as target properties for the parameter fitting, because these are of key importance in characterizing the self-organized surfactant structure in the mesoscale that is the plausible target of CG-MD. By using dozens of small molecular systems for the parameter fitting, the CG model has versatility and transferability. Solvation (hydration) and transfer free energies, which play an essential role in determining of the partition of solute molecules, are also taken into account in our model. For example, our model reproduces the transfer free energy of a hexane molecule from its bulk to water. Two different techniques (rapid growth using steered MD and thermodynamic integration using a series of constraint MDs) are successfully used in the free energy calculations. This approach should be also useful for the CG mapping of a variety of biological molecules, including peptides, cholesterol, and drugs.

The obtained CG model for PEG surfactants self-assembled into micelle, lamellar, hexagonal

structures, showing a good agreement with experiments at given conditions. As an example, a lamellar formation of a PEG surfactant, $C_{12}E_2$, is shown in Fig. 1. The MD simulation is started from a random initial configuration. It takes more than 8 ns to have a defect-free lamellar structure. The molecular area of the PEG surfactant shows a good agreement with the experimental value. The density profile of each component across the CG membrane is also in good accordance with that obtained from AA-MD.

Our approach is useful for a general purpose and will open a way for a systematic CG modeling.

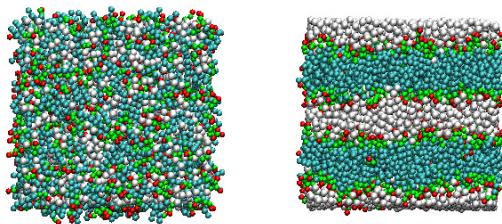


Figure 1. Snapshots of lamellar formation of the $C_{12}E_2$ /water system from a random initial configuration. Initial (left) and final (right) configurations.