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Extended Abstract

A Novel Coarse Grained Model for Simulating Micelles

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I. INTRODUCTION

Soft matter which includes liquid crystals, surfactants and colloids, can organise into various structures of mesoscopic dimensions. Although these phenomena are exceptionally interesting and increasingly relevant to several fields, they are also challenging to computationally model. Difficulties arise from the intermediate length-scales and time-scales of these structures which make the simulation model computationally demanding.

The focus of this study is placed on micelles, specifically on decreasing the time-scale required to observe dynamic phenomena such as formation, fusion and fission.

A. Surfactants and Micelles

A surfactant is a molecule that contains both hydrophilic and hydrophobic moieties. A micelle is a semi-organised aggregation of surfactant molecules in solution. Normally hydrophilic head of the surfactant molecules are orientated towards the solution and hydrophobic tails inside the aggregated structure. (Fig. 1) Although the properties and applications of micelles are well established,[1,2] their dynamics are poorly understood.

B. Computational Model

The coarse-grain method is employed for this simulation. Various continuous potentials are often used in this method to simulate various interactions between different particles.[3] While continuous potentials are desirable to approximate the simulation model as

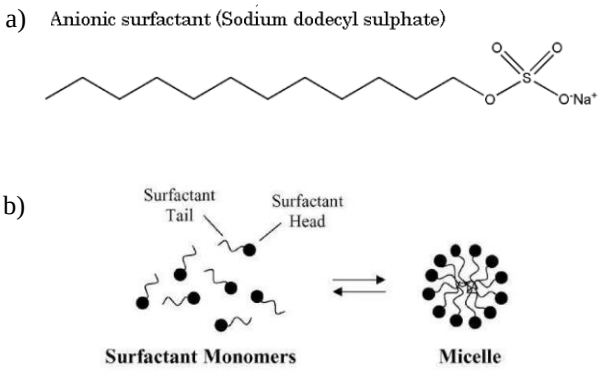

Figure 1. a) The model surfactant used in this simulation. b) Schematic diagram of dynamic equilibrium between a micelle and monomers in solution.[2]

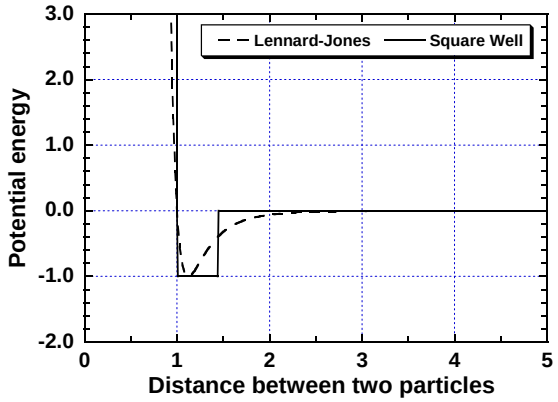

Figure 2. Comparison of the two potentials. Continuous potential (dashed line) is often used to model attractive interactions. The approximation of this potential (solid line) is used in this simulation.

accurately as possible, this sacrifices length of time the simulation may be reasonably run for (time-scale). Since the aim of this study is to extend this time-scale, square well potentials are used instead (Fig. 2).

The model uses 1-head-6-tail particle surfactants, with head groups that are twice the radius of the tail sphere. Tail spheres attract each other, head sphere and solvent sphere attracted, and all other interactions are repulsive. 50 surfactant molecules were used. 28% (volume/volume) of the simulation box was occupied by particles, of which 18 % was solvent.

II. RESULTS AND DISCUSSION

Clear images of aggregation are observed from running this simulation, with more than half of the surfactant molecules involved in forming ordered structures. Up to 20 surfactant molecules were observed in the formation of a micelle.

The program demonstrates that continuous potentials are dispensible in observing the micelle formation.

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