Molecular Dynamics Simulation of Langmuir Monolayers

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For the past 40 years molecular dynamics simulations have been carried out for investigating behaviors of complicated molecular assemblies. In recent years the computer simulation for the monolayer of amphiphile molecules have been conducted by many researchers.

In this study we are going to demonstrate the usefulness of molecular dynamics simulation for the amphiphile molecules on water. The simulation was performed with amphiphile molecules subjected to potentials restricting bond lengths, bond angles, internal rotations and interacting with neighboring " united atoms" according to a truncated Lennard-Jones potential. Water-amphiphile interaction effect was incorporated by choosing a van der Waals type potential function(9-3 type). For the numerical integration of the equation of motion, we used a method suggested by Schofield. At every step temperature control and momentum conservation were performed. Periodic boundary conditions are imposed for the directions parallel to water surface.

The area of the head-group was fixed to calculate the lateral pressure. Special attention was given whether there are phase transitions (the liquid-liquid condensed state,gas-liquid expaned state transitions).