Adsorption of surfactant at air-liquid interface: a molecular dynamics study

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Abstrak

ABSTRAK
The interaction of cationic surfactant (CTAB, Cationic surfactant hexadecyl trimethyl ammonium bromide ((C₁₆H₃₃)N(CH₃)₃BR and TTAB, Tetradecyl
trimethyl ammonium bromide ( )), a prevalent chemical in the industrial
and natural processes, with water ( ) has been studied using GROMACS
program and VMD program. In the following project, to simulate the CTAB and
TTAB at air-water interface, GROMACS (Groningen Machine for Chemical
Simulations) software is used. GROMACS is a molecular dynamics package
designed for primary use of simulation of biochemical molecules like proteins,
lipids, and nucleic acids that have a many complicated bonded interactions
(GROMACS, 2010). Furthermore, to model and display the simulation, VMD
(Visual Molecular Dynamics) program is used. VMD is intended for modeling,
visualization and analysis of biological systems such as proteins, nucleic acids,
lipid bilayer assemblies, etc. In this research project 13 simulations, 6 of these are
successive simulations and the other 7 simulations have been included in the
appendix. The simulations have been simulated to prove the following 3
hypotheses which are ssurfactants has an amphiphilic nature, surfactants adsorb
on the interface between oil and water, lowering the interfacial tension and
promoting mixing and surface potential measurement at the air-water interface
increases surfactant-dependent manner in the air-water expanded transition region.
Therefore with the addition of surfactant to the air-water interface, there will be a
sudden increase of surface potential. The first seven simulations that have been
included in the appendix were simulated to find the right charge distribution. All
the observed results shown by these 13 simulations are not yet predictable or
reliable; this is due to not the right amount of simulation time or the charge
distribution of the cationic surfactant. The three kinds of observations (the density
profile of the cationic surfactant, the surface tension of the cationic surfactant with
water, and the surface potential of cationic surfactant with water) are very
uncertain and therefore many more simulations are required to be completed in
the future.