Molecular Dynamics Study of Classical Complex Systems and Quantum Systems in Condensed Phase

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1. Electrostatic Potential Gap at the Interface between Triethylamine and Water Phases Studied by Molecular Dynamics Simulation[1)]

Molecular dynamics calculations were carried out in order to investigate the interfacial properties of the two-phase coexistence state of the triethylamine (TEA) and water mixture, which is known to have a lower critical soluble temperature. Two kinds of initial configuration were adopted. One was a two-phase coexistence state and the other was a random mixed state of TEA and water molecules. After an equilibration calculation of several nanoseconds, the density profiles converged to the same equilibrated two-phase coexistenc state. In the equilibrated state, anisotropic orientations were observed for both molecules, which makes an electrostatic potential gap between these phases.
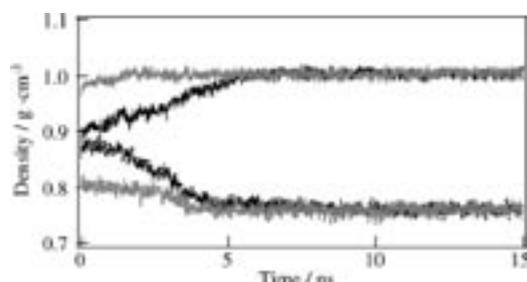
Figure 1. Time evolution of the density of the water phase (solid line) and TEA phase (dotted line) obtained from the MD calculation started from the two-phase state (gray) and from the mixed state (black).
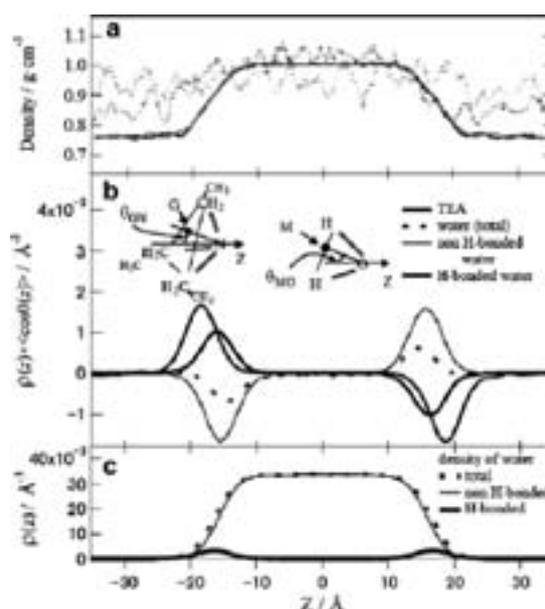
Figure 2. (a) Equilibrated density (solid line) profile calculated from the twophase state (black) and from the mixed state (gray). The corresponding density profile of the initial states is also shown with dotted lines. (b) q(z) A Acosha for TEA molecule (gray) and for water (black) as a function of the z-coordinate. Those with respect to the water molecule, hydrogen bonded (dotted) and non-hydrogen bonded molecules (thin line) to the nitrogen atom of TEA molecule are shown. Definition of hGN and hMO are also shown schematically (see text). (c) Density profile for water molecules.
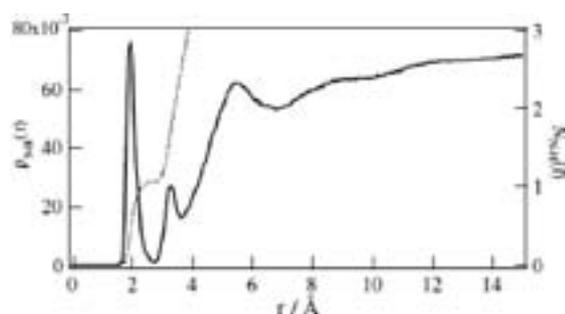
Figure 3. Pair distribution function $\rho_{N-H}(r)$ (solid line) and its running coordination number, $N_{N-H}(r)$ (dotted line), at the vicinity of the interface with a width of 10 Å.
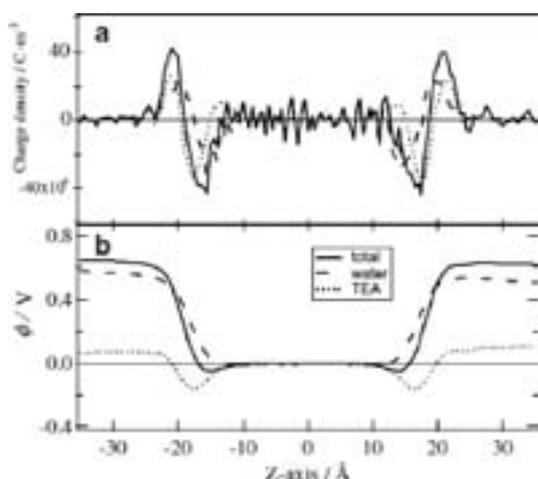
Figure 4. Charge density (a) and electrostatic potential profile (b) as a function of the z-coordinate. Solid line; the total system, dotted line; TEA molecule contribution and broken line: Water molecule contribution.
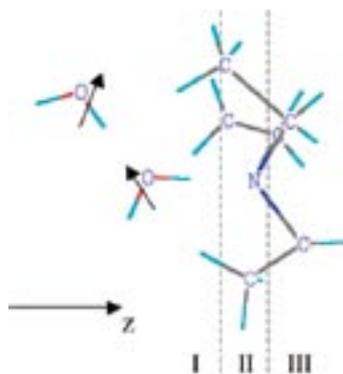
Figure 5. Schematic image of water and TEA molecules at the interface.

We have performed molecular dynamics calculations for the two-phase coexistence state of the TEA and water mixture. At the interface between the two phases, both molecules have unique orientations, which results from hydrogen bonding between TEA and water molecules. These anisotropic orientations lead to a large potential gap of 0.65 V between two phases. Additionally, resulting from the orientation of the TEA molecules, the electric potential has the minimum value in the vicinity of the interface

2. A molecular Dynamics Study of Structure and Dynamics of Surfactant Molecules in SDS Spherical Micelle[2]

An analysis of structure and dynamics of surfactant molecules in SDS micelle is presented based on molecular dynamics calculations. Two-dimensional surface correlation function for the hydrophilic sulfur atoms as well as the bond analysis between the hydrophobic alkyl chains shows that the surfactant molecules are packed sparsely in the micelle such that they form a soccer ball-like structure characterized by the coordination number of three. The hydrophobic bond between the surfactant molecules is produced and annihilated repeatedly in a time scale of about 100 ps but disappears by their diffusion in a time scale of about 1 ns.
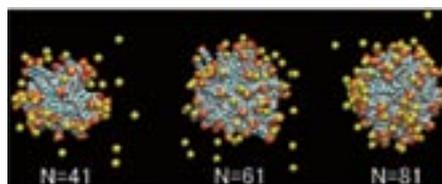
Figure 6. Snapshots of the simulated SDS spherical micelles formed in water. In the figure, water molecules are not drawn just for clarification.

References

1) S. Kajimoto, N. Yoshii, J. Hobley, H. Fukumura and S. Okazaki, *Chem. Phys. Lett.* **448**, 70–74 (2007).
2) N. Yoshii and S. Okazaki, *Cond. Matt. Phys.* **10**, 573–578 (2007).

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