Somyot Srikongrug 2013: The Study of Structure and Dynamics of Water Molecules around Phospholipids Bilayer POPE using Molecular Dynamics Methods. Master of Science (Physics), Major Field: Physics, Department of Physics. Thesis Advisor: Mr. Chalermpol Kanchanawarin, Ph.D. 107 pages.

In this thesis, we investigated the structure and dynamics of water molecules around phospholipids bilayer POPE using molecular dynamics methods. There have been both computational evidence showing a decrease in mobility of water molecules in the vicinity of lipid bilayer due to lipid dipoles. To investigate the issue at atomic details, we performed molecular dynamics (MD) simulations of the POPE membrane bilayer consisting of 144 lipids hydrated in water using TIP3P model (without ions to simplify the problem) and CHARMM forcefields. The POPE membrane system were equilibrated at pressure 1 atm and temperature 310 K for 20 ns. We analyzed the following structural and dynamics properties of water and POPE bilayer (1) area per lipid, (2) bilayer density profile, (3) diffusion of water molecule around the bilayer, (4) number of hydrogen bonds per water molecules, and (5) polarization of water molecules around the bilayer. The analysis was done on the last 1 ns of the MD simulation taken as a 1,000 frame trajectory with the system divided along the z-axis as 460 thin rectangular layers with 4.0 Å thickness by translating the top layer by 0.2 Å distance along the z-axis from the top to the bottom of system. We found that (1) the POPE bilayer has thickness of 36 Å and each lipids occupied an area of 65.03 ± 0.47 Å^2, (2) the POPE bilayer had a density profile consistent with results previously reported by others, (3) diffusion of water molecules were reduced to a third of that in bulk water within the headgroups region of the POPE bilayer, (4) water molecules formed less and less number of hydrogen bonds as they get into the bilayer interior, and (5) water molecules were strongly polarized normal to the membrane bilayer by the dipoles of POPE lipid headgroups. In conclusion, our MD studies show that water molecules are slowed down when they get close to lipid bilayer possibly due to the charges and dipoles on lipids. These slow water molecules may form a planar layer of a hydrogen bonded network that allowed protons to be transported faster along the membrane plane than their diffusion in 3D.

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