

Molecular Dynamics Study of Permeation Process of Small Molecules Through A Lipid Bilayer

Taisuke Sugii, Shu Takagi, Yoichiro Matsumoto

The Univ. of Tokyo, Tokyo, Japan

Recently a cell membrane and a liposome are actively studied in various fields. In this research, the transport characteristics on the lipid bilayer were analyzed using the molecular dynamics method. The free energy profiles of small molecules (O_2 , CO, NO, H_2O , and several artificial diatomic molecules) across the three kinds of pure lipid membranes (DLPC, DMPC, and DPPC) were calculated. We investigated the effect of the polarity of the solute molecules and the length of the hydrocarbon chains of the lipid molecules. Furthermore, we calculated the vdW potential field and the electrostatic potential field. The potential field is very important for the investigation of permeation process because it can represent the local and instantaneous state of the system. In the calculation of the electrostatic potential field, the contribution from the lipid molecules and the water molecules were calculated separately, and it is shown that each profile had own its characteristic.

[View the extended summary](#)