Structure and dynamics of water and lipid molecules in charged anionic DMPG lipid bilayer membranes - DTU Orbit (09/11/2017)

Structure and dynamics of water and lipid molecules in charged anionic DMPG lipid bilayer membranes

Molecular dynamics simulations have been used to investigate the influence of the valency of counter-ions on the structure of freestanding bilayer membranes of the anionic 1,2-dimyristoyl-sn-glycero-3-phosphoglycerol (DMPG) lipid at 310 K and 1 atm. At this temperature, the membrane is in the fluid phase with a monovalent counter-ion and in the gel phase with a divalent counter-ion. The diffusion constant of water as a function of its depth in the membrane has been determined from mean-square-displacement calculations. Also, calculated incoherent quasielastic neutron scattering functions have been compared to experimental results and used to determine an average diffusion constant for all water molecules in the system. On extrapolating the diffusion constants inferred experimentally to a temperature of 310 K, reasonable agreement with the simulations is obtained. However, the experiments do not have the sensitivity to confirm the diffusion of a small component of water bound to the lipids as found in the simulations. In addition, the orientation of the dipole moment of the water molecules has been determined as a function of their depth in the membrane. Previous indirect estimates of the electrostatic potential within phospholipid membranes imply an enormous electric field of 10^8-10^9 V m^{-1}, which is likely to have great significance in controlling the conformation of translocating membrane proteins and in the transfer of ions and molecules across the membrane. We have calculated the membrane potential for DMPG bilayers and found ~1 V (~$2 \cdot 10^8$ V m^{-1}) when in the fluid phase with a monovalent counter-ion and ~1.4 V (~$2.8 \cdot 10^8$ V m^{-1}) when in the gel phase with a divalent counter-ion. The number of water molecules for a fully hydrated DMPG membrane has been estimated to be 9.7 molecules per lipid in the gel phase and 17.5 molecules in the fluid phase, considerably smaller than inferred experimentally for 1,2-dimyristoyl-sn-glycero-3-phosphorylcholine (DMPC) membranes but comparable to the number inferred for 1,2-dilauroyl-sn-glycero-3-phosphoethanolamine (DLPE) membranes. Some of the properties of the DMPG membrane are compared with those of the neutral zwitterionic DMPC bilayer membrane at 303 K and 1 atm, which is the same reduced temperature with respect to the gel-to-fluid transition temperature as 310 K is for the DMPG bilayer membrane.

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