Driving Force for Water Permeation Across Lipid Membranes

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J. Phys. Chem. Lett. **2013**, *4*, 3233-3237.

The diffusion of water, and many small molecules including CO_2 and O_2, across cell membranes is of paramount biological and biotechnological importance. For instance, the permeation of water has a significant role in regulating the ionic concentrations inside of cells. The exchange of CO_2 and O_2 between the red blood cells and the environment is critical for respiratory systems. Given the significance of such permeations, the diving force has never been depicted. In particular, such diffusions across cell membranes are energetically unfavorable processes.

In this regards, we performed atomistic molecular dynamics simulations of water diffusion across zwitterionic dipalmitoyl phosphatidylcholine (DPPC) bilayers and anionic 1,2-dilauroyl-*sn*-glycero-3-phosphol-L-serine (DLPS) bilayers. The membrane conformations of the liquid-crystalline and the gel phases are investigated for both membranes.

- The water permeation across the lipid bilayers is verified regardless of the types of the lipids, and the membrane conformations
- The free energy barrier of water permeation is calculated to be around 23 kJ/mol for the membranes in the liquid-crystalline phase, and around 28 kJ/mol in the gel phases, with a negligible effect of the types of the lipids.
- The fluctuations in the potential energy are found to have a significant, if not the exclusive, role in the transportation of water across lipid membranes

In addition to the permeation of water, this work is valuable to understanding the diffusion of small molecules and ions across cell membranes, as well as the formation of single-file water hydrogen bonding chain inside of carbon nanotubes.

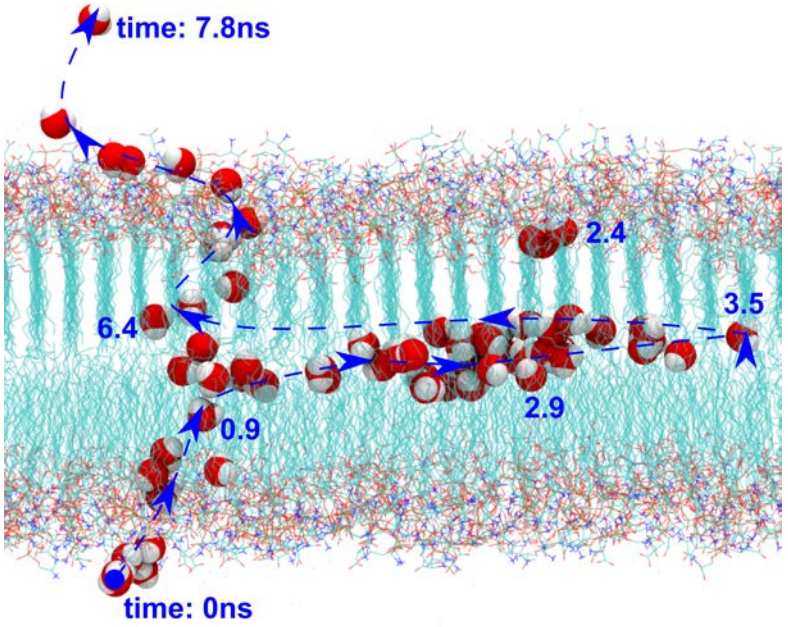

***Figure**:* The permeation process of a single water molecule (highlighted) across a DLPS membrane. The trajectory of this water molecule within 7.8 ns is drawn in the same illustration with the dashed line to guide the eyes and some typical occupations labeled with the time. The other water molecules are removed for clarity..

Funded by the Office of the Director of Defense Research and Engineering (DDR & E) under Award No. FA9550-10-1-0167.