Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Why Hydrophilic Water can Permeate Hydrophobic Interior of Lipid Membranes[1] BAOFU QIAO, MONICA OLVERA DE LA CRUZ, Northwestern University — Water molecules as well as some small molecules have long been found to be able to diffuse across lipid membranes. Such permeation is of significant biological and biotechnological importance. For instance, the permeation of water across lipid membrane plays a important role in regulating ionic concentrations inside of cells. Such water permeation without the assistance of proteins embedded in membranes has been found to be a energetically unfavorable process. We, for the first time, explicitly depict the driving force for such an energetically unfavorable process. Atomistic molecular dynamics simulations are employed to investigate water diffusion in both liquid-crystalline and ordered gel phases of membranes containing zwitterionic DPPC or anionic DLPS lipid. The membrane conformation is calculated to have a critical role in water permeation, regardless of the type of lipid. 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. Our results are also informative for the diffusion of small molecules of CO_2, O_2 and drug molecules, the absence of diffusion of ions, and the diffusion of water into the hydrophobic pores of carbon nanotubes.

[1]The authors acknowledge the support from the Office of the Director of Defense Research and Engineering (DDR & E) under Award No. FA9550-10-1-0167.

Baofu Qiao
Northwestern University

Date submitted: 14 Nov 2013 Electronic form version 1.4