Title: Thermodynamics of pore formation in lipid bilayers

Date: Dec 05, 2013 03:45 PM

URL: http://pirsa.org/13120022

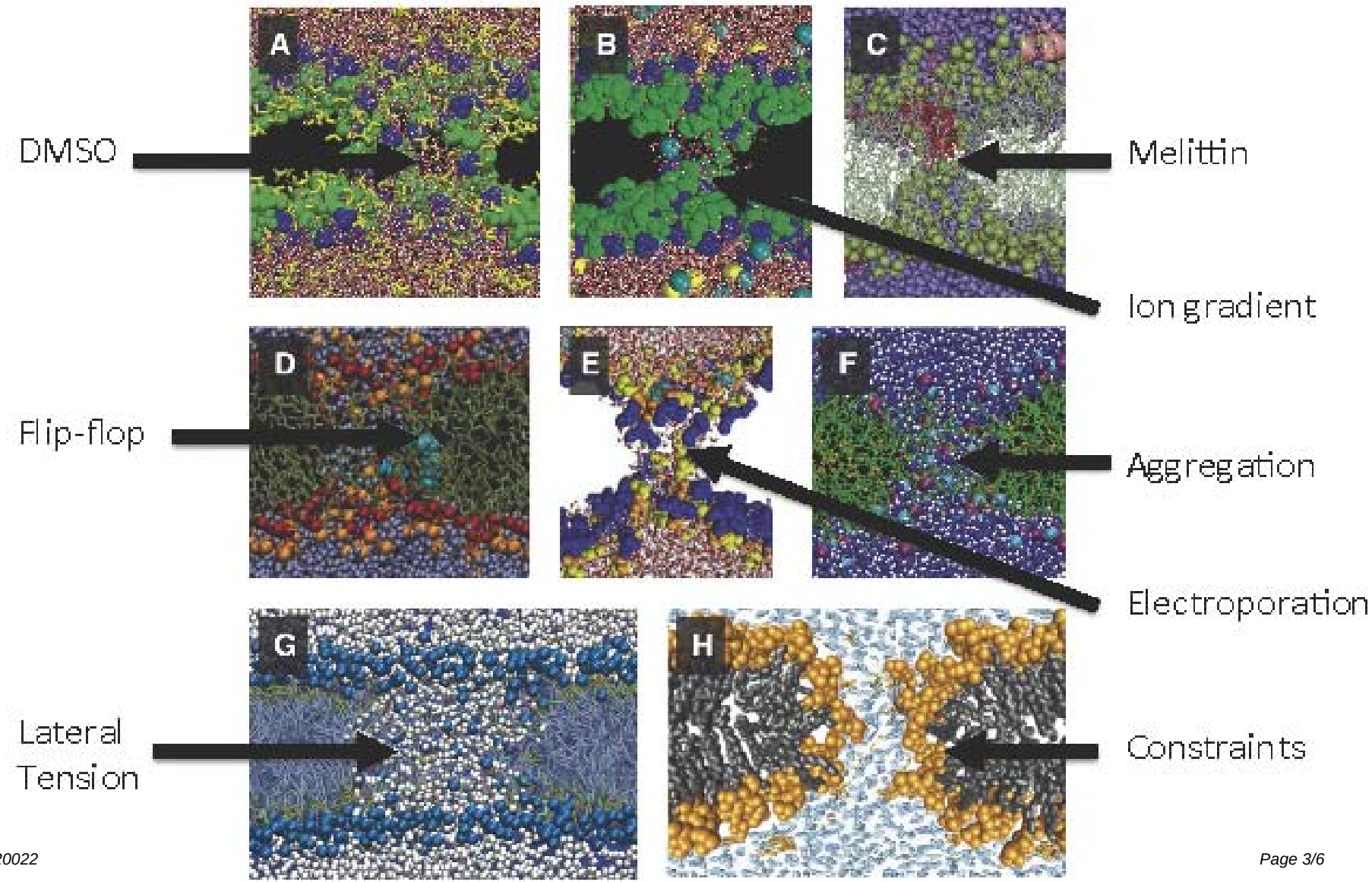
Abstract: Lipid bilayers form the basic structure of cellular membranes creating a semi-permeable barrier necessary for separating distinct chemical environments. Hydrophilic pores can form in bilayers that breach the barrier potentially causing cell death or enhance the uptake of hydrophilic molecules. We use molecular dynamics simulations and free energy calculations to investigate pore formation in model bilayers. The free energy barrier for pore formation is much lower in thinner phosphatidylcholine bilayers compared to thicker bilayers. The free energy barrier is due to an unfavourable change in entropy while the enthalpy of pore formation is favourable. These results have implications on a wide range of biological and biotechnological applications such as drug delivery antimicrobial peptides and transmembrane structure and stability.

Atomistic Simulations of Pore Formation in Model Membranes

Dr. W.F. Drew Bennett
University of Waterloo

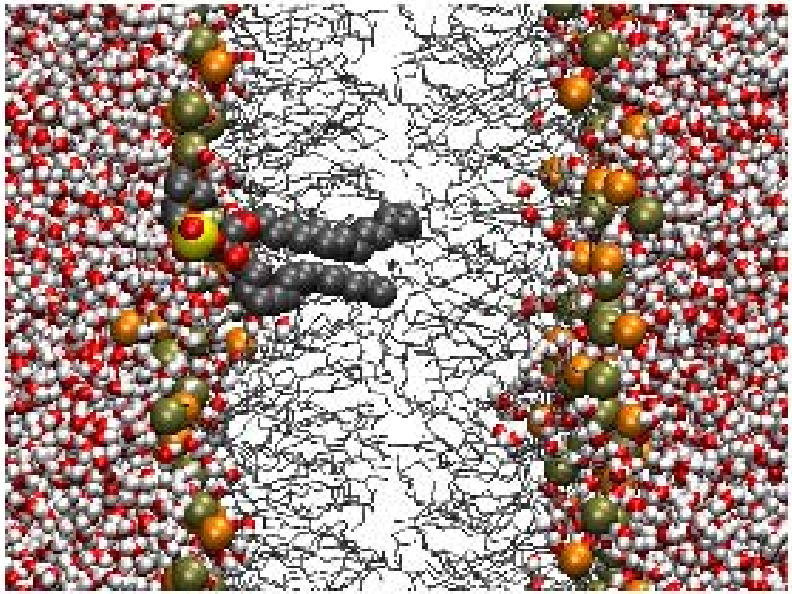
Supervisor: Dr. Mikko Karttunen
Website: www.softsimu.net

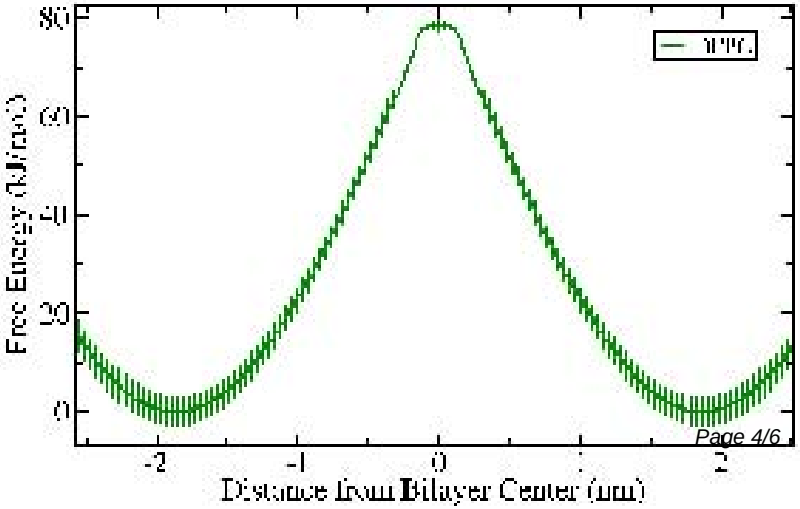
Previous Simulations



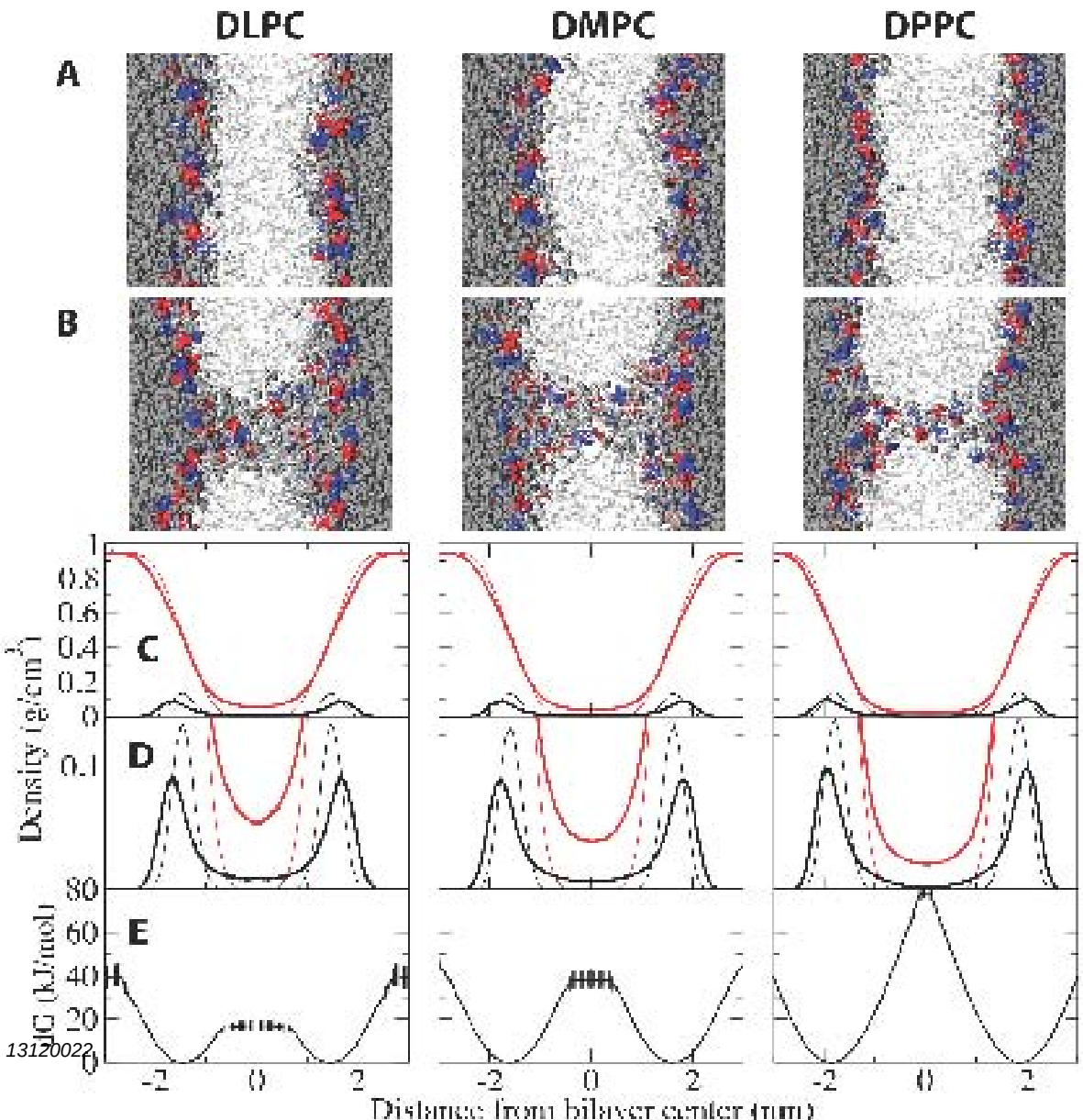
Pore formation: Free energy calculations

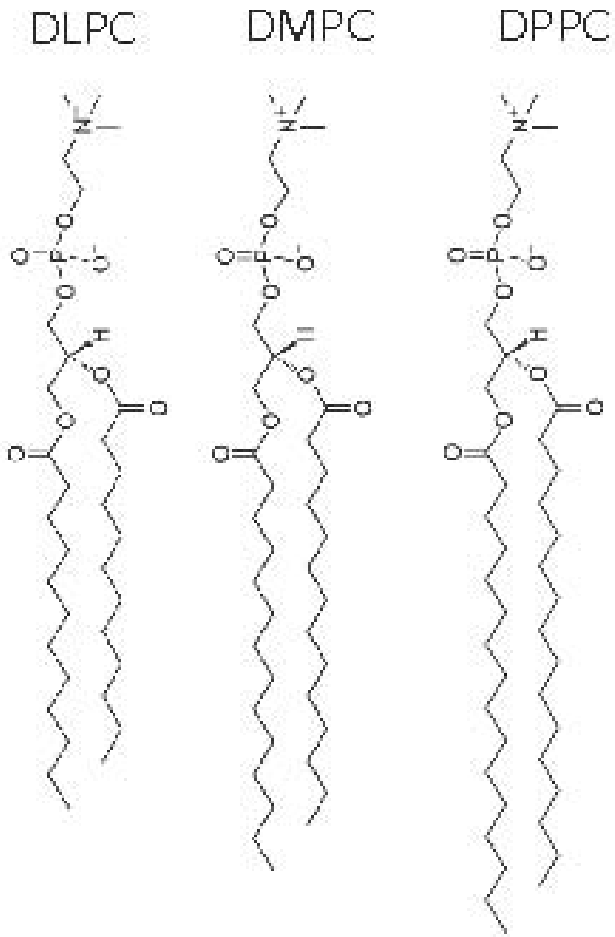
- Atomistic simulations:
  -GROMACS
  -Berger lipids
- Umbrella sampling
- Restrain the phosphate of one lipid with respect to the bilayer center.
- 50 simulations for ~50 ns

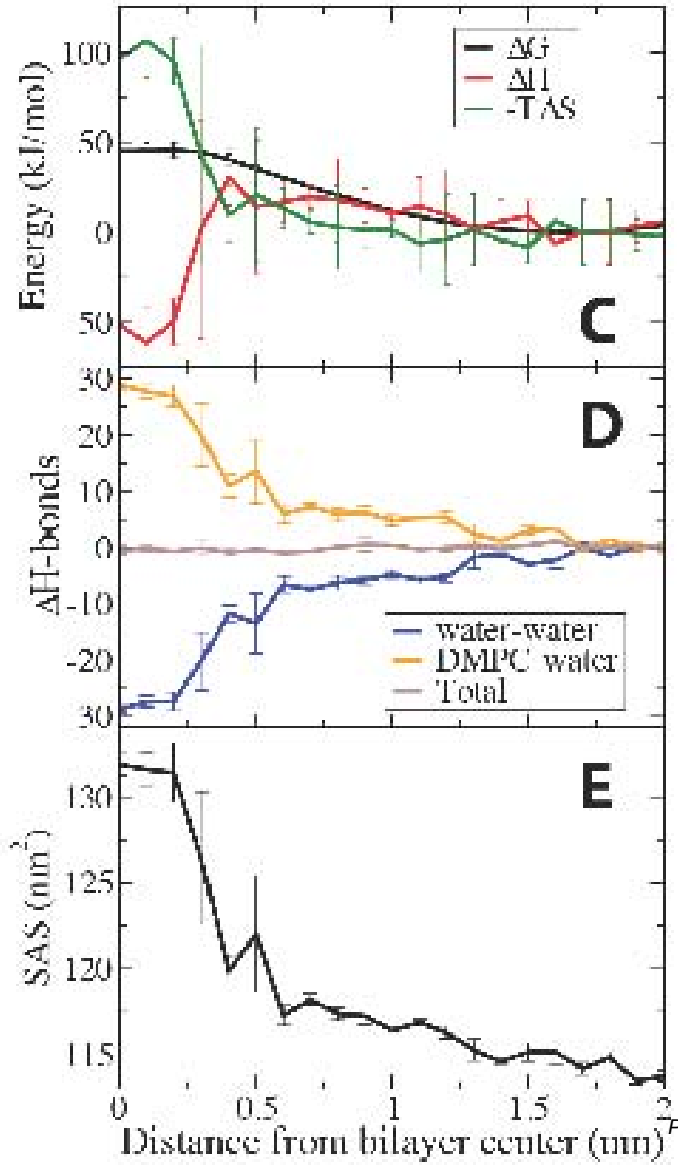




Saturated PC Bilayers





Free Energy Decompositions

- DMPC PMF for lipid flip-flop
- 4 independent US simulations
- ΔH is from the average total energy for the system at each umbrella position
- ΔG = ΔH - TΔS
- mean +/- standard deviation of the mean