

A DPD Simulation Study of Active Membranes

Sanoop Ramachandran*, Mohamed Laradji** and P. B. Sunil Kumar*

*Indian Institute of Technology Madras, Chennai, India

**University of Memphis, USA

sanoop@physics.iitm.ac.in

Lipid asymmetry is actively maintained between the two leaflets of a bilayer membrane by a certain class of proteins known as phospholipid translocators or "flippases" with the expenditure of ATP. By building on the Dissipative Particle Dynamics [1][2] simulation model of a lipid bilayer, we incorporate the action of such proteins on the membrane. We then use this to investigate its effect on the membrane tension profiles and rigidity modulus.

Both cases of symmetric (equal number of up-down lipid flips) and asymmetric (unequal number of up-down) flipping of lipids are considered. We find that the symmetric flipflop activity results in a lowering of the membrane tension without any effect on the bending modulus.

Asymmetric flipping in a localized area results in a lipid number density difference between the two layers. Depending on the rate of flipping, we observe both blister and bud formation. Blister formation occurs at fast flip-rates, where as a bud is formed when the flip-rate is much slower. An interesting observation is that blister formation can result in encapsulation of water particles (which are on the same side as the blister). Where as slow flipping results in encapsulation of water particles from the opposite side. We believe that both these mechanisms are possible in the case of real membranes.

We thus observe that both blister and bud formation can occur as a response to a perturbation in the local lipid number density in a bilayer membrane.

References

- [1] Hoogerbrugge, P. J., and Koelman, J. M. V. A., 1992. Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics, *Europhys. Lett.* 19:155.
- [2] Espanol, P., and Warren, P., 1995. Statistical mechanics of dissipative particle dynamics, *Europhys. Lett.* 30:191.