Molecular Insight into the Line Tension of Bilayer Membranes

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- Lipid bilayer membranes, mainly created by two layers of lipid molecules, are crucial components of cellular machinery (See Fig 1A). Lipids, i.e, amphiphilic phospholipids, possess a hydrophilic phosphate head and two hydrophobic fatty acid tails. In addition to serving diverse biochemical functions like facilitating cellular transport and signal trafficking, lipid bilayer membranes also play a crucial role as barriers, effectively separating cells and organelles from their surrounding environment.
- During important biological processes, such as membrane fusion and fission, the membrane changes its shape. Therefore, objects such as membrane pores and bends can occur, leading to the formation of membrane edges (See Fig 1B). In this project, we will study the physical properties of such edges, including line tension. Line tension acts as a force counteracting the expansion of the membrane edges, working to minimize their presence.
- **Your Task:** Study how different lipid types affect the line tension using simplified versions of membrane models – coarse-grained membrane models – such as Martini (See Fig 1C)
- You will gain experience conducting molecular dynamics (MD) simulations which are a robust and valuable tool for studying the dynamic behavior, energetics, and interactions of diverse biological systems, including membrane lipids, proteins, protein-ligand complexes, nucleic acids.

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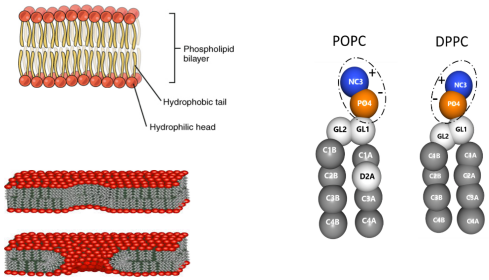

Figure 1 A) Lipid bilayer membrane. B) Two possible conformations of the lipids at the edge of a pore. C) POPC and DPPC Martini lipid model.

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