IITB-Monash Research Academy

An Indian-Australian research partnership

Indian Institute of Technology Bombay | MONASH University

Project Title:	**Multiscale modeling and simulation of bilayers and vesicles**	
Project Number	IMURA0473	
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Research Academy Themes:

Highlight which of the Academy's Theme(s) this project will address?

(Feel free to nominate more than one. For more information, see www.iitbmonash.org)

1. Advanced computational engineering, simulation and manufacture
2. Infrastructure Engineering
3. Clean Energy
4. Water
5. Nanotechnology
6. Biotechnology and Stem Cell Research

he Research Problem

Phospholipid bilayers are important constituents of cellular membranes, and are used to compartmentalize various biomolecules within the cell. These membranes also house macro-molecular assemblies responsible for recognizing and controlling the transport of various biologically active molecules. In fact, more than fifty percent of known drug targets reside in biological membranes. We are interested in understanding how the composition of the bilayer modulates its structural properties (such

as area compressibility modulus, bending stiffness, lysis tension) as well as functional response (including permeability to water and other solutes, adsorption and incorporation of relevant biomolecules such as drugs, peptides etc.).

Project Aims

To this end we plan to use multiscale modelling approach which includes molecular dynamics (MD) and smooth dissipative particle dynamics (S-DPD) to simulate bilayer membranes and vesicles. The model will also account for active materials where force generation takes place via actin polymerization or through molecular motors. The model results will be validated using experimental results including those obtained by micro-pipette aspiration assays, high speed microscopic analysis of vesicle rupture due to osmotic swelling and time-lapse microscopy of active vesicle deformation.

Expected Outcomes

Our efforts will provide a deeper understanding of how bilayer composition and its interaction with biomolecules affects the properties of the membrane and thereby help develop a rational approach towards engineering smart liposomes for drug delivery applications. Furthermore, these studies will also provide insights into the role of molecular motors in the dynamic structural integrity of cells as well as cell motility.

How will the project address the Goals of the above Themes?

The models and simulations developed in this study address Goal 1. The subject of these simulations is biologically relevant membranes and its interaction with biomolecules – this addresses Goal 6.

Capabilities and Degrees Required

- Undergraduate degree in chemical or mechanical engineering
- Good academic background in thermodynamics, fluid mechanics, transport phenomena, numerical computation.