IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Molecular simulations of graphene-polymer composite membranes**	
Project Number	**IMURA0421**	
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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

The research problem

The novel two-dimensional material graphene has attracted tremendous attention for a its widely ranging potential industrial applications. One such application of graphene is in separation and capture technologies, where a composite hybrid material consisting of graphene and polymers can be used to fabricate membranes and thin films with tunable morphologies.The morphology of the hybrid material is a result of the self-assembly process of the two phases, which in turn is governed by the interactions between the polymer and graphene oxide phases. The assembly process is complex because it depends not only on specific chemistry, but on physical aspects such as polymer conformations and entropic effects. A number of these effects occur at the nanometer length scales and are difficult to probe by experiments. In this context, molecular simulations offer a powerful tool to investigate the processes that control the morphologies of these hybrid systems.

This project will utilize multi-scale molecular simulations to study the assembly process of layered graphene-oxide/polymer materials. The multi-scale simulations will consist of large-scale parallel molecular dynamics simulations and coarse-grained simulations.

Project aims

The aims of the project are,

1. Simulate the adsorption of polymers onto a single graphene oxide surface for different surface chemistry using both fully atomistic and coarse-grained molecular simulations
2. Simulate the simultaneous adsorption of polymers onto multiple graphene oxide surfaces using both fully atomistic and coarse-grained molecular simulations
3. Simulate the self-assembly of graphene oxide particles and polymers into layered hybrid systems

Expected outcomes

The following outcomes are expected,

1. Publications in high-impact journals
2. A PhD scholar witha demonstrated expertise in multi-scale molecular simulations
3. This project is expected to provide new knowledge for the molecular design of composite graphenemembranes. Moreover, modelling studies will provide microscopic insight and complement experimental studies.

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

1. This project involves multi-scale simulations requiring high-performance computing to design membrane materials, and hence is aligned with the theme of Advanced Computational Engineering, Simulation and Manufacture.

2. The key structural features and the molecular phenomena of the materials of interest are essentially nano-scale and impact the overall macroscopic performance. Thus tailoring the structure at the nano-scale is a major aspect of this project and makes it highly relevant for the theme of Nanotechnology.

Capabilities and Degrees Required

The prerequisite skills needed in this project are a combination of mathematical modelling capabilities and knowledge of materials science.

Candidates with the following degrees are desirable,

1. B.Tech./M.Tech. in Chemical Engineering, Materials Engineering, Metallurgical Engineering, Mechanical Engineering
2. M.Sc. in Physics, Chemistry (Physical Chemistry with Mathematics in undergraduate program)

Capabilities: An ideal candidate will have a strong interest in computational studies of nanoscale materials. The candidate with some experience and interest in basic programming languages (Fortran/C/ C++/MATLAB) will be preferred

Potential Collaborators

Please visit the IITB website www.iitb.ac.in OR Monash Website www.monash.edu to highlight some potential collaborators that would be best suited for the area of research you are intending to float.

Please provide a few key words relating to this project to make it easier for the students to apply.

Graphene, membranes, hybrid nanomaterials, molecularsimulations,