IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Atomistic Simulations of Graphene–Boron Nitride Hybrid Nanostructures**
Project Number	**IMURA0258**
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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

Define the problem

Graphene—a 2D structure with a honeycomb carbon lattice—is attracting tremendous attention as a promising material for next generation optoelectronic and NEMS applications. Recent developments have shown that it is possible to obtain hybrid 2D structures by combining sp^2-graphene lattice with sp^2-lattice of non-carbon materials such as hexagonal Boron Nitrides. The atomically thin sheets containing both hexagonal-Boron Nitride and graphene can result in new materials with properties complementary to their individual properties and further enrich their potential applications. In this project, using first-principles atomistic and molecular dynamics simulations, we will elucidate thermal, electronic and optical properties of 2D hybrid h-BN and graphene materials.

Project aims

Define the aims of the project

Our aim in the project will be to:

i) Analyze the structure and stability of the composite nanoscale hybrid structures composed of graphene and monolayer hexagonal boron nitride with various shapes, sizes and interface structures.

ii) Once the geometries of these nanoscale structures have been determined we will employ molecular dynamics and first principles calculations to study how their thermal, electronic and optical properties are influenced by the atomic-level structure.

Expected outcomes

Highlight the expected outcomes of the project

By means of the atomistic calculations, we will understand the possible geometrical shapes these composites can acquire, and their optoelectronic structure. By examining the structure-property relations, one can achieve insights about obtaining the ideal heterostructures, which will have optimal and desired thermal and optoelectronic properties. Such information will be used to guide design strategies for the application of graphene in next-generation nanoscale device and architecture.

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

Describe how the project will address the goals of one or more of the 6 Themes listed above.

This project will involve atomistic simulations requiring high-performance computing. Secondly the objects of these studies, namely graphene-h-BN composites are ideal candidates for NEMS, nanoelectronics and nano-optical devices, with tunable properties. Therefore, our project will address the goals of both the themes highlighted above.

Capabilities and Degrees Required

List the ideal set of capabilities that a student should have for this project. Feel free to be as specific or as general as you like. These capabilities will be input into the online application form and students who opt for this project will be required to show that they can demonstrate these capabilities.

Persons with the following degrees should be considered eligible:

i) M.Sc. In Physics or Chemistry
ii) B.Tech/M Tech degree in various engineering disciplines.

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.