

An Indian-Australian research partnership

Project Title: **Experimental and modeling studies of metal/2D layered semiconductor interfaces**

Project Number **IMURA0630**

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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

The recent emergence of 2D materials such as graphene, MoS₂ and other transition metal dichalcogenides (TMDCs) has led to the need to take a fresh look at fundamental understanding of standard semiconductor devices and physics such as metal-semiconductor contacts/interfaces, metal-insulator-semiconductor (MIS) devices, physical/chemical doping, etc for these materials. One of the challenges is in obtaining low resistance contacts as well as the ability to tune the metal/semiconductor interface from being an electron injecting to a hole injecting contact. While low contact resistance is a must have for most high performance devices semiconductor used in computation, communications, etc., tunability of contact properties is important for the ability to design different kinds of p-n devices such as solar cells, p-n junctions, CMOS etc. Specifically in the case of MoS₂, high contact resistance and strong Fermi-level pinning near the conduction band have emerged as problems that need to be

overcome to realize the potential of this promising material in a variety of semiconductor device applications.

Project aims

Define the aims of the project

The project aims at understanding the Schottky barrier formation, contact resistivity for various metals and metal/interfacial layer stacks on mono and bulk 2D layered semiconductor (e.g. MoS₂ layers). This will involve development of metrology/test structures to understand metal/2D material interfaces such as TLM, diode and Kelvin devices. In addition, novel ideas (e.g., interfacial layers, doping etc.) to modulate contact resistivity and carrier injection will need to be developed and tested. The project will aim to fundamentally understand metal/2D semiconductor interfaces through simulations, material and device characterization as well as to develop low resistance, tunable contacts.

Expected outcomes

Highlight the expected outcomes of the project

Objectives: The project's key objectives are:

- 1) Demonstrate high-impact work in the area of 2D materials and devices, more specifically in the area of metal/2D semiconductor interfaces.
- 2) Identify and utilize synergistic capabilities and expertise at Monash and IITB in the areas of device and materials simulations and modelling, materials characterization, device fabrication, device test and analysis
- 3) Strike the right balance between fundamental understanding of metal/2D semiconductor interfaces and developing contact solutions that can enable technology development using 2D layered semiconductors.

Expected Outcomes:

The project will result in the following key outcomes:

- 1) Publications in premier conferences (viz. DRC, IEEE SISC, IEDM, VLSI Tech. Symp. etc.) and high impact journals such as Applied Physics Letters, IEEE Electron Device Letters, Nanoletters, ACS Materials and Interfaces, ACS Nano etc.
- 2) Fundamental understanding of metal/2D semiconductor interfaces and development of metal contact technology for 2D semiconductors.
- 3) Expression of interest and/or engagements with industry partners such as Applied Materials and Sematech
- 4) Identification of key capabilities at both IITB and Monash in the fast emerging area of 2D layered semiconductors that are complementary and can be used to define future projects

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.

The project can address the goals of the following themes:

(I) Nanotechnology:

-It will build semiconductor devices using a 2D semiconductor whose thickness can be controlled at the nanometer scale, i.e. a nanostructured material which can be used in devices for various applications ranging from computation and communications to energy.

(ii) Clean energy:

- A more specific outcome of this project could be in the area of photovoltaics where, if successful, the project may end up demonstrating carrier-selective photovoltaic devices using a nanostructured 2D semiconductor.

(iii) Advanced computational engineering:

- A key aspect of this project is to investigate the electronic structure of metal/semiconductor interfaces using first principles quantum mechanical simulations. These simulations require state-of-art massively parallel high performance computing systems.

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.

The student should have exposure to a good theoretical understanding (coursework and projects) in the areas of :

- (i) Quantum mechanics and solid state physics
- (ii) Solid state devices and materials
- (iii) VLSI fabrication and technology

Qualifying Degrees:

- (i) MSc Physics, Electronics Science
- (ii) B.E/B.Tech/M. Tech in Materials Science, ECE, Engineering Physics

The following experience can be considered as a plus:

- (i) Exposure to hands-on semiconductor device fabrication and cleanroom processes
- (ii) Exposure to materials modelling such as ab-initio/DFT calculation tools
- (iii) Exposure to scientific programming

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.

2D semiconductors, metal-semiconductor contacts, photovoltaics, computational modelling, device transport simulation, first principles simulations