

An Indian-Australian research partnership

Project Title: "Experimental and modeling studies of 2D/2D layered semiconductor heterointerfaces"

Project Number IMURA0970

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Electrical Engineering

Research Clusters:

Research Themes:

Highlight which of the Academy's CLUSTERS this project will address?

(Please nominate JUST **one**. For more information, see www.iitbmonash.org)

- 1 **Material Science/Engineering (including Nano, Metallurgy)**
- 2 Energy, Green Chem, Chemistry, Catalysis, Reaction Eng
- 3 Math, CFD, Modelling, Manufacturing
- 4 CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control
- 5 Earth Sciences and Civil Engineering (Geo, Water, Climate)
- 6 Bio, Stem Cells, Bio Chem, Pharma, Food
- 7 Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng
- 8 HSS, Design, Management

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
- 7 Humanities and social sciences
- 8 Design

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, semiconductor-semiconductor heterointerfaces, physical/chemical doping, etc for these materials. One of the challenges is in obtaining clean 2D/2D heterointerfaces as well as the ability to tune the heterointerface from being type-I to type-II and type-III. While type-II heterointerfaces are essential for most high-performance semiconductor devices used in computation, communications, etc., tunability of heterointerface 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 2D materials, the ability to use electrostatic gating and the van der Waals nature of the heterointerface gives unprecedented control over the heterointerface properties that can lead to novel physics and device applications.

Project aims

Define the aims of the project

The project aims at understanding 2D-2D heterointerface formation, interface band offsets/charge transfer/bandstructure for various 2D-2D layer stacks for mono as well as few layer 2D layered semiconductors (e.g. MoS₂, WSe₂ etc.). This will involve development of metrology/test structures to understand 2D/2D material interfaces such as diodes, Hall bars and transistors. In addition, novel ideas (e.g., electrostatic gating, suspended layers, strain, optical modulation etc.) to modulate interface properties and carrier transport across the heterointerface will need to be developed and tested. The project will aim to fundamentally understand 2D/2D semiconductor interfaces through simulations, material and device characterization as well as to develop tunable 2D/2D heterostructure diodes and transistors.

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 2D-2D semiconductor heterointerfaces.
- 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 2D-2D semiconductor heterointerfaces and developing novel heterostructures 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 2D-2D semiconductor heterointerfaces and development of novel heterostructure technology for 2D semiconductors.
- 3) Expression of interest and/or engagements with industry partners such as Applied Materials
- 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.

(i) Advanced computational engineering:

- A key aspect of this project is to investigate the electronic structure of 2D-2D semiconductor heterointerfaces 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

Necessary Courses

Name three tentative courses relevant to the project that the student should complete during his/her coursework at IITB (the student will require to secure 8 point in these courses)

- (i) EE 733: Solid-State Devices
- (ii) EE 672: Microelectronics Lab
- (iii) EE 724: Nanoelectronics

(iv) EE 784: 2D Materials and Devices

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.

NA

Select up to **(4)** keywords from the Academy's approved keyword list (**available at <http://www.iitbmonash.org/becoming-a-research-supervisor/>**) relating to this project to make it easier for the students to apply.

Nanotechnology, nanoscience, Computer Simulation, Semi Conductors, Materials
Chemistry/Science