IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Atomistic Thermal Transport in Semiconducting Solids**	
Project Number	**IMURA0979**	
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IITB Department:	Mechanical Engineering	

Research Clusters:

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*

Research 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*
7	*Humanities and social sciences*
8	Design

The research problem

The understanding of thermal transport physics in semiconducting solids is crucial for applications such as thermoelectric energy conversion, heat management, nuclear energy, etc. As opposed to metals with plenty of free electrons, the thermal transport in semiconductors is predominantly due to atomic vibrations (phonons). The contribution of phonons towards the thermal transport can be obtained using the classical Molecular Dynamics Simulations and/or quantum/classical Lattice Dynamics Calculations. Semiconducting superlattices, where two different lattices are arranged in a periodic array, such as PbTiO3/SrTiO3/PbTiO3/SrTiO3, are interesting in this regard as this superlattice arrangement results in the scattering of heat-carrying phonons and hence reduced material thermal conductivity which is beneficial for thermoelectric figure of merit. In this project, we will investigate the thermal transport physics in semiconducting superlattices using molecular dynamics simulations and lattice dynamics calculations.

Project aims

Understanding of thermal transport physics in semiconducting superlattices using Molecular Dynamics Simulations and Lattice Dynamics Calculations.

Expected outcomes

Other than several high-impact publications and seeding collaboration between IIT and Monash PI, the project will be helpful in understanding of thermal transport physics in superlattice-like materials. These materials have low lattice thermal conductivity and have potential applications as thermal barriers or thermoelectrics.

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

The project is focussed on the use of computational simulations to understand the thermal transport physics in superlattices which are actively investigated for thermoelectric applications. The thermoelectric energy conversion has a potential to recover waste heat and convert it directly to electricity and thus reducing our energy dependence.

Potential RPCs from IITB and Monash

Prof. Dipanshu Bansal, Mechanical Engineering, IITB – Vibrational spectroscopy and phonons
Prof. Amrita Bhattacharya, MEMS, IITB – Atomic Simulations

Capabilities and Degrees Required

Strong computational and analytical skills. Comfortable with any one of the high-level programming languages (Python, Matlab, Shell, etc). Basic understanding of Materials Science (from undergrad, Intro to Materials Science Course)

Necessary Courses

1. Materials modelling using atomistic first-principles calculations
2. Solid-state/Condensed Matter Physics
3. High-performance computing
4. Any introductory course on Density Functional Theory and Molecular Dynamics Simulations

Potential Collaborators

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.

Modelling and Simulation, Novel Functional Materials, Energy, Materials Science