

An Indian-Australian research partnership

Project Title: **Unravelling the charge and heat transport in thermoelectric Heusler**

Project Number **IMURA0981**

Monash Main Supervisor
(Name, Email Id, Phone)

Prof. Nikhil Medhekar,
nikhil.medhekar@monash.edu

Full name, Email

Monash Co-supervisor(s)
(Name, Email Id, Phone)

**Monash Head of
Dept/Centre** (Name,Email)

Prof. Neil Cameron

Full name, email

Monash Department:

Materials Science and Engineering, Monash

Monash ADGR
(Name,Email)

Timothy scott

Full name, email

IITB Main Supervisor
(Name, Email Id, Phone)

Dr. Amrita Bhattacharya, b_amrita@iitb.ac.in,

Full name, Email

IITB Co-supervisor(s)
(Name, Email Id, Phone)

Full name, Email

IITB Head of Dept
(Name, Email, Phone)

Prof. K. Narasimhan, nara@iitb.ac.in

Full name, email

IITB Department:

Metallurgical engg. And materials science, IITB

Research Clusters:

Research Themes:

Highlight which of the Academy's CLUSTERS this project will address? <i>(Please nominate JUST one. For more information, see www.iitbmonash.org)</i>		Highlight which of the Academy's Theme(s) this project will address? <i>(Feel free to nominate more than one. For more information, see www.iitbmonash.org)</i>	
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8	HSS, Design, Management	8	Design

The research problem

Recovery of waste heat is one of the exploratory areas of research for achieving energy stability worldwide. Thermoelectric (TE) materials have the ability to convert temperature gradient to useful electricity and can be a viable contributor to waste heat recovery. These materials, if optimized, may aid to the improvement of the efficiency of the existing power sector which otherwise incurs a loss of about 66% of the produced energy. The efficiency of thermoelectric devices is governed by a dimensionless parameter, figure of merit (ZT). ZT depends directly on transport properties Seebeck (S), electrical conductivity (σ) and inversely on thermal conductivity (K). These properties are interdependent on carrier concentration (n) are intrinsic to the materials/ compounds used. Among the many compound class explored for potential TE application, the half-Heusler (HH) have emerged as one of the promising ones; having huge chemical space and tunable bandgap for optimization of its performance. In the past, most of the work done in the field of thermoelectrics relied on extensive trial and error synthesis and characterization of compounds, followed by prolong test series for analysing the thermoelectric performance of samples in the laboratory. Apart from being hugely cost ineffective, this also suffers from the possibility of missing out the appropriate dopant or host. After the recent surge of data driven techniques, many studies have been performed on high throughput DFT calculations for identification of TEMs based on their ab initio transport properties. However, the main drawback of these studies is that they do not follow up and verify these ab initio predictions by performing the synthesis and analysis in the laboratory. Ideally one should combine these two approaches in order to effectively screen the compositional space and maximize the performance of the TEMs. We plan to employ a bottom-up hierarchical approach. We propose to perform high through ab initio screening of the compounds for their thermodynamic stability and thermoelectric performance. After selecting the compositions based on their theoretical figure of merit, we plan to synthesize, characterize and analyse the compounds in the laboratory.

Project aims

The proposed research aims at predicting, realizing, and understanding the transport properties of Heusler compounds for their application as typical TEMs. The current work will employ a non-traditional route. State of art first principles calculations and advanced machine learning techniques will be employed to scan a large number of compounds and filter the ones with high electronic transport and low thermal transport coefficients. Thus, the compounds that show a promising zT, will be synthesized using traditional solid state synthesis techniques as has been proposed in the work. Finally, the transport coefficients of these compounds will be measured. Given that the ab initio calculations of thermoelectric transport coefficients act as the backbone here, this work will contribute significantly by shedding light on the various microscopic phenomena that drive the transport properties of these compounds. The experimental results will establish the proof of the concept. Moreover, this route will save wastage of resources, since only the prior identified most promising compounds will be synthesized. We expect our studies to reveal novel and hitherto unknown phenomena, which will provide the guide-lines to improve the thermoelectric efficiency of the Heusler compounds.

Expected outcomes

Thermoelectrics are one of the indispensable, promising, and steadily growing alternatives towards a green and efficient energy economy. The only challenge, for their cost effective and large-scale deployment in devices, is their low figure of merit vis-a-vis their high production cost. The proposed research aims to provide a cost-effective solution for both. This research aims not only to enable a thorough, systematic identification of the efficient thermoelectrics, but also their realisation in the laboratory. Thus, the chances of maximizing the device efficiency are consequential and cost effective. More explicitly the following outcomes can be expected;

- (a) The microscopic phenomena that drive the transport properties in Heusler and similar materials class will be identified.
- (b) The experimental results will establish the proof of the concept.
- (c) Results may reveal novel and hitherto unknown phenomena and guide-lines to improve the thermoelectric efficiency of the Heusler and many similar compound classes.
- (d) Efficient thermoelectric devices can be made.

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

The project addresses directly to the green energy sector since thermoelectrics are very promising alternatives towards achieving one via waste heat recovery. This project has a computational component which will involve state of art simulation techniques as well as machine learning methods. Furthermore, it also will involve the synthesis, characterization and analysis of the transport properties in the laboratory. Thus, it also falls in advanced computational engineering, simulation and manufacture category.

Potential RPCs from IITB and Monash

Prof. Titas Dasgupta
Prof. Satish Vitta
Dr Julie Karel
Prof. Jacek Jasieniak

Capabilities and Degrees Required

Degree: (1) MSc in Physics/ Applied Physics/ Materials science/ Chemistry (specialization in physical chemistry)
(2) BTech/ MTech in Materials Science/ Materials engineering/ Applied physics/ Electronics/ Electrical
Prerequisites: Quantum Mechanics I and II, Basic solid state physics, Basic programming and plotting skills, Numerical methods

Necessary Courses

- (a) Electronic properties of materials (MM318)
- (b) X ray diffraction and electron microscopy (MM684)
- (c) First principles approach to materials science (MM747)
- (d) Thermoelectric materials (MM747)

Potential Collaborators

- (a) Prof. Titas Dasgupta (MEMS, IITB)
- (b) Prof. Satish Vitta (MEMS, IITB)

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.

Green Chemistry and Renewable Energy, Computational and Theoretical Chemistry, Materials Chemistry/Science, Modelling and Simulation