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Indo-German workshop

On

THERMOELECTRIC DEVICES FOR EMERGING APPLICATIONS (IG-WTEA)

26-28th FEB 2024

Generators (TEGs) Space Applications Sensors and IoT Micro - thermoelectric Modules Active Cooling

IGSTC

Indo-German Workshop on

Thermoelectric

Devices for Emerging Applications

(IG-WTEA) Devices

26th - 28th Feb 2024

IISER THIRUVANANTHAPURAM

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VENUE

Trivandrum, India

INDO-GERMAN SCIENCE AND TECHNOLOGY CENTRE

Indo-German workshop

On

THERMOELECTRIC DEVICES FOR EMERGING APPLICATIONS

IG-WTEA

Coordinators

VINAYAK KAMBLE
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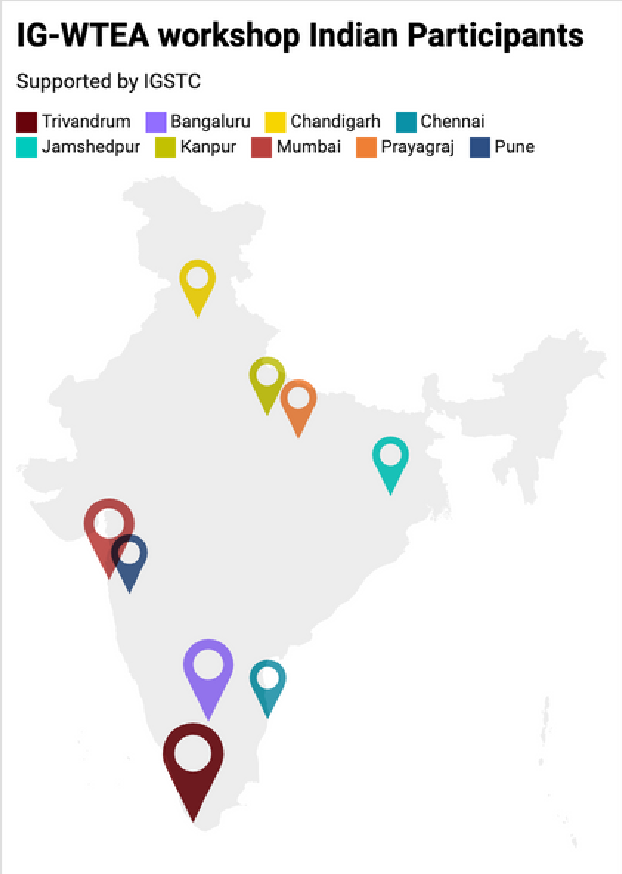
About
School of Physics, IISER Trivandrum

IISER Thiruvananthapuram (IISER TVM, in short) is part of the Western Ghats Mountain ecosystem located at Vithura, 40 km away from Thiruvananthapuram, Kerala, at the foothills of the Agasthyamalai hills. The School of Physics at IISER TVM is nestled amidst lush greenery and provides a breathtaking setting for academic work. We have a total of 29 faculty members where 15 work in theoretical areas whereas 14 are experimentalists. We offer five-year BS-MS and two-year MSc programs to provide high quality education, integrating it with outstanding research at the undergraduate level itself to develop a spirit of enquiry across the disciplines. Furthermore, a newly conceptualized five-year BS-MS programme in Integrated and Interdisciplinary Physics (i2 Physics) is launched to equip tomorrow's workforce with skill that meet the evolving needs and challenges of the modern word. This require integrated expertise and interdisciplinary knowledge across physics, chemistry, biology and mathematics. We are proud to have vibrant Integrated-Ph.D. and Ph.D. programs dedicated to train and prepare future scientists.

IG-WTEA

Participants



IG-WTEA

German Participants

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Nils Katenbrink	Quick-Ohm Küpper & Co.
Mofasser Mallick	Karlsruhe Institute of Technology
Dennis Hohlfeld	University of Rostock
Peter Woias	IMTEK, Albert-Ludwigs-Universität Freiburg

IG-WTEA

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Name	Affiliation
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Arindam Ghosh	IISc Bangalore
Titas Dasgupta	IIT Bombay
Tanmoy Maiti	IIT Kanpur
Bivas Saha	JNCASR, Bangalore
Surjeet Singh	IISER Pune
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Chandan Bera	INST Mohali
Amrita Bhattacharya	IIT Bombay
Sivaprahasam D	ARCI, Chennai, India
Ravi Golani	Tata Steel, Jamshedpur
Joy Mitra	IISER Thiruvananthapuram
Vinayak Kamble	IISER Thiruvananthapuram

Program Schedule

Indo-German Workshop on Thermoelectric devices for Emerging Applications

Venue: IISER Thiruvananthapuram, India

Venue: Chemical Sciences Block, Seminar hall.

Day 1 : 26th Feb 2024		
Inaugaration and IGSTC session	10.00 - 10.30 am	Opening Remarks by **Prof. S. Srinivasula Murthy** Deputy Director, IISER Thiruvananthapuram Brief overview of R&D activities at IISER TVM by **Dr. R. S. Swathi,** Associate Dean (R&D, Consultancies), IISER TVM
	10.30 -11.00 am	**IGSTC session: Dr. Lalitha P. V** Funding opportunities with Indo-German Center
Group photo		
11.00 - 11.30 am Tea / Coffee break		
Session 1 **Chair: Vincent Linseis** **Disruptive developments in TE Material and Applications**	11.30 - 12.00 noon	**Kanishka Biswas, JNCASR, Bangalore** Enhanced Atomic Ordering Leads to Ultra-High Thermoelectric Performance
	12.00 - 12.30 pm	**Dennis Hohlfeld, University of Rostock** Fabrication and Characterization of a TEG for Electrically Active Implants
12.30 - 1.30 pm Lunch break		
Session 2 **Chair: Titas Dasgupta** **Modelling and simulation in TE devices I**	1.30 -2.00 pm	**Chandan Bera, INST Mohali** Theoretical and Computational Studies of Thermoelectric Nanomaterials
	2.00 - 2.30 pm	**Amrita Bhattacharya, IIT Bombay** First principles approach to predict the stability and transport properties of Heusler compounds for thermoelectric applications
2.30 - 2.45 pm Tea / Coffee break		
Session 3 **Chair: Surjeet Singh** **TE in engineered 2D hybrids**	2.45 - 3.15 pm	**Bivas Saha, JNCASR Bangalore** Functional Nitride Thin Films and Superlattices for Thermoelectric Application
	3.15 - 3.45 pm	**Arindam Ghosh, IISc Bangalore** Flow of charge and heat in high-quality graphene and hybrids.
3.45 - 4.00 pm Tea / Coffee break		
Session 4 **Chair: Saskia Fischer** **Recent advances TE materials and application**	4.00 - 4.30 pm	**Peter Woias, IMTEK, Albert-Ludwigs-Universität Freiburg (online)** Thermoelectric energy harvesting: From generator design to system application
	4.30 -5.00 pm	**Tanmoy Maiti, IIT Kanpur** Oxide composites: A viable route for high temperature thermoelectric power generation
7.00 - 9.00 pm Cultural program and Conference Dinner Venue: Hotel Rohini international, Vithura		

Indo-German Workshop on Thermoelectric devices for Emerging Applications

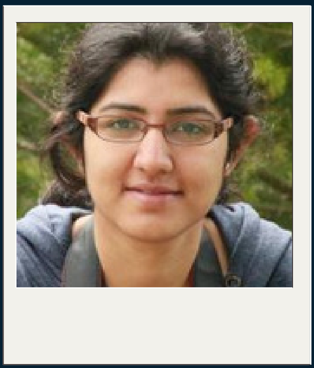
Venue: IISER Thiruvananthapuram, India

Day 2: 27th Feb 2024		
Session 5 Chair: Johannes de Boor **TE Measurement and Metrology**	9.30 - 10.00 am	**Saskia Fischer, HU Berlin** Influence of geometry and size on transport processes: Considerations for thermoelectric device design
	10.00 - 10.30 am	**Joy Mitra, IISER Thiruvananthapuram** Measuring thermal and electrical transport of anisotropic nanocomposites
	10.30 -11.00 am	**Vincent Linseis, Linseis Messgeräte GmbH** Thermoelectric Metrology: A Comprehensive Review from a Manufacturer's Perspective
11.00 - 11.30 am Tea / Coffee break		
Session 6 Chair: Biswapriya Deb **Talks on Industry TE research**	11.30 12.00 noon	**Ravi Golani, Tata Steel, Jamshedpur** Harnessing High-temperature Radiant Waste Heat from Hot Steel Slab using Thermoelectric Generator at Tata Steel Ltd
	12.00 - 12.30 pm	**Nils Katenbrink, Quick-Ohm Küpper & Co.** Thermoelectric Cooling – Applications, Challenges and Potentials
	12.30 - 1.00 pm	**Sivaprahasam D., ARCI, Chennai** Fabrication and characterization of P-type the rigid thermoelectric devices composed of NaxPb1-xTe – Mg2Si1-xSnx, BixSb1-xSe-(Bi1-x-ySbxMy)Te3 compounds
1.00 to 2.00 pm Lunch break		
2.00 - 2.30 pm		**Discussion: industrial ventures, possible collaborations,** project specific requirements and looking for a certain expertise.
Session 7 Chair: Dennis Hohlfeld **Modelling and simulation in TE devices II**	2.30 - 3.00 pm	**Titas Dasgupta, IIT Bombay** Multi-band Modelling of Thermoelectric Materials: Applications in Materials and Devices
	3.00 -3.30 pm	**Rekha Varma, IIIT Allahabad** Electron-phonon coupling and related transport properties in two-dimensional semiconductors
3.30 -3.45 Tea / Coffee break		
Session 8 Chair: Deepshikha Jaiswal-Nagar **Recent advances: TE alloys composites and TE application**	3.45 -4.15 pm	**Ran He, IFW (Online)** Half-Heusler thermoelectric materials: Towards the decoupling between electrons and phonons
	4.15 -4.45 pm	**Surjeet Singh, IISER Pune** Enhancing Thermoelectric Performance through Innovative Strategies in Defective Half-Heusler Alloys
	4.45 -5.15 pm	**Johannes de Boor, DLR** Mg_2Si-based thermoelectric materials and devices: progress and challenges, in particular interdiffusion phenomena
7.00 - 9.00 pm Dinner and Networking Session Venue: River County Restaurant.		

Day 3 : 28th Feb 2024		
Session 9 Chair: Rekha Varma **Material challenges for TE devices**	9.30 -10.00 am	**Vijaykumar, NIIST Thiruvananthapuram** Thiophene-based Organic Thermoelectric Materials: Insights into Structure-Property Relationships and Doping Mechanisms
	10.00 - 10.30 am	**Vinayak Kamble, IISER Thiruvananthapuram** Thermoelectric energy harvesting using chalcogenide thin films.
10.30 - 10.45 am		Tea / Coffee break
Session 10 **Chair:** Nils Katenbrink **Printed and Flexible TE devices**	10.45 – 11.15 am	**Biswapriya Deb, NIIST Thiruvananthapuram** Polymer composites for Lightweight Thermoelectric Generators
	11.15 -11.45 am	**Mofasser Mallick, KIT** Ag2Se/Sb1.5Bi0.5Te3-based fully printed origami thermoelectric module for low-grade thermal energy harvesting
Session 11 Chair: Vinayak Kamble **Industry talk**	11.45 - 12.00 noon	**Subash Pai,** Excel Instruments, India Our encounters with TEG and related instrumentation
12.00 - 1.00 pm		Lunch break
Session 12	1.00 pm	**Rajasekhar P. VIT Vellore.** Thermoelectric Properties of Higher Manganese Silicide Synthesized through Molten Salt Shielded Synthesis Method
Chair: Ravi Golani **Young Researchers session**	1.15 pm	**Pintu Singha, IISER TVM** Thermoelectric and magneto transport properties of Bismuth Chalcogenide topological insulator
	1.30 pm	**Nithin P., IFW** Geometry optimization of micro thermoelectric devices
	1.45 pm	**Sanyukta Ghosh, DLR** Magnesium Silicide-based Composites: Correlating Composition with Transport Properties at the Micro and Nano-Scale for Effective Energy Filtering
2.00 to 3.00 pm		**Concluding session and vote of Thanks**

INVITED TALKS

Amrita Bhattacharya



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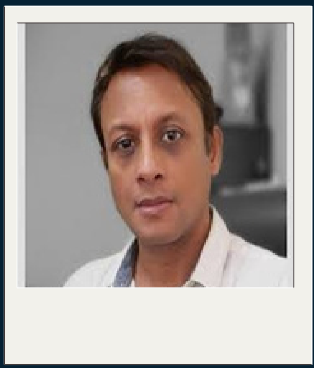
First principles approach to predict the stability and transport properties of Heusler compounds for thermoelectric applications

First principles density functional theory calculations may aid to the issue of cost effective way of rapid prescreening of the periodic table for predicting the properties of compounds prior to their synthesis in the laboratory. The stability prediction from first principles hold the foremost challenge. Using first principles based high throughput calculations and machine learning approaches, we present a pathway to predict the thermodynatic stability of Heusler compounds as a representative class of materials. Thereby, for several thermodynamically stable compounds the electronic properties are studied for their application as thermoelectric materials [1]. Parallely, focussing on half Heusler materials class (XYZ), we perform high throughput calculations to investigate transport properties of stable half Heusler compounds [2]. Thereby, we show that Y site doping is detrimental for enhancing the electronic transport coefficients. However, we find that a small amount of off stoichiometric excess self doping with the Y site elements in these half Heusler compounds, may lead to drastic lowering of the lattice thermal conductivity [3]. Further, we use machine learning to predict the lattice thermal conductivity of semiconducting half Heusler compounds [4].

[1]. P. R. Raghuvanshi, Suman Mondal, and Amrita Bhattacharya, “A high throughput search for efficient thermoelectric half-Heusler compounds”, Journal of Materials Chemistry A, 8 , 25187 (2020).
[2]. Nagendra S. Chauhan, Bhasker Gahtori, Bathula Sivaiah, Subhendra D. Mahanti, Ajay Dhar, and Amrita Bhattacharya*, "Modulating the lattice dynamics of n-type Heusler compounds via tuning Ni concentration", Appl. Phys. Lett., 113, 013902 (2018).
[3]. P. R. Raghuvanshi, D. Bhattacharya, and Amrita Bhattacharya, “Self-Doping for Synergistically Tuning the Electronic and Thermal Transport Coefficients in n-Type Half-Heuslers”, ACS Applied Materials & Interfaces, 13, 55060 (2021).
[4]. D. Bhattacharya, K. Kundayu, D. Saraswat, P. R. Raghuvanshi and Amrita Bhattacharya, “A thorough descriptor search to machine learn the lattice thermal conductivity of half-Heusler alloys”, ACS applied energy materials, 5 (7), 8913, (2022).

Arindam Ghosh



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Flow of charge and heat in high-quality graphene and hybrids.

Biswapriya Deb

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Polymer Composites for Lightweight Thermoelectric Generators

Portable and lightweight power generators are extremely appealing for self-powered electronic devices such as wearables, sensors/actuators, IoT (Internet of Things) devices, and round-the-clock health/environmental monitoring systems [1]. The unique heat/carrier transport of printable polymer nanocomposites, such as quasi-1-dimensional (1D) carbon nanostructures hybridized with π-conjugated polymeric systems, is advantageous for thermoelectric (TE) applications [2,3]. Here, we will focus on the systematic chemical doping-assisted TE performance improvements in benzodithiophene-thienothiophene (BDT-TTE) carbon nanotube composites. Investigations found that a proper doping technique could concurrently increase the Seebeck coefficient and electrical conductivity via low-energy carrier filtering at the polymer-CNT interfaces. It was discovered that the fundamental electronic transport mechanism and doping efficiency are highly dependent on CNT types (MWCNT/SWCNT), molecular structure, and polymer side chain variations. The findings provide vital insight into the underlying scientific principles and device design criteria.

[1] J. Cao, J. Zheng, H. Liu, C.K.I. Tan, X. Wang, W. Wang, Q. Zhu, Z. Li, G. Zhang, J. Wu, L. Zhang, J. Xu, A. Suwardi, Mater. Today Energy. 25 (2022), 100964
[2] Vijitha I, N. Raveendran, A. Prabhakaran, Y. Tanjore Puli, V. Chakkooth, Biswapriya Deb, Chem. Eng. J. 409 (2021), 128294
[3] Vijitha I., Navin J., Neethi R., Vijayakumar C., Biswapriya Deb, Materials Today Energy 32 (2023), 101233

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Functional Nitride Thin Films and Superlattices for Thermoelectric Application

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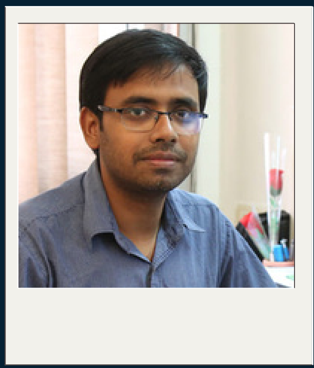

Theoretical and Computational Studies of Thermoelectric Nanomaterials

Two-dimensional (2D) materials possess different properties, which leads to worldwide research in this area. We will show our recent work on 2D chalcogenides and their heterostructure using first principle calculation based on Density functional theory and Boltzmann transport equation. Computational simulation of the electronic structure and lattice dynamics and theoretical simulation of the transport properties will be presented in 2D materials.

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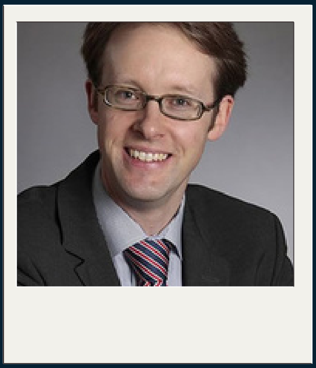

Fabrication and Characterization of a TEG for Electrically Active Implants

Johannes de Boor

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Mg2Si-based thermoelectric materials and devices: progress and challenges, in particular interdiffusion phenomena

J. de Boor[1,2], A. Duparchy[1], S. Ghosh[1], A. Sankhla[1], G. Oppitz[1], M. Abdelbaky[3], W. Mertin[3], B.K. Ryu[4], S.J. Park[4], S.D. Park[4], E. Müller[1,5]
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5 Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, D-35392 Giessen, Germany

Alternative thermoelectric materials that can substitute the commercially dominant bismuth telluride technology are highly desirable for heat conversion and thermal management applications. Magnesium silicide based solid solutions Mg2X (X = Si, Ge, Sn) are among the most promising thermoelectric (TE) materials due to very good thermoelectric properties, low cost of raw materials and environmental compatibility. We have demonstrated technological maturity with prototypes of p- and n-type Mg2X and p-MgAgSb/n-Mg2X, the latter reaching conversion efficiencies > 6.5% (Tc = 25 °C; Th = 300 °C) and power densities of ~1 W/cm2, comparable in performance to commercial bismuth telluride modules.
However, stable thermoelectric properties are of utmost importance for successful large-scale application. Intrinsic defects like Mg interstitials and Mg vacancies affect the properties of Mg2X significantly, therefore Mg diffusion is a potential concern here. Annealing experiments and in-situ measurements at high temperature show that degradation of Mg2X is a two-step process, where in the first step loosely bound excess Mg sublimates from the surface, reducing the charge carrier concentration, and only in the second step, after the solubility limit of Mg vacancies has been reached, Mg2X decomposes into other phases. Variation of the annealing temperature allows us to develop a kinetic model which can be used to predict material stability at different application temperatures, we also find indications that this process can be decelerated by sealing of the surfaces.
Furthermore, we find that diffusion phenomena are relevant even at room temperature, changing the thermoelectric properties on a scale of months to years if stored under laboratory atmosphere. Microstructural investigations by SEM, EDX and AFM indicate that the observed changes are related to Mg diffusion inside the material, in line with conclusions from high temperature experiments. They furthermore show that the diffusion constant is approximately independent of the Si:Sn ratio of the material. Comparison of different microscopic mechanisms of bulk diffusion by first-principles calculations reveals that Mg transport via Mg vacancies is the most relevant mechanism and the increase in vacancy density explains the experimentally observed faster change of Sn-rich Mg2X.

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Measuring thermal and electrical transport of anisotropic nanocomposites

Eutectic $NiTiO_3$–TiO_2 samples and their H_2 reduced Ni TiO_2 samples, where high aspect ratio TiO_2 nanostructures are axially decorated with nodular Ni glob ules, are thoroughly explored to understand their effect in photo-response. We show that by employing this novel eutectic architecture, effectively exploiting the nano-structuring process along with the chosen material properties, the overall effi ciency of the ensuing photoactive device is improved. We also show the competing photo-driven and photo-thermal-driven carrier mechanisms to define the total photo response of the system. Additionally, the ability to function self-powered poses this approach as a potential strategy for achieving efficient photodetectors.

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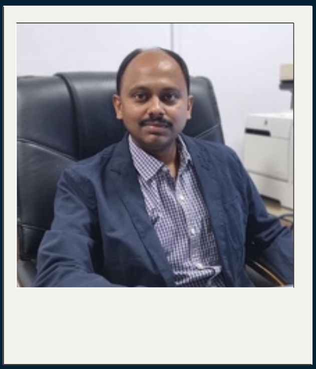

Enhanced Atomic Ordering Leads to Ultra-High Thermoelectric Performance

High thermoelectric performance is generally achieved through either electronic structure modulations or phonon scattering enhancements, which often counteract each other. A leap in performance requires innovative strategies that simultaneously optimize electronic and phonon transports. We demonstrate high thermoelectric performance with a near room-temperature figure of merit, ZT ~ 1.5, and a maximum ZT ~ 2.6 at 573 kelvin, by optimizing atomic disorder in cadmium-doped polycrystalline silver antimony telluride (AgSbTe2). Cadmium doping in AgSbTe2 enhances cationic ordering, which simultaneously improves electronic properties by tuning disorder-induced localization of electronic states and reduces lattice thermal conductivity through spontaneous formation of nanoscale (~2 to 4 nanometers) superstructures and coupling of soft vibrations localized within ~1 nanometer around cadmium sites with local strain modulation. The strategy is applicable to most other thermoelectric materials that exhibit inherent atomic disorder.

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$Ag_2Se/Sb_{1.5}Bi_{0.5}Te_3$-based fully printed origami thermoelectric module for low grade thermal energy harvesting

M. Mallick[1], L. Franke[1], A. Rösch[1], Q. Zhang, M.I.Khan, I.Brunetti, and U.Lemmer[1]*
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Printed electronics has the potential to reduce the manufacturing cost of electronic devices significantly. Here, we demonstrate a scalable manufacturing route for high-performance fully printed thermoelectric generators (TEGs) as a cost-effective solution for energy harvesting applications. In this work, we present a facile one-pot synthesis method to develop a high performance Ag_2Se-based printable n-type thermoelectric (TE) material. We proceeded to fabricate a fully printed origami TEG (o-TEG) by employing the thermally annealed Ag_2Se-based material as n-type legs and incorporating photonic sintered Bi-Sb-Te based TE material as p-type legs. The printed n-type Ag_2Se-based material exhibits a power factor of ~ 14 $\mu Wcm^{-1}K^{-2}$ and a maximum figure-of-merit zT of ~ 0.92 at ambient temperature. Furthermore, we introduce a printed carbon layer as an effective interface material that minimizes the diffusion of metal elements across the thermoelectric and electrode materials. Hence, a low contact resistance is achieved in o-TEGs. The origami folded TEG exhibits an open-circuit voltage (VOC) of 284 mV and a record high power density (pmax) of ~11 W m^{-2} for a printed TEG at a temperature gradient (ΔT) of 80.7 K. These results underscore the capability of printed origami TEGs in efficiently converting low-grade heat into electricity, signifying a promising opportunity for powering Internet-of-Things (IoTs) devices.

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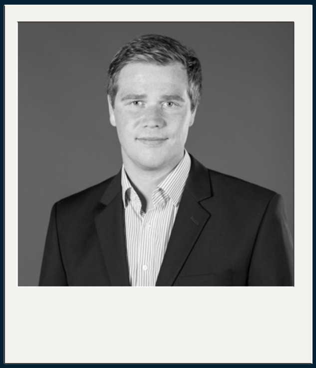

Thermoelectric Cooling – Applications, Challenges and Potentials

Thermoelectric cooling has been used for many decades in a wide variety of applications. In addition to an overview of the applications, the challenges in system integration and the limits and possibilities are given in particular. An outlook on future applications and market requirements rounds off the presentation.

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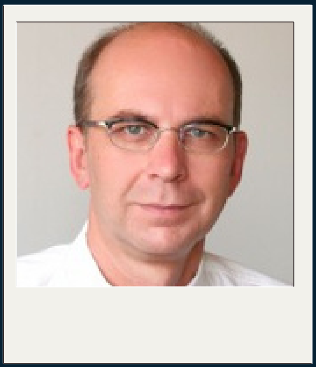

Thermoelectric energy harvesting: From generator design to system application

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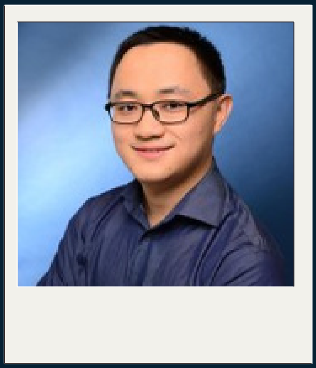

Half-Heusler thermoelectric materials: Towards the decoupling between electrons and phonons

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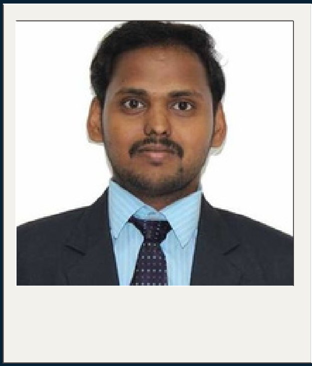

Thermoelectric Properties of Higher Manganese Silicide Synthesized through Molten Salt Shielded Synthesis Method

*Nishath Begum J, Rajasekar P**

Among the various class of materials studied for thermoelectric applications, transition metal silicides continue to attract the curiosity of working metallurgists because of their thermal, mechanical and chemical stability at increased temperatures. Silicides are considered as one of the potential candidates for commercial thermoelectric applications, as they are non-toxic, stable and made up of earth abundant elements[1,2]. Mg_2Si, $MnSi_{1.7}$, $CrSi_2$, and β-$FeSi_2$, are some of the silicides studied for thermoelectric applications. Among these silicides, $MnSi_x$ show good thermoelectric performance at mid-temperature range with good mechanical stability. In literature manganese silicides are synthesized by various preparation methods such as arc melting, ball milling, hot pressing, chemical vapor transport and spark plasma sintering. Although Mn and Si are cheap, the steps with high temperature and vacuum requirement in these synthesis and processing methods increases the cost[3]. Hence in this work we have focused on the synthesis of $MnSi_{1.7}$ by a cost-efficient molten salt shielded synthesis method[4]. The synthesized silicide samples have then been sintered by spark plasma sintering. The phase, morphology and elemental composition of the synthesized materials have been characterized through X-ray diffraction, scanning electron microscopy and EDX. The Rietveld refinement of diffraction pattern confirms the formation of higher manganese silicide along with a minimal MnSi impurity phase. The temperature dependent thermoelectric properties of the sample were measured upto 623 K. The electrical conductivity and Seebeck coefficient of the synthesized sample at 623 K has been measured to be 205 Scm^{-1} and 202 μV/K, respectively. The calculated power factor is 8 $Wcm^{-1}K^{-2}$. The measured total thermal conductivity of the sample is 2.19 $Wm^{-1}K^{-1}$ at 623 K. With this the peak thermoelectric figure of merit zT obtained is 0.24 at 623 K. This shows that by molten salt shielded method can be used as a cost-effective method to synthesize manganese silicide in atmospheric condition with good thermoelectric properties. Further, the thermoelectric properties of the manganese silicide synthesized by molten salt shielded synthesis can be improved by suitable chemical doping and microstructural tuning.

References

1. Schlesinger, M. E. Thermodynamics of Solid Transition-Metal Silicides. Chem. Rev vol. 90 (1990).
2. Chen, L. Metal Silicides: An Integral Part of Microelectronics.www.tms.org/pubs/journals/JOM/0509/Chen-.
3. Liu, et. al.. Eco-Friendly Higher Manganese Silicide Thermoelectric Materials: Progress and Future Challenges. Adv Energy Mater 8, 1800056 (2018).
4. Dash et.al. Molten salt shielded synthesis of oxidation prone materials in air. Nature Materials vol. 18 465–470.

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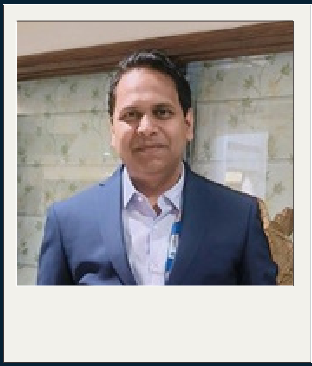

Harnessing High-temperature Radiant Waste Heat from Hot Steel Slab using Thermoelectric Generator at Tata Steel Ltd

The objective of present work was to harness the enormous potential of untapped waste heat by using thermoelectric to convert high-grade waste heat in the form of heat radiation into electric power. A customised thermoelectric generator (TEG) system was developed, suited for heat sources that generate thermal radiation, such as hot steel slabs (300 0C–350 0C), to make use of the high temperature radiation waste heat during the continuous casting of steel. Advanced heat transfer modelling and simulation studies were done to develop & optimize the design parameters for Thermoelectric generator. The system of capacity producing 0.75 KWhr of electricity was installed in the Continuous Slab Casting line. The system underwent extensive testing and demonstration to confirm its dependability, efficiency, and performance in the challenging steel environment. Plant trials successfully demonstrated the feasibility and stability of designed thermoelectric generator system for caster lines in actual steel works environment. This is an important step towards adopting sustainable energy practices, which will cut down on energy waste and advance sustainability.

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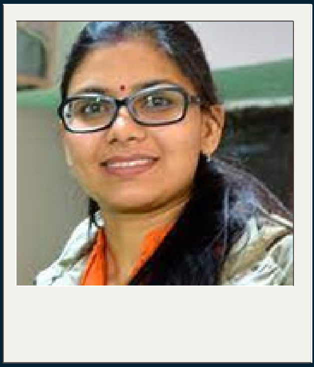

Electron-phonon coupling and related transport properties in two-dimensional semiconductors

Two-dimensional semiconductors have shown immense potential in future electronics, optoelectronics and energy applications. Materials with high electron transport and low phonon transport properties are considered to be the potential candidates for thermoelectric applications [1-3]. Recent studies have shown that sub-nanostructuring (lattice imperfections like dislocations/interstitial sites/clusters) enhances the overall thermoelectric figure of merit. This is due to the fact that sub-nanostructuring slightly hampers the carrier transport and helps in maintaining high carrier mobility while significantly disrupts the phonon transport [4]. However, experimental realization of these nanostructures poses significant challenges and expenses. In recent decades, there has been a growing demand for ab-initio based theoretical calculations of transport properties in materials, primarily due to their precise and efficient calculations that require relatively less computational expenses. Through the utilization of ab-initio based computational tools like electron-phonon Wannierization, it becomes possible to calculate the temperature-dependent scattering rate of charge carriers, carrier mobility, electrical conductivity, line-widths, etc., by analyzing the electron-phonon interactions in the system [5]. This is done by calculating the electron-phonon self-energies arising from the electron-phonon coupling.
In the present work, we calculate these coupling energies for the electron-phonon transport properties in two-dimensional hexagonal layered structures (silicene, germanene and tungsten carbide) using ab-initio techniques for effective calculations of thermoelectric power factor. The methodology thus developed can further be extended to estimate the thermoelectric transport properties in bulk/low-dimensional structures with sub-nanostructures, before practical realization of such materials.

References
[1] L. D. Hicks, M. S. Dresselhaus, Phys. Rev. B, 47, 12727 (1993)
[2] G. D. Mahan, J. O. Sofo, National Academy of Sciences, 261, 7436 (1996)
[3] R. Venkatasubramanian, E. Siivola, T. Colpitts, B. O'quinn, 263, Nautre, 413, 597 (2001).
[4] Y. Qin, Y. Xiao, APL Materials, 8, 010901 (2020).
[5] F. Giustino, M. L. Cohen, S. G. Louie, Phys. Rev. B, 76, 165108 (2007).

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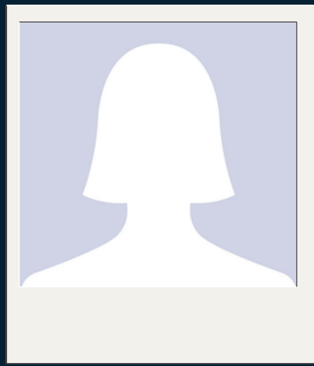

Influence of geometry and size on transport processes: Considerations for thermoelectric device design

Understanding of charge and heat transfer processes in thermo-electric and electronic materials is important for optimal and sustainable device operation. Dimensionality and size control may be advantageously introduced into material and device design. Commonly, charge and heat flow are considered to be well-understood by taking into account established transport material parameters for the bulk, such as the electrical and thermal conductivity. However, at the micro- and nanoscale considerable deviations in electron-phonon and phonon-phonon interactions may occur when surfaces and interfaces effects come into play. Examples of the influence of size effects on material parameters in the wide range from pure metals to wide-band gap semiconductors will be given with a focus on changes in the Seebeck coefficient and the phonon drag effect. Challenges for measurements at the micro- and nanoscale will be outlined and examples of recent progress demonstrated.

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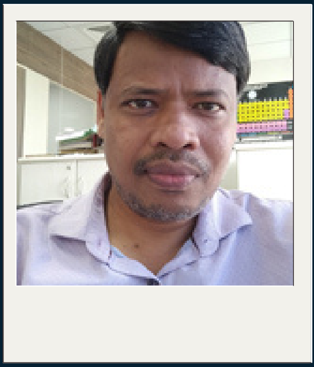

Fabrication and characterization of rigid thermoelectric modules composed of $Na_xPb_{1-x}Te$ – $Mg_2Si_{1-x}Sn_x$, $Bi_xSb_{1-x}Se$-$(Bi_{1-x-y}Sb_xM_y)Te_3$ compounds

Two types of thermoelectric p and n material pair, low-temperature $Bi_xSb_{1-x}Se$ and $Bi_{1-x-y}Sb_xM_yTe_3$, and medium temperature $Na_{0.02}Pb_{0.98}Te$ and $Mg_2Si_{0.38}Sn_{0.6}Bi_{0.02}$ are fabricated into rigid modules consist of up to 100 legs. These modules hold immense potential for converting waste heat into electrical energy in the 25-400°C temperature range, addressing the growing demand for sustainable energy solutions. This work delves into the synthesis and processing techniques employed to assemble these thermoelectric modules. The fabrication process involves the TE compounds prepared by melting and powder processing into more than 99.0% dense sintered pellets, along with diffusion barriers and contacts that offer low specific contact resistance. The pellets thus prepared were diced to various dimensions using automated diamond wire cutting or electric discharge machining (EDM). These optimized dimension leg materials were assembled into thermoelectric modules using manufacturing methods such as reflow soldering and solid, liquid interface diffusion (SLID) bonding. The module's internal resistance, integrity, structural stability, and V-I and P-I characteristics were evaluated. Various materials' characteristics and processing parameters critical for fabricating stable modules are discussed.

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Enhancing Thermoelectric Performance through Innovative Strategies in Defective Half-Heusler Alloys

Half-Heusler materials have long been explored for their thermoelectric potential, yet challenges such as low carrier mobilities and high lattice thermal conductivity persist. To overcome these limitations, a new generation of half-Heusler materials, including "defective" alloys stabilized by vacancies, shows promise. In this study, we focus on $Nb_{0.8}CoSb$ as a base material and present two innovative approaches to enhance its thermoelectric properties. Firstly, we investigate the efficacy of Sn-doping in $Nb_{0.8}CoSb$. Secondly, we propose a modulation doping strategy in $Nb_{0.8}CoSb$-TiCoSb composites to achieve synergistic improvements in thermoelectric performance. These novel methodologies demonstrate the potential for significant advancements in thermoelectric materials through tailored compositional engineering and innovative design approaches.

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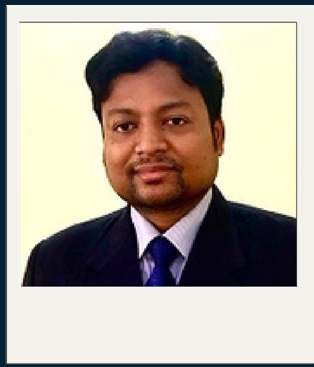

Oxide composites: A viable route for high temperature thermoelectric power generation

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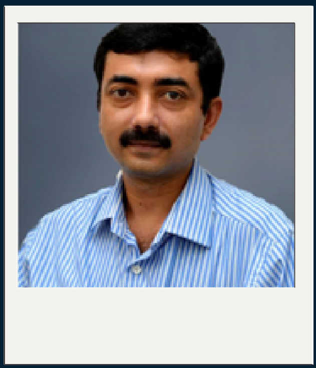
The challenges in oxide thermoelectrics are manifold as thermoelectric device figure of merit, *ZT* of oxides suffer from lower electrical conductivity as well as relatively higher thermal conductivity compared to state-of-the-art materials like chalcogenides. Especially, achieving *ZT*>1 remained elusive for bulk oxide thermoelectrics. Electrons in oxide perovskites suffer from Anderson's localization due to the presence of multi-valent transition metals and point defects giving rise to variation in local electric field and strain. Recently, we have posited a strategy of boosting the electron transport by manipulating semiconductor to metal transition temperature in donor doped $SrTiO_3$ by synthesizing nanocomposites with graphene oxide (GO), graphite (G), CNT and MXene. Presence of these nano-inclusions in perovskite matrix provide high momentum electrons and impart enough strain to facilitate these localized electrons to attain the itinerant state. As a result, we could achieve single-crystal like electron mobility in ceramic nanocomposites. Thus, we reported the first experimental demonstration of ZT>1 in oxide thermoelectrics. Furthermore, we could restrain the increase in thermal conductivity by attaining enhanced Umklapp scattering along with phonon-glass-like temperature-independent phonon mean-free-path above Debye temperature. We have achieved the maximum ZT ~1.42 in $SrTi_{0.85}N_{0.15}O_3$ perovskite composite with 0.5wt% G, which is highest ever ZT reported for oxide ceramics. We have further fabricated 4-legged n-type thermoelectric power generator demonstrating milliwatt-level power output, hitherto remained unattainable for oxide thermoelectrics. Our proposed way of designing rare-earth-free composites with graphite, graphene and MXene can potentially open up the possibility of fabricating novel thermoelectric generators capable of recycling high grade (>1000 K) waste-heat.

Titas Dasgupta



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Multi-band Modelling of Thermoelectric Materials: Applications in Materials and Devices

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Investigation of electronic band structure (EBS) plays a significant role in the advancement of thermoelectric materials and devices. In this presentation, details of a new multi-band modelling technique, referred as multi-band refinement technique (MBRT)1, for analyzing EBS of thermoelectric (TE) materials will be presented. MBRT uses a least square minimization based approach for extracting EBS information, with the input being experimental electrical properties and an electronic structure model. The methodology and the validation of the technique using standard materials will be presented. In addition, the applicability of MBRT for analyzing the EBS of TE materials and utility in development of high efficiency TE devices will be discussed based on specific examples.

References:

[1] Agrawal B., de Boor J., Dasgupta T., A multi-band refinement technique for analyzing electronic band structure of thermoelectric materials, Cell Reports Phys. Sci. 5, 101781 (2024)

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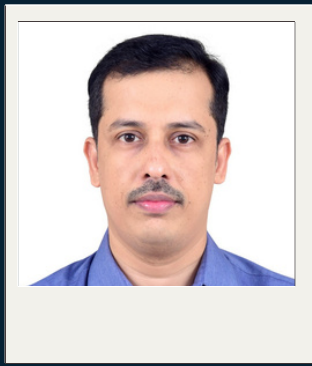

Thiophene-based Organic Thermoelectric Materials: Insights into Structure-Property Relationships and Doping Mechanisms

Thiophene-based organic materials have garnered significant interest in thermoelectric applications because of their excellent electrical conductivity and chemical versatility. These properties allow for the fine-tuning of their thermoelectric properties, making them efficient for energy conversion. Our studies have explored the intricate roles of doping and charge transfer in optimizing the thermoelectric properties of thiophene-based systems. By strategically using dopants, we have achieved significant improvements in electrical conductivity and Seebeck coefficient in these systems. We have prepared, characterized, and studied thiophene-based small molecules and polymers with different doping agents. The structure of the conjugated backbone, doping mechanism, and degree of polymer aggregation are critical factors that affect the thermoelectric performance. We have used advanced analytical methods to elucidate the structure-property relationships. Our study provides critical insights for designing high-performance thermoelectric materials, which have implications for sustainable energy-conversion technologies.

References

1. Raveendran et.al. Mater. Today Energy 2023, 34, 101296.
2. Vijitha, et.al.Mater. Today Energy 2023, 32, 101233.
3. Vijith Thermoelectric material and process for the preparation thereof. US Patent Application, US20200411743A1.
4. VJau kumar et.al. Conjugated polymer-carbon nanotube thermoelectric composite film and thermoelectric application thereof. Indian Patent Application 202311013444.

Vijayakumar, C.; Deb, B.; Jacob, N.; Vijitha, I.; Raveendran, N.; Poovattil, S.; Kumar. S.; Maurya, L. K.; Yuvaraj, T. P. A n-type thermoelectric composite film and preparation thereof. Indian Patent Application 202311013443.

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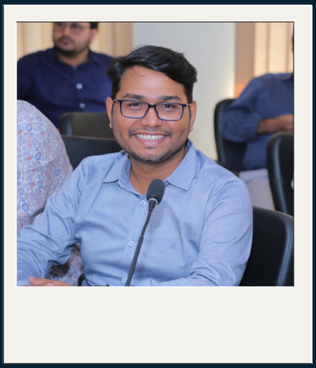
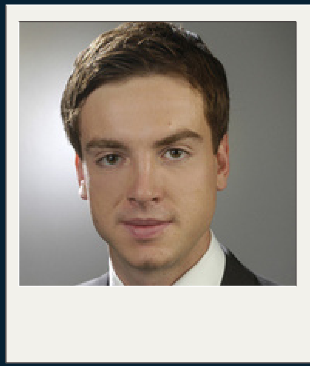


Thermoelectric energy harvesting using chalcogenide thin films.

Photothermoelectric devices utilize the photothermoelectric effect, which involves the generation of an electric current in response to a temperature gradient induced as a result of photon flux. The operating principles of photothermoelectric devices, which rely on the Seebeck effect to convert a temperature gradient into an electric voltage and the photovoltaic effect to convert light into electricity for low to high grade of heat recovery. Applications of photothermoelectric devices across different sectors include renewable energy harvesting, waste heat recovery, sensing, and optoelectronics. These devices show promise for powering remote sensors, wearable electronics, etc. Researchers are exploring novel materials and device architectures to improve efficiency, stability, and scalability. Challenges such as optimizing device performance under varying environmental conditions and cost-effective fabrication remain areas of active investigation. My talk highlights some recent developments and challenges in the field of photothermoelectric devices, explores the underlying fundamental principles and some of our early result with CVD grown chalcogenide films.

Vincent Linseis



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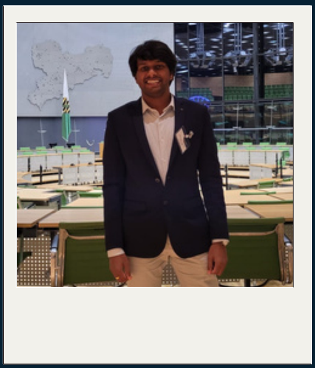
Thermoelectric Metrology: A Comprehensive Review from a Manufacturer's Perspective

Thermoelectric metrology, situated at the intersection of thermoelectricity and metrology, plays a pivotal role in optimizing thermoelectric materials as well as ensuring the accuracy and reliability of thermoelectric devices across various applications. We want to provide a comprehensive overview of recent advancements and challenges within thermoelectric metrology, from the perspective of an established commercial manufacturer and partner of the scientific community. Beginning with elucidating the state-of-the-art techniques and methodologies employed in the characterization of thermoelectric bulk materials and devices, including Seebeck coefficient measurement, thermal conductivity determination, and figure of merit evaluation. Furthermore, this overview highlights established setups for characterizing nano-scaled thermoelectric films, such as a unique chip-based system, utilizing the three-omega technique, as well as a FDTR setup, which is optimized from a commercial perspective. Analogous to an academic project progress, after the material characterization, a brief insight into the state-of-the-art characterization of thermoelectric devices will be provided. Finally, attention is drawn to open questions in measurement technology, underscoring areas ripe for further exploration and potential collaborations within the field of thermoelectric metrology.

References:
[1] Linseis, V., Völklein, F., Reith, H., Nielsch, K., and Woias, P. 2018. Advanced platform for the in-plane ZT measurement of thin films. Review of Scientific Instruments 89, 1, 15110.

Young Researcher Talks

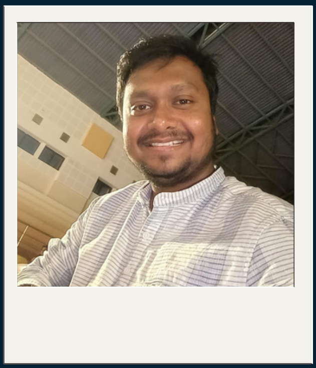


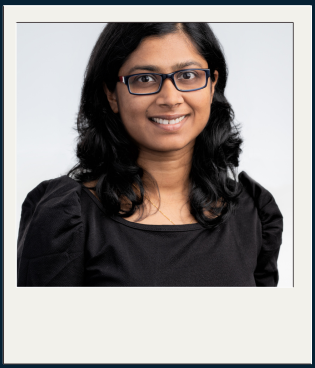
Nithin P., IFW

Geometry optimization of micro thermoelectric devices

Pintu Singha, IISER TVM

Thermoelectric and magneto transport properties of Bismuth Chalcogenide topological insulator

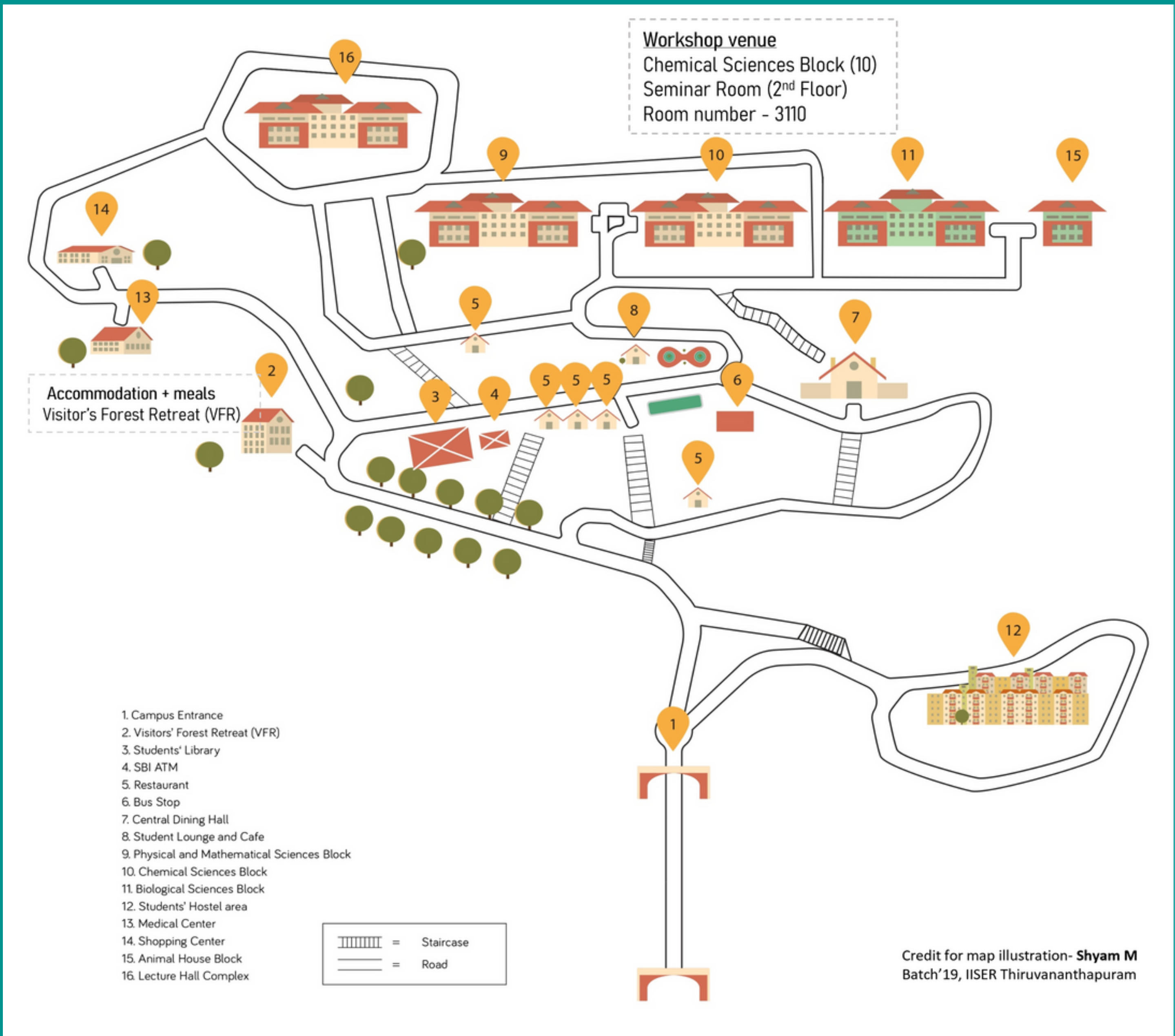




Sanyukta Ghosh, DLR

Magnesium Silicide-based Composites: Correlating Composition with Transport Properties at the Micro and Nano-Scale for Effective Energy Filtering

Campus Map



Workshop venue
Chemical Sciences Block (10)
Seminar Room (2nd Floor)
Room number - 3110
Accommodation + meals
Visitor's Forest Retreat (VFR)
1. Campus Entrance
2. Visitors' Forest Retreat (VFR)
3. Students' Library
4. SBI ATM
5. Restaurant
6. Bus Stop
7. Central Dining Hall
8. Student Lounge and Cafe
9. Physical and Mathematical Sciences Block
10. Chemical Sciences Block
11. Biological Sciences Block
12. Students' Hostel area
13. Medical Center
14. Shopping Center
15. Animal House Block
16. Lecture Hall Complex
= Staircase
= Road
Credit for map illustration- **Shyam M**
Batch'19, IISER Thiruvananthapuram

Local Organizing Committee

SMaRT Lab

- Pintu Singha
- Soumya Biswas
- Silpa S
- Dipanjana Mondal
- Satarupa Mandal
- Varsha Biswas
- Shivam Singh
- Nithin P. (IFW)
- Harikrishna G
- K. Savio
- Saptak Majumder
- Gaurav Bolegave
- Niharika P V
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INDO-GERMAN SCIENCE & TECHNOLOGY CENTRE

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