

# Anuj Goyal

Assistant Professor, Department of Materials Science & Metallurgical Engineering

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## Major Areas of Research:

- Electronic structure and atomistic materials modeling
- Defects in semiconductors
- Materials discovery for clean energy applications

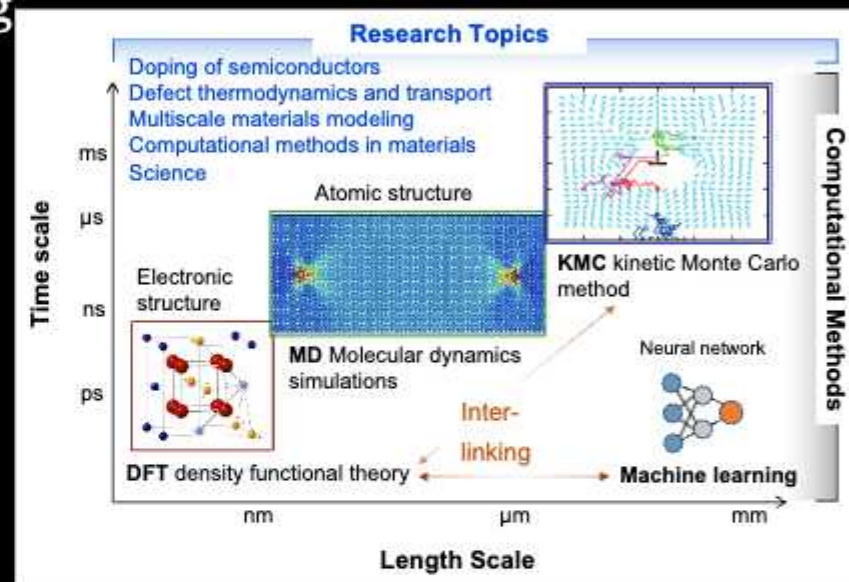
## Major Research Facilities in the Group:

Supercomputing facilities at IITH

- NSM Param Seva
- High Performance Computing

## Publications:

- A. Goyal, P. Gorai, H. Peng, S. Lany and V. Stevanovic, "A computational framework for automation of point defect calculations", *Computational Materials Science* 130, 1-9 **2017**. DOI:10.1016/j.commatsci.2016.12.040
- A. Goyal, P. Gorai, S. Anand, E. S. Toberer, G. J. Snyder and V. Stevanovic, "On the dopability of semiconductors and governing material properties", *Chemistry of Materials* 32, 11, 4467-4480 **2020**. DOI:10.1021/acs.chemmater.9b05126
- A. Goyal, A. Zakutayev, V. Stevanovic and S. Lany, "Computational Fermi level engineering and doping-type conversion of Mg:Ga<sub>2</sub>O<sub>3</sub> via three-step synthesis processing", *Journal of Applied Physics* 129, 245704 **2021**. DOI:10.1063/1.5000000



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Indian Institute of Technology Hyderabad



**Ashok Kamaraj**

**Assistant Professor ,Process Metallurgy Lab**

**Department of Materials Science & Metallurgical Engineering**

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**Major Areas of Research/Up to 3 major sponsored projects**

Physical Modelling & simulation of metallurgical processes

Metal extraction, recycling & life cycle analysis of metallurgical processes

Development of alloy steel products & Certified Reference Materials

**Major Research Facilities in the Group**

Vacuum Induction melting furnace

High-temperature furnace for slag-metal equilibrium studies<sup>#</sup>

FactSage Software package<sup>#</sup>

<sup>#</sup> under procurement stage

**Technology/Product Developed/Up to 3 most significant Publications**

Design of an auto dip mold simulator for simulation of initial solidification behavior during continuous casting process: Equipment Design Patent: NML/PAT0569/2019/IN, P/1152/12/2019, India.

DeoxyCalc-Version 1.0” A computer model for prediction of the amount of deoxidizers in Ladle Furnace: Software copyright: Ashok K, Gopi K Mandal, D Bandyopadhyay: CR-0092/2014, India.

Know-How for Hydrogen standard in steel (Technology): Certified Reference Materials (CRM): Ashok K, J K Sircar, A K Upadhyay, D Bandyopadhyay, M M Humane, J N Patel, D P Singh: CRM -501, July 2020, India.



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### Major Areas of Research

Powder Metallurgy, Sintering, Metal Additive Manufacturing, Ultra High Temperature Composites, Nanostructured Materials, Microstructure-mechanical Properties of Steels, High Entropy Alloys, Surface Engineering, 2D-Mxene for Super-capacitors and Energy storage, Electro Spark Coatings, Wear And Tribology, Hard Carbides Tool Materials

### Major Research Facilities in the Group

High Temperature Furnace, Vacuum Hot Press, Tubular Furnaces, Cold Compaction, Planetary Ball Mill, DSC, TGA, Pin-On-Disc Wear Test, Electro-Spark Deposition Unit

### Publications

- ❑ Subhendu Naskar, S. Rohila, S. Suryakumar, B. B. Panigrahi, Influence of Heat treatments on Microstructure and Mechanical Properties of Additive Manufactured Inconel 718 Superalloy, Trans. INAE (2021). <https://doi.org/10.1007/s41403-021-00247-6>
- ❑ S.S.N. Murthy, Manish Patel, T. Sreekantha Reddy, V.V. Bhanu Prasad, Bharat B. Panigrahi, Processing and characterization of carbon fibres reinforced ZrB<sub>2</sub> ultra high temperature ceramic matrix composite, Ceramics International, (2021) <https://doi.org/10.1016/j.ceramint.2021.08.145>.
- ❑ K. Godbole, C. R. Das, J. Joardar, S. K. Albert, M. Ramji, B.B. Panigrahi, Toughening of AISI 410 stainless steel through quenching and partitioning and effect of Prolonged Aging on microstructure and mechanical Properties, Metall and Mat Trans A (2020), <https://doi.org/10.1007/s11661-020-05809-x>.





# Chandrasekhar Murapaka

Assistant Professor, Spintronic Device Lab

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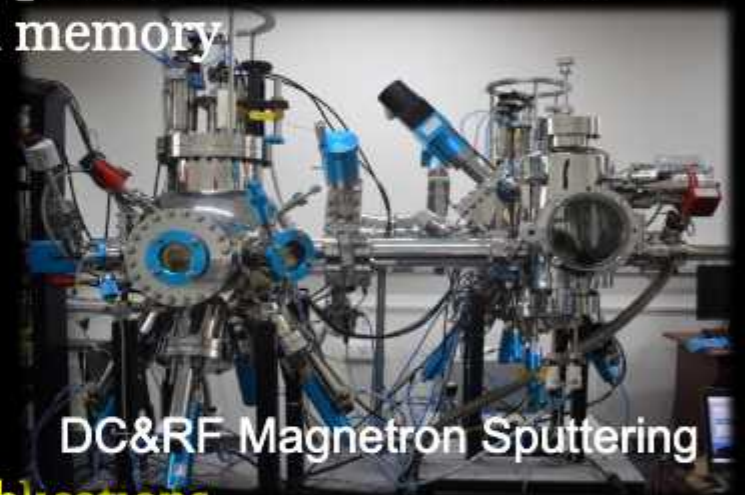
## Major Areas of Research/Up to 3 major sponsored projects

Spinorbitronics, Skyrmion based devices, Pure spin current generation and detection

- ❖ Ferrimagnet based synaptic device for neuromorphic computing (SERB-CRG)
- ❖ Harnessing pure spin current by tailoring molecular spinterface (DAE-BRNS)
- ❖ Novel spin Hall materials for spin-orbit torque based memory and logic devices (JICA friendship 2023)

## Major Research Facilities in the Group

- ❑ DC&RF Magnetron sputtering system (8 Targets)
- ❑ 2D Maskless lithography system
- ❑ Kerr Microscopy
- ❑ DC Probe station
- ❑ Magnetoresistance setup



DC&RF Magnetron Sputtering

## Technology/Product Developed/Up to 3 most significant Publications

- ✓ B Paikaray, K. Mahathi, A Haldar, C. Murapaka, "Reconfigurable logic operations via gate controlled skyrmion motion in a nanomagnetic device", ACS Applied Electronic Materials 4, 2209 (2022)
- ✓ T. Manoj, H. Perumal, B. Paikaray, A. Haldar, J. Sinha, P. P. Bhattacharjee, C. Murapaka, "Perpendicular magnetic anisotropy in a sputter deposited nanocrystalline high entropy alloy thin film", Journal of Alloys and Compounds, 167337 (2022).
- ✓ K. Sriram, Jay Pala, B. Paikaray, A. Haldar, C. Murapaka, "Effect of Seed layer on Ta crystalline phase and spin Hall angle", Nanoscale 13, 19985 (2021).



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**Deepu J. Babu**

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## Major Areas of Research

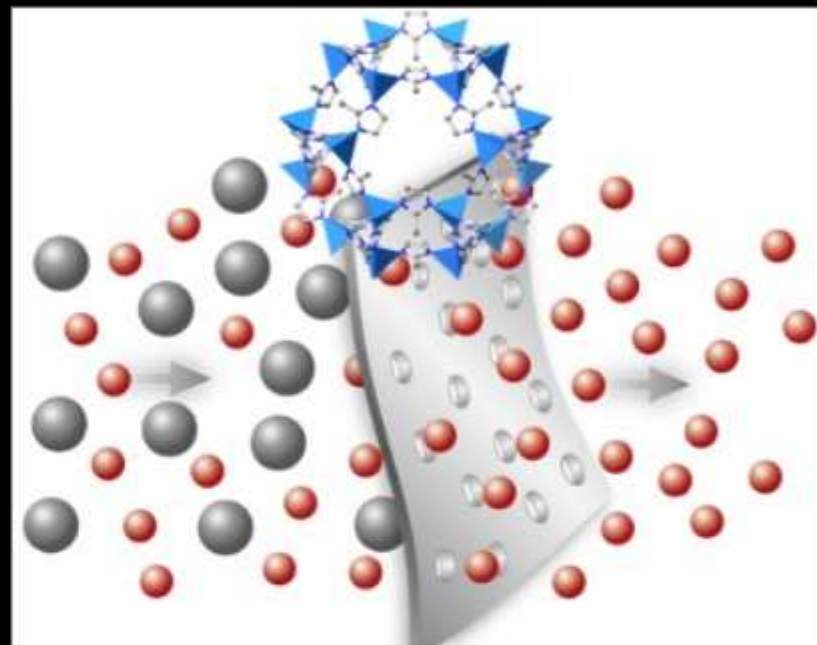
- Carbon Capture
- Adsorption/Membrane separation
- Nanoporous Materials
- CVD synthesis

## Major Research Facilities in the Group

- Gas adsorption setup
- Membrane permeation setup
- BET surface area analyzer
- Plasma cleaner
- CVD setup for 2D materials growth

## 3 most significant Publications

1. D.J. Babu, G. He, K.V. Agrawal et al., Restricting Lattice Flexibility in Polycrystalline Metal–Organic Framework Membranes for Carbon Capture, *Advanced Materials*. 31 (2019) 1900855.
2. D.J. Babu, M. Bruns, J.J. Schneider, Unprecedented CO<sub>2</sub> uptake in vertically aligned carbon nanotubes, *Carbon*. 125 (2017) 327–335.
3. J. Hao, D.J. Babu, K.V. Agrawal et al., Synthesis of high-performance polycrystalline metal–organic framework membranes at room temperature in a few minutes, *J. Mater. Chem. A*. 8(2020) 7633–7640.



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# Mayur Vaidya

Assistant Professor, Department of Materials Science & Metallurgical Engineering

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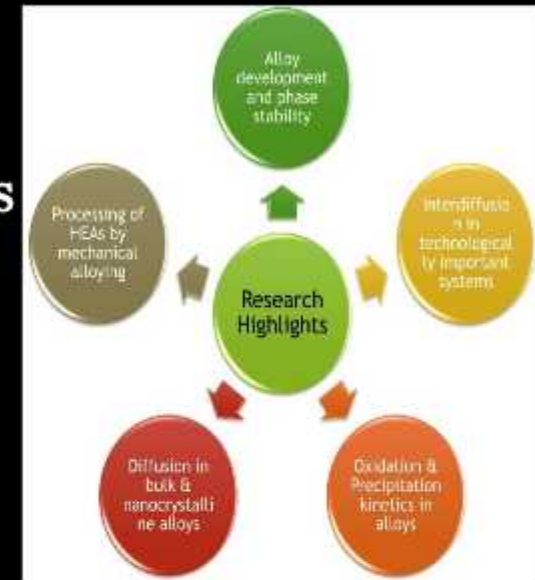


## Major Areas of Research/Up to 3 major sponsored projects

1. Oxidation behaviour of multicomponent alloys
2. Size and temperature effects on diffusion in materials
3. Design and development of steels and multicomponent alloys
4. Nanocrystalline multicomponent alloys by mechanical alloying and spark plasma sintering

## Major Research Facilities in the Group

1. Thermal Evaporation System
2. Tubular Furnaces (max. temp - 600 °C and 1100 °C)
3. Low Speed Cutter, Diamond Wire Saw



## Technology/Product Developed/Up to 3 most significant Publications

1. Burla, A., Khandelwal, M., & Vaidya, M. (2022). Antibacterial properties of Cu containing complex concentrated alloys. Materials Today Communications, 33, 104915.
2. M. Vaidya, Sandipan Sen, Lena Frommeyer, Lukas Rogal, S. Sankaran, Blazej Gabrowski, G. Wilde, S. V. Divinski, Phenomenon of ultra-fast tracer diffusion of Co in HCP high entropy alloys, Acta Mater. 196 (2020) 220-2303.
3. M. Vaidya, A. Karati, K. Guruvidyathri, M. Nagini, K.G. Pradeep, B.S. Murty, Suppression of  $\sigma$ -phase in nanocrystalline CoCrFeMnNiV high entropy alloy by unsolicited contamination during mechanical alloying and spark plasma sintering, Mater. Chem. Phys. 255 (2020) 123558



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**Mudrika Khandelwal**

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## Major Areas of Research:

Drug Delivery, Antimicrobial Materials, Battery, Soft Actuators, Food Packaging, Depth Filters, Hydrophobic Surfaces

## Major Research Facilities in the Group:

Microbial Culture Facility, Lyophilizer, Humidity Chamber, Water Bath, Centrifuge, Vacuum Oven, Battery Cycler, UV-VIS Spectrophotometer

## Technology/Product Developed:

**SthriVIn** – A Antifungal & Antibacterial product for intimate wear with Microcapsule formulation



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# Saswata Bhattacharyya

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## Major Areas of Research

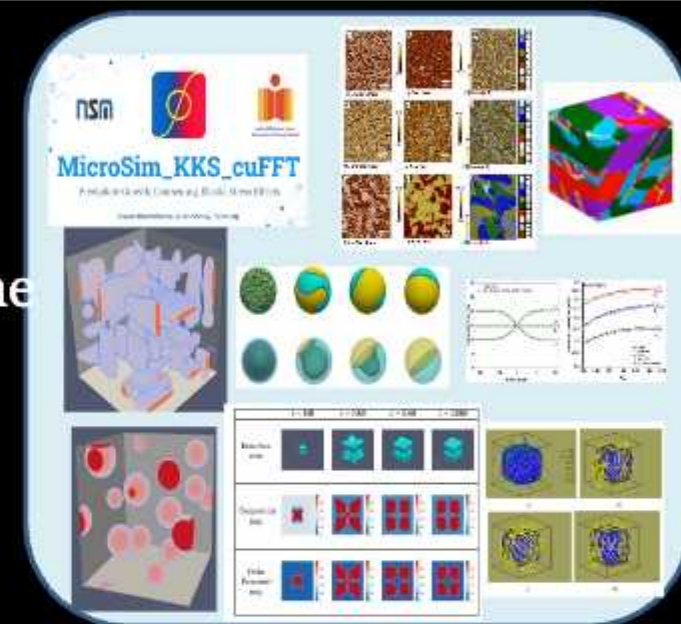
Optimization of diffusivities in Ni-base alloys and their influence on Microstructural evolution (SERB)

Development of high-performance phase-field codes (DST-NSM) through Process Modeling of Single crystalline Ni-base superalloy – validation using CMSX-4 (GTMAP)

## Major Research Facilities

HPC cluster (Tesla GPUs + InfiniBand)

ThermoCalc



## Technology/Product Developed/Up to 3 most significant Publications

**MicroSim** - Open-source HPC software package to simulate microstructural evolution using Phase-field method <https://microsim.co.in/> (Current version: 2.0)

Evolution of Janus, core-shell, and inverse core-shell configurations in bimetallic nanoparticles and morphological stability map – Pankaj, Saswata Bhattacharyya, Subhradeep Chatterjee, Acta Materialia 2022  
<https://doi.org/10.1016/j.actamat.2022.117933>

A physics-informed neural network-based numerical inverse method for optimization of diffusion coefficients in NiCoFeCr multi principal element alloy – Hemanth Kumar, Dash, Alope Paul, Saswata Bhattacharyya, Scripta Materialia  
<https://doi.org/10.1016/j.scriptamat.2022.114639>



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# Shourya Dutta Gupta

Assistant Professor, NODe Lab

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## Major Areas of Research

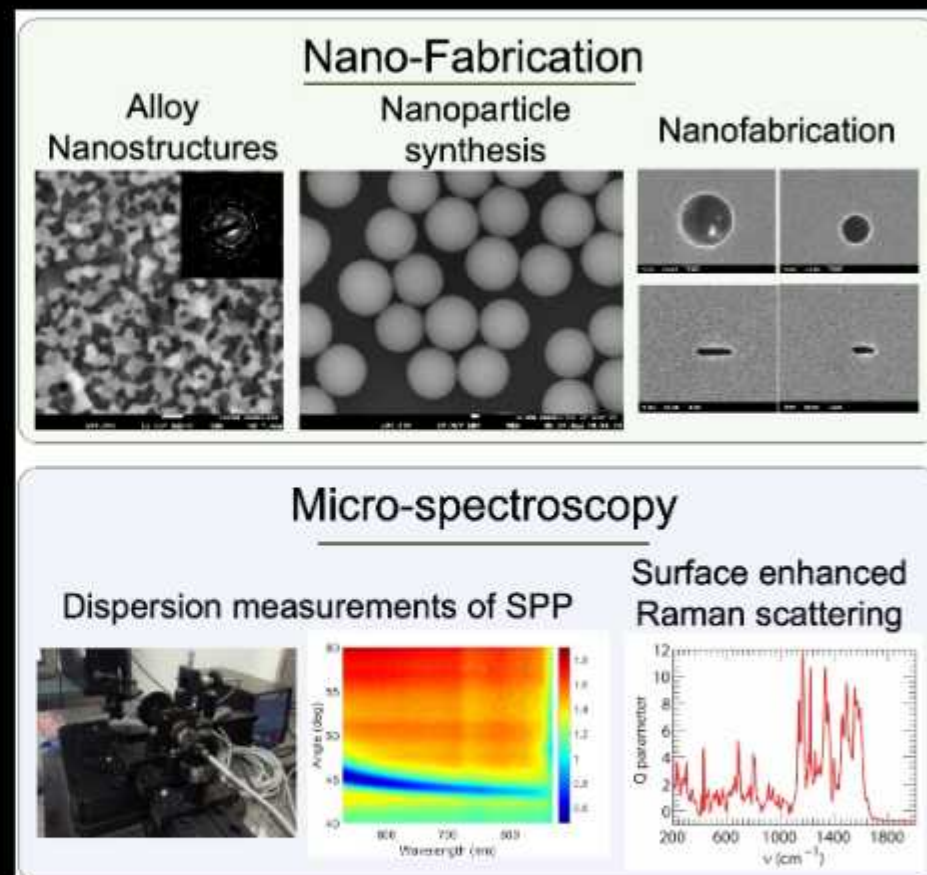
- Plasmonics & Nanophotonics
- Metamaterials & metasurfaces
- Optical Sensors & Modulators

## Major Research Facilities in the Group

- Micro-optical spectroscopy (including Raman)
- Magnetron sputtering
- Nanoparticle synthesis & characterization tools

## Technology/Product Developed

- Phase separated Ag-Cu thin films for plasmonic applications
- SERS based biosensors using nanoparticle-nanoaperture configuration



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**Subhradeep Chatterjee**

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## Major Areas of Research/Up to 3 major sponsored projects

Metallurgy of welding and solidification processing

Alloy design and phase transformations

Microstructural characterization and modeling

## Major Research Facilities in the Group

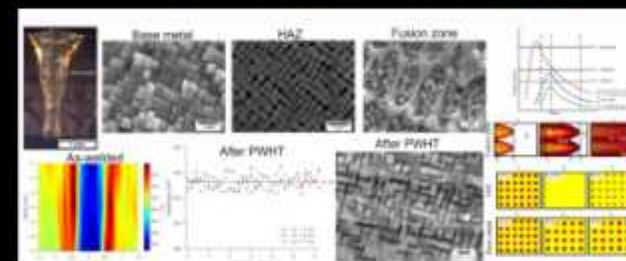
Robotic keyhole GTA welding set-up (Fronius ArcTIG)

## Technology/Product Developed/Up to 3 most significant Publications

Welding and additive manufacturing of superalloys ([link](#))

Alloy design and welding of high entropy alloys ([link](#))

Predicting morphology of bimetallic nanoparticles through phase field simulations ([link 1](#), [link 2](#))



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**Suhash Ranjan Dey**

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## Major Areas of Research

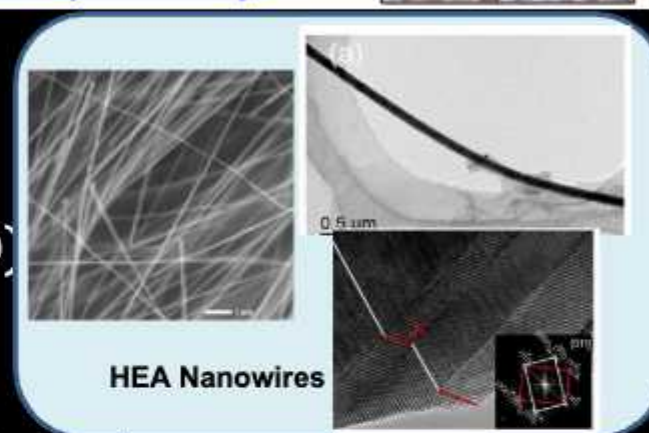
Electrochemical Materials Design & Processing

(High Entropy Alloy Design & Manufacturing (0D, 1D, 2D))

Metals Recovery from Scraps/E-Wastes (Solar PVs, LiBs)

4D Printing of Shape Memory Alloys

Electrochemical Additive Manufacturing Corrosion (cold & hot)



HEA Nanowires

## Major Research Facilities in the Group

Electrochemical Setup

Corrosion Setup

Electrochemical Modelling & Simulation

## Technology/Product Developed

Anti-viral Coatings on any substrates

High Entropy Alloys Coatings and Nanowires

Sequential Recovery of Critical Metals from E-

Wastes/Scraps



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### **Major Areas of Research/Up to 3 major sponsored projects**

- printed and flexible electronics, oxide semiconductors, organic electronics, gas sensors, and memristors
- A General route towards low voltage high current power printed electronics (SERB)
- Low-cost sensor technology to detect different biological warfare agents (ATB)

### **Major Research Facilities in the Group**

- Inkjet printer, Ink preparation unit, Hot plates
- Spin coater, Fume hood, Probe station
- Memristor measurement system, Source measurement unit



### **Technology/Product Developed/Up to 3 most significant Publications**

- Garlapati, S. K., et al., (2018). Advanced Materials, 30(40), 1707600. [IF: 32.09]
- Garlapati, S. K., et al., (2017). Advanced Electronic Materials, 3(9), 1600476. [IF: 7.295]
- Garlapati, S. K., et al., (2015). Small, 11(29), 3591-3596. [IF: 15.15]



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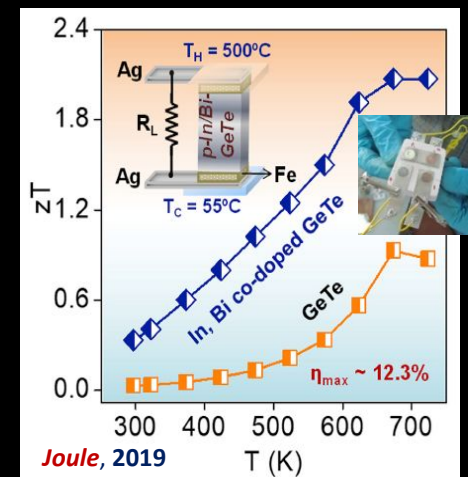
## Major Areas of Research/Up to 3 major sponsored projects

### Research Interests:

- ◆ Energy Materials and Devices
- ◆ Thermoelectric Power Generation
- ◆ Thermoelectric Metrology
- ◆ Magnetic Refrigeration

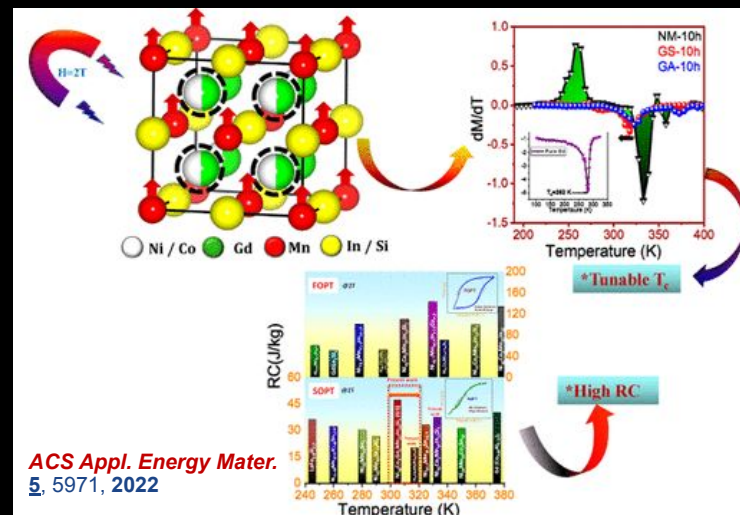
### Sponsored Projects:

- ◆ Nanostructured Thermoelectric Materials for power generation: Seed Grant IITH, Rs. 30 Lakhs (Ongoing)
- ◆ Microstructural Engineering of Higher Manganese Silicides: CEFIPRA, Govt. of India, Rs.160 Lakhs (Ongoing).



## Major Research Facilities in the Group

- ◆ Vacuum Arc Melting Machine
- ◆ Induction hot-pressing Machine
- ◆ High Energy Ball Milling Machine
- ◆ High Temperature Furnaces



## Technology/Product Developed/Up to 3 most significant Publications

1. Jothilal Palraj, Muhammad Sajjad, Manojkumar Moorthy, Madhuvathani Saminathan, Bhuvanesh Srinivasan, Nirpendra Singh, Rajasekar Parasuraman, Shashikant P Patole, Kiran Mangalampalli, **Suresh Perumal\***, *J. Mater. Chem. A*, 12, 13860, **2024**.
2. Manojkumar Moorthy, Bhuvanesh Srinivasan, David Berthebaud, Rajasekar Parasuraman, **Suresh Perumal\***, *ACS Appl. Energy Mater.* 6, 723, **2023**.
3. Shaleni Venkatesan, E M Abhinav, N Pavan Kumar, S Kavita, M Manivel Raja, Rajasekar P., Durai Murugan K., **Suresh Perumal\***, *ACS Appl. Energy Mater.* 5, 12, 15959, **2022**.
4. **Suresh Perumal**, Manisha Samanta, Tanmoy Ghosh, U. Sandhya Shenoy, Anil K. Bohra, S. Bhattacharya. Ajay Singh, U. V. Waghmare, and K. Biswas, *Joule*, 3, 2565, **2019**.