

PRANOY RAY: A Biographical Sketch

Pranoy is a Mechanical Engineering PhD Student at GeorgiaTech. His advisor is [Dr. Surya Kalidindi](#) and he works as a doctoral researcher at the MINED Group in GeorgiaTech. He is also pursuing his MS in Computational Science and Engineering at the College of Computing, GeorgiaTech in parallel with his doctoral degree. Broadly speaking, he works in the area of Materials Informatics and his research is focused on building data-driven models and automation tools to address fundamental and applied problems in the pursuit of accelerated materials discovery. His work involves developing autonomous systems for materials design and modeling to support materials design and discovery at the atomistics scale.

He has previously worked on projects related to Computational Materials Science in the atomistics scale and has experience working with DFT (Density Functional Theory) and MD (Molecular Dynamics) Simulations. He completed his undergraduate studies from the National Institute of Technology Durgapur, in India, and graduated with a Bachelor's in Technology in Metallurgical and Materials Engineering in 2020. He completed his undergraduate thesis at the Bhabha Atomic Research Centre in Mumbai, India under the guidance of [Dr. Brahmananda Chakraborty](#), working on predicting new materials for solid-state Hydrogen Storage with the application of Density Functional Theory and MD Simulations. His work done here resulted in a journal article in the Elsevier-International Journal of Hydrogen Energy as well as a Poster Presentation at the Department of Atomic Energy Computational Chemistry Symposium (DAE-CCS) in 2019. He continued working as a Project Assistant at BARC, transitioning from his role as a research Intern, and completed two more projects predicting two new materials for Hydrogen Storage, before joining the PhD program at GeorgiaTech in Fall 2021.



Pranoy has held many leadership roles in the past, during his undergraduate degree at NITD, which include being the President of the Entrepreneurship Development Cell, amongst other positions. When Pranoy doesn't code, he loves to get off the grid and go on treks. He is fascinated often by the progress in the aeronautical sciences spectra and aims to research for and contribute to the industry in the near future.

His publications, past projects, technical skills and some relevant graduate coursework have been enlisted below.

PUBICATIONS:

1. Chakraborty, Brahmananda, Pranoy Ray, Nandini Garg, and Srikumar Banerjee. "High capacity reversible hydrogen storage in titanium doped 2D carbon allotrope Ψ -graphene: Density Functional Theory investigations." *International Journal of Hydrogen Energy* 46, no. 5 (2021): 4154-4167.
2. Pranoy Ray, Brahmananda Chakraborty. "Ti-doped Carbon Nanostructure as an Efficient Medium for Hydrogen Storage", *Proceedings - DAE CCS*, F-5 191-192 (2019)

PAST PROJECTS:

Pranoy has worked on multiple academic and research projects, some of which have resulted in the above publications (2 more papers under review):

1. Accelerated Materials Discovery using advanced AI and Statistical Methods, GeorgiaTech - This ongoing project is being conducted under the supervision of Dr. Surya Kalidindi. The determination of Physical & Mechanical Properties of various 2D/3D Materials using advanced statistical methods like 2-point correlations is being analyzed, at the atomistics scale.
2. Prediction of Mechanical Properties of Materials using Machine Learning, IIT Bombay - This project was conducted under the supervision of Dr. Alankar (Prof. IIT-B & Director, IMaGen Lab). The determination of Mechanical Properties of various binary and ternary alloys with the aid of Materials Informatics and ML-driven approaches was analyzed.
3. Phase Modelling Computation of Interfacial Energies of HEA, IIT Kharagpur - This ongoing project is being conducted under the supervision of Prof. Shibayan Roy (Materials Science Centre, IIT KGP). My current project is an undisclosed one, using Aluminum Alloys, where I am working on phase modelling problems using DFT & MD Simulations.
4. Prediction of Nuclear Coolant Materials for MSRs, HP & SRPD, BARC - This ongoing project is being conducted under the supervision of Dr. B. Chakraborty (Scientist G, BARC). The variation of properties of fluoride and chloride salts against various factors & conditions are being studied.
5. First Principles Studies of Efficient Hydrogen Storage in Transition-Metal doped Carbon-Nanostructures, HP & SRPD, BARC - This completed project was conducted under the supervision of Dr. B. Chakraborty (Scientist G, BARC). The determination of Hydrogen Storage Capabilities of various new materials in accordance with the DOE's standards has being analyzed using BARC's super-computing facility. A full article paper has been submitted for publication.
6. Determination of Water Contamination Content Profile in a Steel Plant Belt(Durgapur) - This project was completed under the supervision of Prof. Hirok Chaudhari (Physics Department, NITD). The determination of the content profile and their effect in our daily lives, besides a few other detrimental physical factors were measured, which were further used as inputs to fabricate an anti-polluting membrane.

TECHNICAL SKILLS:

- Languages: Python, Java, R, C, \LaTeX, HTML
- Frameworks: PyTorch, Flask, PyQt4, PyCalphad, Shell Scripting, CSS, Firebase
- Simulation Packages: VASP, LAMMPS
- Softwares: VESTA, Origin, THERMOCALC, Ovito, BlueJ, Adobe Photoshop, MS Office

RELEVANT GRADUATE COURSEWORK:

- ME8803: Materials Informatics (Instructor: Dr. Surya Kalidindi) Fall 2021
- ME8883: ML Foundations for ME (Instructor: Dr. Aaron Stebner) Fall 2021
- MSE6140: Computational Materials Science (Instructor: Dr. Rampi Ramprasad) Fall 2021
- ME8813: Artificial Intelligence for ME (Instructor: Dr. Wang/Dr. Kalidindi) Spring 2022
- MSE8803-D: Density Functional Theory (Instructor: Dr. Rampi Ramprasad) Spring 2022