PRANOY RAY

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ABOUT

I'm a computational materials science researcher focused on building data-driven models and automation tools to address fundamental and applied problems in the pursuit of accelerated materials discovery at the atomistic scale. In particular, I am currently working on:

- Accelerated Materials Discovery using Artificial Intelligence Methods
- Development of Novel Materials using Computational Chemistry (Atomistic Scale)
- Discovery and Prediction of Material Systems for Renewable Energy (Atomistic Scale)

My advisor is Dr.Surya Kalidindi and I work as a doctoral researcher at the MINED Group in GeorgiaTech. My research involves developing physics-informed DL models to significantly accelerate materials discovery and promote product design. I have experience in using and handling datat extracted from various open-source DFT-generated databases like JARVIS, Materials Project, etc. to develop models for such projects.

EDUCATION

- Ph.D - Mechanical Engineering, MINED Lab, Georgia Institute of Technology - Atlanta, 2026
- MS - Computational Science and Engineering, MINED Lab, Georgia Institute of Technology - Atlanta, 2024
- Summer School - Computational Materials Science, CMS3, Texas A&M University - College Station, 2022
- B.Tech - Metallurgical & Materials Engineering, National Institute of Technology - Durgapur, 2020
- High School - Computer Science, Don Bosco School Park Circus-Kolkata, 2016

INVITED TALKS

- **Feature engineering of electron charge density fields for building AI/ML models to predict material properties**
  P.Ray, S. Kalidindi | December 2022
  Energy & Informatics Symposium, Oahu, HI, USA
  Invited Talk - Published in Proceedings (TBD)
- **Voxelized representations of atomic systems for machine learning applications**
  S. Kalidindi, M. Barry, P.Ray | March 2023
  TMS Annual Meeting, San Diego, CA, USA
  Invited Talk - Published in Proceedings (TBD)

JOURNAL PUBLICATIONS

- **High Capacity Reversible Hydrogen Storage in Titanium Doped 2D Carbon Allotrope PSI-Graphene: DFT Investigations**
  B. Chakraborty, P.Ray, N.Garg, S. Banerjee | November 2020 | Citations: 53 (as of 09-2022)
  International Journal of Hydrogen Energy (Elsevier) | Volume 46 | Issue 5 | Pages 4154-4167
  Full Article - Journal Paper

CONFERENCES & SYMPOSIUMS

- **Ti-doped Carbon Nanostructure as an Efficient Medium for Hydrogen Storage**
  P.Ray, B. Chakraborty | November 2019
  Department of Atomic Energy, Computational Chemistry Symposium, BRNS-Govt. of India
  Poster Presentation- Published in Proceedings

GRANTS & ACCOLADES

- Energy & Informatics Symposium 2022 Fellow: Tokyo Tech (Hawaii, USA)
- CMS3 2022 Fellow: NSF + Texas A&M University (College Station, TX, USA)
- Best Poster Award: TEQIP III Grant (NIT Durgapur) to present my poster at DAE-CCS 2019 (Mumbai, MH, India)

RESEARCH EXPERIENCE

Georgia Institute of Technology, Atlanta — **MINED Group**
Graduate Research Assistant (advised by Dr. Surya Kalidindi) — *August 2021 to Present*
- Working on an undisclosed Materials Discovery project using AI at the atomistics scale (using PyTorch and VASP)

Bhabha Atomic Research Centre, Mumbai — **HP & SRPD**
Research Assistant (advised by Dr. Brahmananda Chakraborty) — *July 2019 to August 2021*
- Completed 3 projects where we predicted a Novel Material System for Hydrogen Storage (1 Journal Paper pub., 2 under-Rev)

Summer Research Intern — *May 2019 to July 2019*
- Completed a project which involved new Material Discovery using DFT (Density Functional Theory), Bader Charge Ananly. & MD.

Indian Institute of Technology, Bombay — **IMaGen Lab**
Research Intern (advised by Dr. Alankar Alankar) — *July 2020 to Nov 2020*
- Worked on a Materials Informatics project using the Random Forest - Machine Learning Algorithm in Python.

Indian Institute of Technology, Kharagpur **SRMSC Lab**
Research Intern (advised by Dr. Shibayan Roy) *June 2020 to Oct 2020*
- Worked on a Phase-Field Modelling project involving DFT & MD Simulations (colab with Washington University at St. Louis).

Hindustan Aeronautics Limited, Bangalore **Foundry & Forge Division**
Project & Industrial Intern *May 2018 to July 2018*
- Completed two Projects: (1) ID of Post Investment Casting Defects (2) Preventive Measures for QC using Lean Management

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

ACADEMIC PROJECTS

- **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 statsitical methods like 2-point correlations is being analyzed, at the atomistics scale.
- **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.
- **Phase Modelling Computation of Interfacial Energies of HEA, IIT Kharagpur** - This ongoing project is being conducted under the supervision of Dr. Shibayan Roy (Prof. at the Materials Science Centre, IIT KGP). My current project is an undisclosed one, using Aluminium Alloys, where I am working on phase modelling problems using DFT & MD Simulations.
- **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.
- **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.
- **Determination of Water Contamination Content Profile in a Steel Plant Belt(Durgapur)** - This project was completed under the supervision of Dr. Hirok Chaudhari (Prof.of the 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.

TEACHING AND MENTORING EXPERIENCE

- 2016-20 : Mentored 5 on-campus startups from idea stage to execution
- 2018-20 : Taught classes on Entrepreneurship & Innovation at the Institute Innovation & Incubation Cell, NITD. I received a Certificate of Appreciation from the Ministry of Human Resource Development, Govt. of India for the same.

LEADERSHIP EXPERIENCE

- President at the Entrepreneurship Development Cell, NIT Durgapur (2016-2020)
- Treasurer at the Art & Photography Club, NIT Durgapur (2017-2020)

MENTIONS IN THE NEWS

- **Backyard Startups** - The Telegraph (India) - 1st August, 2018 :
  #JustHashtags is a startup that I co-founded with a school friend of mine. We were interviewed by this newspaper as we made headlines with our foolproof business model when we launched in the city of Calcutta. I continue to play a non-profit advisory role in this startup.

EXTRACURRICULAR ACTIVITIES

Convened and Organized 3 Entrepreneurship-Summits, namely:
- E-Summit 2018: First of it's kind in NITD
- E-Summit 2019: Second Largest in Eastern India
- E-Summit 2020: Largest Virtual E-Summit in India

Convened and Organized 6 exhibitions and 5 graffiti arts across campus, and played a pivotal role in associating the college with external art projects.