

PRANOY RAY

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OVERVIEW

Demonstrated leadership of multidisciplinary teams of engineers and student scientists in high profile R&D projects in industrial and academic settings. Key responsibilities include overseeing project timelines and deliverables within a start-up / entrepreneurial (fast-paced) environment. Demonstrated the ability to build a diverse group, on-boarding key skill sets into critical project roles, ensuring clear communication of project deliverables. Comprehensive communication of project results and milestones. Demonstrated innovator and problem solver with a background in materials chemistry, molecular simulations and novel feature engineering within product-driven Materials Informatics and ICME workflows.

EDUCATION

- Ph.D: Mechanical Engineering, Georgia Institute of Technology - Atlanta, USA (exp-2026)
- [MS](#): Computational Science and Engineering, Georgia Institute of Technology - Atlanta, USA (2024)
- B.Tech: Metallurgical & Materials Engineering, National Institute of Technology - Durgapur, India (2020)

PROFESSIONAL CERTIFICATIONS

- Management of Technology ([MOT](#)), Scheller College of Business, GeorgiaTech - Atlanta, USA (2025)
- Computational Materials Science & Engineering ([CMSE](#)), School of MSE, GeorgiaTech - Atlanta, USA (2023)

RESEARCH EXPERIENCES

George W. Woodruff School of Mechanical Engineering (Atlanta, USA)

Graduate Research Assistant (Advisor: [Dr. Surya R. Kalidindi](#))

MINED Group @ GT

Aug 2021 to Present

- Formulating efficient spatial featurization protocols for lower-order ML models, promoting accelerated materials design and UQ
- Head Teaching Assistant (ME8813 & ME4853) Spring 2023 & Spring 2025
- Instructed & graded classes of 100 graduate and UG students on ML Fundamentals for AI4Science applications (MSE/ME)

Indian Institute of Technology (Bombay, India)

Research Intern (Advisor: [Dr. Alankar Alankar](#))

IMaGen Lab

July 2020 to Nov 2020

- Workflows for predicting the mechanical properties of materials from composition using lower order ML models (RF, SVMs, etc.)

Indian Institute of Technology (Kharagpur, India)

Research Intern (Advisor: [Dr. Shibayan Roy](#))

SRMSC Lab

June 2020 to Oct 2020

- Participated in a Phase-Field Modelling project involving DFT & MD Simulations (collab with Washington University at St. Louis)

INDUSTRY EXPERIENCES

Multiscale Technologies Inc (Seattle, USA)

Data Science Manager (Advisor: [Srikanth Kasam](#))

R&D Team

April 2024 to Aug 2024

- Led global, interdisciplinary data science teams in delivering materials design solutions to Fortune 100 clients.

Materials Scientist (Advisor: [Vasu Kalidindi](#))

Jan 2024 to April 2024

- Developed AI workflows for federal, private and international labs to accelerate materials discovery at the molecular scale.

Bhabha Atomic Research Centre (Mumbai, India)

Research Assistant (Advisor: [Dr. Srikumar Banerjee](#) & [Dr. Brahmananda Chakraborty](#))

HP & SRPD

May 2019 to Aug 2021

- Theoretically discovered 3 distinct novel material systems for solid-state Hydrogen Storage using DFT & MD

Hindustan Aeronautics Limited (Bangalore, India)

Project & Industrial Intern (Advisor: [Soumya Mandi](#))

Foundry & Forge Division

May 2018 to July 2018

- Completed two Projects: (1) ID of Post Investment Casting Defects (2) Preventive Measures for QC using Lean Management

GRANTS & ACCOLADES

- Woodruff School Fellow (2025): GWW School of Mechanical Engineering, GeorgiaTech (Atlanta, GA, USA)
- Novelis Graduate Scholar (2024): Novelis Innovation Hub & Novelis Inc (Kennesaw, GA, USA)
- EIIF Fellow (2022): TokyoTech & Strategic Energy Institute @GT (Honolulu, HI, USA)
- CMS3 Fellow (2022): NSF + Texas A&M University (College Station, TX, USA)
- Best Poster Award: TEQIP III Grant (NIT Durgapur) @ DAE-CCS 2019 (Mumbai, MH, India)

TECHNICAL SKILLS

- **Machine Learning/AI**: Neural Networks, Gaussian Process Regression, Bayesian Optimization, Normalizing Flows, Autoencoder
- **Programming & Data Science**: Python (with key libraries like PyTorch, GPyTorch, BOPorch, Pyvista, SciPy, scikit-learn), R, Java, C
- **Computational Materials Science**: VASP, LAMMPS, GROMACS, DFT, Molecular Dynamics, CG-Martini3, ORCA
- **HPC/Cloud Platforms**: MPI, familiarity with cloud platforms (AWS, GCP, Azure), Shell Scripting, Flask, Firebase
- **Advanced Graduate Courses**: Parallel Computing (HPC), Density Functional Theory, Materials Informatics, DOX, ML, DL

MEDIA MENTIONS

- [Novelis Graduate Scholar](#) - Georgia (USA) - 12th January 2024: based on the scholarship awarded by [Novelis Inc](#) (world's largest aluminium rolling and recycling) as a top scholar conducting research in aspects of sustainability, techno-economics of circularity, high-throughput materials discovery, and AI/data science applications in materials/manufacturing/supply chains.

- **2nd EIIIF TokyoTech** - Hawaii (USA) - 13th January 2023: based on an invited talk at the 2nd Energy & Informatics Forum @ Oahu in December 2022 supported by the Strategic Energy Institute (SEI) at GeorgiaTech
- **Backyard Startups** - The Telegraph (India) - 1st August 2018: based on #JustHashtags (a startup that Ray co-founded) which was launched in the city of Calcutta, India without the assistance of investors.

RESEARCH WORK

JOURNAL PUBLICATIONS [Google Scholar]

- **Refining Coarse-Grained Molecular Topologies: A Bayesian Optimization Approach**
P. Ray, A. P. Generale, N. Vankireddy, Y. Asoma, M. Nakauchi, H. Lee, K. Yoshida, Y. Okuno, S.R. Kalidindi | July 2025
npj Computational Materials | Volume 11 | Article 234
- **Lean CNNs for Mapping Electron Charge Density Fields to Material Properties**
P. Ray, K. Choudhary, S.R. Kalidindi | January 2025
Integrating Materials and Manufacturing Innovation | Volume 14 | Issue 1 | Pages 1-13
- **Zr doped C_{24} fullerene as efficient hydrogen storage material: insights from DFT simulations**
A. Kundu, A. Jaiswal, P. Ray, S. Sahu, B. Chakraborty | August 2024
Journal of Physics D: Applied Physics | Volume 57 | No. 49 | Pages 495502-13
- **Ti-decorated C_{30} as a High-capacity Hydrogen Storage Material: Insights from Density Functional Theory**
H.T.Nair, A.Kundu, P.Ray, P.K.Jha, B.Chakraborty | August 2023
RSC Sustainable Energy & Fuels | Volume 7 | Issue 20 | Pages 5109-19
- **High Capacity Reversible Hydrogen Storage in Titanium Doped 2D Carbon Allotrope Ψ -Graphene: DFT Investigations**
B. Chakraborty, P.Ray, N.Garg, S. Banerjee | January 2021
International Journal of Hydrogen Energy (Elsevier) | Volume 46 | Issue 5 | Pages 4154-67

CONFERENCES & SYMPOSIUMS

Oral Presentations/Talks

- **Structure-aware Bayesian optimization for efficient design of disordered CCAs**
P.Ray, S.R. Kalidindi | October 2025 | SES Annual Technical Meeting, Atlanta, GA, USA
- **(INVITED) Bayesian frameworks for advanced materials design at the atomistic scale**
P.Ray, S.R. Kalidindi | October 2024 | Novelis' Global Research and Technology Center, Kennesaw, GA, USA
- **(INVITED) Bayesian optimization of Coarse-Grained topologies: Applications to common polymers**
P.Ray, A.P. Generale, et. al. | October 2024 | TMS Fall Meeting, Pittsburgh, PA, USA
- **(INVITED) Feature engineering of electron charge density fields for building AI/ML models to predict material properties**
P.Ray, S.R. Kalidindi | December 2022 | 2nd Energy & Informatics International Forum, Oahu, HI, USA

Posters

- **Accelerating Molecular Design with generalizable Bayesian Optimization**
P.Ray, S. R. Kalidindi | October 2024 | MSE Research Showcase, GeorgiaTech, Atlanta, USA
- **Ti-doped Carbon Nanostructure as an Efficient Medium for Hydrogen Storage**
P.Ray, B. Chakraborty | November 2019 | Department of Atomic Energy Computational Chemistry Symposium, Mumbai, India

EXTRA-CURRICULAR RESPONSIBILITIES

Academic:

- Peer Reviewer (AI4Mat): NeurIPS 2025, San Diego, CA (USA)
- Peer Reviewer (AI4Mat): CVPR (IEEE Computer Vision & Pattern Recognition) 2025, Nashville, TN (USA)
- Peer Reviewer: PEARC25 (ACM Practice and Experience in Advanced Research Computing), Columbus, OH (USA)
- Session Chair/Reviewer: GT Undergraduate Research Symposium (UOPS) 2025, Atlanta, GA (USA)
- Reviewer/Committee-Member: Scipy Conference 2025, Tacoma, WA (USA)
- Peer Reviewer: Springer Nature Journal Of Materials (2023-current)
- Reviewer/Committee-Member: Scipy Conference 2024, Tacoma, WA (USA)
- Reviewer/Committee-Member: Scipy Conference 2023, Austin, TX (USA)

Leadership:

- Board Member: Emerging Leaders Advisory Board @GT (2025-2026)
- Internal VP: Mechanical Engg Grad Association (MEGA) @GT (2023-2024)
- President: Entrepreneurship Development Cell, NIT Durgapur, India (2016-2020)
- Treasurer: Strokes (Art & Photography Club), NIT Durgapur, India (2017-2020)

REFERENCES

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| Dr. Surya R. Kalidindi (surya.kalidindi@me.gatech.edu)
Regents' Professor, Rae S. and Frank H. Neely Chair
Mechanical Engineering, Georgia Institute of Technology
Atlanta, GA, USA 30332 | Dr. Brahmananda Chakraborty (brahma@barc.gov)
Scientist G, HP&SRPD, Bhabha Atomic Research Center
Associate Professor, Homi Bhabha National Institute
Mumbai, MH, India 400085 |
| Dr. Manoj Kolel-Veetil (manoj.k.kolel-veetil.civ@us.navy.mil)
Research Scientist, Chemistry Division
Naval Research Laboratory
Washington, DC 20375 | |