

# PRANOY RAY<sup>ID</sup>

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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 and root cause analysis of new & existing issues. 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)

## INDUSTRY EXPERIENCES

### Multiscale Technologies Inc (Seattle, USA)

Data Science Manager

R&D Team

April 2024 to Aug 2024

- Commercialized optimized manufacturing solutions for Fortune 100, cutting production costs. Led interdisciplinary teams.

Materials Scientist Intern

Jan 2024 to April 2024

- Deployed AI workflows that accelerated time-to-market for newer materials, cutting R&D cycle time by 80% for federal labs.

### 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 alternative fuels (Hydrogen Storage) using DFT & MD

### Hindustan Aeronautics Limited (Bangalore, India)

Project & Industrial Intern (Advisor: Soumya Mandi)

Foundry & Forge Division

May 2018 to July 2018

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

## PROFESSIONAL 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)

## 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)

- EII 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, BOTorch, Pyvista, SciPy, scikit-learn), R, Java, C
- Computational Materials Science: VASP, LAMMPS, GROMACS, DFT, Molecular Dynamics, CG-Martin3, ORCA
- HPC/Cloud Platforms: MPI, AWS, GCP, Azure, Shell Scripting, Flask, Firebase, Hadoop, BigData
- 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 & recycling) as a top scholar conducting research in aspects of sustainability (de-carbonization), techno-economics of circularity, high-throughput materials discovery, & AI/data science in materials/manufacturing/supply chains.

- **2nd EIIF 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

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### JOURNAL PUBLICATIONS [Google Scholar]

- **Assessing the accuracy of Bayesian-optimized CGMD in predicting polymer miscibility**  
P. Ray, Y. Asoma, N. Vankireddy, A. P. Generale, M. Nakauchi, H. Lee, K. Yoshida, S.R. Kalidindi, Y. Okuno | Nov 2025  
RSC Chemical Science | Under Review
- **ML workflows for assisting in the treatment and removal of forever chemicals**  
P. Ray, A. Castillo, M. Kolel-Veetil, S.R. Kalidindi | Oct 2025  
Advanced Science | Under Review
- **Unraveling the PFAS helix: A statistical approach**  
P. Ray, H. Cavalli, K.D. Tynes, G. Bizana, A. Castillo, S. Vyas, R. Siefert, S.R. Kalidindi, M. Kolel-Veetil | Sep 2025  
ACS Journal of Chemical Information and Modeling | Under Review
- **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  $\Psi$ -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

### ORAL PRESENTATIONS/TALKS (CONFERENCES)

- **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

## PROFESSIONAL SERVICES/RESPONSIBILITIES

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### Academic:

- Reviewer & Committee Member: SciPy Conference (2023, 2024, 2025)
- Peer Reviewer (AI4Mat): NeurIPS 2025, CVPR 2025
- Peer Reviewer: PEARC25, Springer Nature Journal of Materials (2023-Present)
- Session Chair & Reviewer: GT Undergraduate Research Symposium (2025)

### 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](mailto: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](mailto: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](mailto:manoj.k.kolel-veetil.civ@us.navy.mil))  
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