

PRANOY RAY

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CAREER OBJECTIVE

Interdisciplinary scientist leveraging applied statistics and physics-informed AI to accelerate materials discovery and manufacturing optimization. Driving industrial innovation by translating complex, multiscale data into robust, scalable engineering solutions.

EDUCATION

- Ph.D: Mechanical Engineering, Georgia Institute of Technology - Atlanta, USA (expected May 2026)
 - Advisor: [Dr. Surya R. Kalidindi](#)
 - Thesis Title: "Computationally efficient voxelized approaches for structure-property relationships in molecular systems"
- [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)

TECHNICAL SKILLS

- **Applied Statistics & Process Informatics:** Bayesian Optimization, Gaussian Processes (GPyTorch, BoTorch), Active Learning, Uncertainty Quantification (UQ), Pareto Frontier Analysis, Design of Experiments (DoE), Scikit-learn.
- **Machine Learning & Generative AI:** PyTorch, Graph Neural Networks (GNN), CNN, Autoencoders, Normalizing Flows, GANs.
- **Engineering Simulations:** VASP, LAMMPS, GROMACS, MACE, Density Functional Theory (DFT), Molecular Dynamics (MD), CGMD.
- **Programming, HPC & Cloud:** Python, R, C, Java, MPI, AWS, GCP, Azure, SLURM/PBS, Flask, Shell Scripting.

RESEARCH & INTERNSHIP EXPERIENCES

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

Graduate Research Assistant

Led collaborative projects domestically and internationally. Architected physics-informed, interpretable, and robust ML Models to solve complex inverse problems and capture relevant process-structure-property relationships, leveraging UQ with multiscale simulations to calibrate for multimodal fidelity. Published 5+ research papers in top journals (see [Google Scholar](#) and [LinkedIn](#))

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)

Multiscale Technologies Inc (Seattle, USA)

Data Science Manager & Materials Scientist Intern

R&D Team

Jan 2024 to Sep 2024

Defined product strategy and executed the roadmap for semiconductor manufacturing process optimization (SMPO) and AI-driven manufacturing solutions. Led cross-functional teams to deliver and deploy high-fidelity cost-saving tools for Fortune 100 clients, focusing on product lifecycle and ROI requirements. Results published in scientific journals.

Bhabha Atomic Research Centre (Mumbai, India)

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

May 2019 to Aug 2021

Theoretically discovered and published 3 distinct novel material systems for alternative fuels (Hydrogen Storage) using DFT & AIMD

Indian Institute of Technology (IIT) 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 (IIT) 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)

Hindustan Aeronautics Limited (Bangalore, India)

Project & Industrial Intern (Advisor: Soumya Mandi)

Foundry & Forge Division

May 2018 to July 2018

Led and deployed projects on shop floors: (1) Led failure analysis investigations on casting defects, implementing process control measures that improved yield. (2) Applied Lean management principles to manufacturing quality control.

LEADERSHIP & COMMUNITY SERVICES

- Board Member: Emerging Leaders Advisory Board @GT (2025-2026)
- Internal VP: Mechanical Engg Grad Association (MEGA) @GT (2023-2024)
- Peer Reviewer: Springer Nature, Journal of Materials, Chemical Papers (since 2023)
- Peer Reviewer: SciPy Conference (2023, 2024, 2025), NeurIPS 2025, CVPR 2025, PEARC 2025, GT UG Research Symposium (2025)

HONORS & AWARDS

- **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)
 - Featured in: [GTRI News](#) as a top scholar advancing sustainability, circularity, and AI-driven materials discovery.
- **EIIF Fellow** (2022): TokyoTech & Strategic Energy Institute @GT (Honolulu, HI, USA)
 - Invited Scholar: Selected by [GT Strategic Energy Institute](#) for the 2nd Energy & Informatics Forum.
- **CMS3 Fellow** (2022): NSF + Texas A&M University (College Station, TX, USA)

Other "selected" Media & Press

- **TMS Standout Article** (2025): Highlighted by TMS Editors as a standout 2025 publication for novel work on Lean CNNs.
- **The Telegraph (India)** (2018): Featured in "Backyard Startups" for launching the bootstrapped venture #JustHashtags.

SELECTED RESEARCH

JOURNAL PUBLICATIONS

- **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) | [Code](#)

- **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

Angewandte Chemie (Under Review)

- **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

ChemRxiv preprint | RSC Chemical Science (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 | [Code](#)

ORAL PRESENTATIONS/CONFERENCE TALKS

- **Statistical quantification of helicity in linear PFAS**

P. Ray, H. Cavalli, et. al. | March 2026 | ACS Spring, Atlanta, GA, USA

- **(INVITED) Lean CNNs for materials discovery using electron charge density fields**

P. Ray, S.R. Kalidindi | October 2025 | Host: Prof. Stefano Sanvito | Trinity College, Dublin, Ireland

- **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

REFERENCES

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. Manoj Kolel-Veetil (manoj.k.kolel-veetil.civ@us.navy.mil)
Research Scientist, Chemistry Division
US Naval Research Laboratory, Washington DC, USA 20375

Dr. Brahmananda Chakraborty (brahma@barc.gov)
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Associate Professor, Homi Bhabha National Institute
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Dr. Andrew J. Medford (ajm@gatech.edu)
Associate Professor, Georgia Institute of Technology
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