

# 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), Failure Modes & Effects Analysis (FMEA).
- Machine Learning & Generative AI:** PyTorch, Graph Neural Networks (GNN), CNN, Autoencoders, Normalizing Flows, Scikit-learn.
- 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

**MINED Group @ GT**

Aug 2021 to Present

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)

**R&D Team**

Data Science Manager & Materials Scientist Intern

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)

**HP & SRPD**

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)

**IMaGen Lab**

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

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)

**SRMSC Lab**

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

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)

**Foundry & Forge Division**

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

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: ICLR 2026, NeurIPS 2025, CVPR 2025, PEARC 2025, SciPy Conference (2023, 2024, 2025), GT UGRS 2025

## HONORS & AWARDS

- Woodruff School Fellow** (2025): GWW School of Mechanical Engineering, GeorgiaTech (Atlanta, GA, USA)
- TMS Standout Article** (2025): Highlighted by TMS Editors as a standout 2025 publication for novel work on Lean CNNs.
- 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.
- ELIF 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)
- The Telegraph (India)** (2018): Featured in "Backyard Startups" for launching the bootstrapped venture #JustHashtags.

## SELECTED RESEARCH

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### 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 | Novartis' 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

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