# PRANOY RAY

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## CAREER OBJECTIVE

Interdisciplinary scientist leveraging **materials science**, applied statistics, and **process informatics** to accelerate **manufacturing optimization** and yield improvement. Driving industrial innovation by translating complex, multiscale data into robust **Design for Manufacturing (DFM)** solutions and scalable engineering processes for microelectronics and material systems.

## 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

•**Manufacturing Statistics & Process Control:** Failure Modes & Effects Analysis (FMEA), Design of Experiments (DoE), Bayesian Optimization, Uncertainty Quantification (UQ), Pareto Frontier Analysis, Process Informatics, Root Cause Analysis.
•**Engineering Experiments, Simulations & Physics:** Density Functional Theory (DFT), Molecular Dynamics (MD), VASP, LAMMPS, GROMACS, Multiscale Modeling, Material Property Prediction, Materials Characterization (SEM), Microscopy.
•**Machine Learning & Data Analysis:** PyTorch, Graph Neural Networks (GNN), CNN, Scikit-learn, Autoencoders, Normalizing Flows.
•**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)** — **MINED Group @ GT**
*Graduate Research Assistant* — *Aug 2021 to Present*

- Architected physics-informed, interpretable models to solve complex inverse problems and capture relevant **process-structure-property** relationships, leveraging UQ with multiscale simulations to calibrate for multimodal fidelity & manufacturing tolerances.
- Led collaborative projects domestically & internationally. Published 5+ research papers in top journals (Google Scholar & 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. 10+ digital twins developed for manufacturing process simulation.

**Bhabha Atomic Research Centre (Mumbai, India)** — **HP & SRPD**
*Research Assistant (Advisor: Dr. Srikumar Banerjee & Dr. Brahmananda Chakraborty)* — *May 2019 to Aug 2021*

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

**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.

- **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)
- **The Telegraph (India)** (2018): Featured in "Backyard Startups" for launching the bootstrapped venture #JustHashtags.

## SELECTED RESEARCH

**JOURNAL PUBLICATIONS**

- **ML Workflows for Screening Degradation-Relevant Properties of Forever Chemicals**
  *P. Ray, A. Castillo, M. Kolel-Veetil, S.R. Kalidindi* | *Jan 2026*
  **Advanced Science | e23817 | Code**
- **Universal electronic manifolds for extrapolative alloy discovery**
  *P. Ray, S. Bhowmik, P. Suryanarayana, S.R. Kalidindi, A.J. Medford* | *Jan 2026*
  **RSC Digital Discovery (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*
  **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 Techincal 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. Brahmananda Chakraborty* (brahma@barc.gov)
Scientist G, HP&SRPD, Bhabha Atomic Research Center
Associate Professor, Homi Bhabha National Institute
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*Dr. Manoj Kolel-Veetil* (manoj.k.kolel-veetil.civ@us.navy.mil)
Research Scientist, Chemistry Division
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*Dr. Andrew J. Medford* (ajm@gatech.edu)
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