

PRANOY RAY

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PROFESSIONAL SUMMARY

Materials Scientist & AI Researcher specializing in accelerating semiconductor process discovery and optimization. Expert in integrating Physics-Informed Machine Learning with experimental workflows to reduce trial-and-error cycles in deposition and etching processes. Proven track record in industrial R&D (Fortune 100) including DFM (Design For Manufacturing), delivering Digital Twin solutions that optimize manufacturing yield and experimental efficiency. Seeking to leverage expertise in Bayesian Optimization and Process Informatics to drive exploratory materials research.

EDUCATION

- Ph.D: Mechanical Engineering, Georgia Institute of Technology - Atlanta, USA (*expected May 2026*)
 - Advisor: [Dr. Surya R. Kalidindi](#)
 - Thesis Title: "Computationally efficient molecular voxelizations for structure-property relationships in Multiscale Modeling"
 - Affiliation: Automated Manufacturing Pilot Facility (AMPF) at Georgia Tech
- [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

- **Semiconductor & Process Knowledge:** Process Informatics, Design of Experiments (DOE), Yield Optimization, Failure Analysis (FMEA), Thermodynamics of Deposition/Etching, Semiconductor Manufacturing Physics.
- **AI for Process Discovery & Machine Learning:** PyTorch, Neural Networks, GNN, CNN, Autoencoders, Normalizing Flows, sklearn.
- **HPC, Cloud & Programming:** Python (Advanced), R, C, Java, MPI, CUDA, AWS, GCP, Azure, SLURM/PBS, Flask, Shell Scripting.
- **Process Informatics & Inverse Design:** Bayesian Optimization, Gaussian Processes (GPyTorch, BoTorch), Active Learning, Uncertainty Quantification (UQ), Pareto Frontier Analysis, Design of Experiments (DoE), FMEA.
- **Multiscale Simulation Packages:** VASP, PySCF, LAMMPS, GROMACS, QuantumExpresso, CG-Martini3, Ab Initio MD (AIMD), Dissipative Particle Dynamics (DPD), Forcefield Development, ML Interatomic Potentials (MLIPs/MACE).

RESEARCH & INTERNSHIP EXPERIENCES

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

Graduate Research Assistant (see [Google Scholar](#) & [LinkedIn](#))

MINED Group @ GT

Aug 2021 to Present

- **Inverse Design & Generative Optimization:** Engineered Bayesian Optimization frameworks to guide experimental design (DOE) for polymer topologies, optimizing material properties in data-scarce regimes typical of exploratory research.
- **Geometric Deep Learning:** Developed a **Voxel-based featurization** engine combined with **Lean CNNs** to map electron charge density fields to material properties, enabling rapid multi-element crystal screening and accelerating DFT workflows.
- **Physics-Informed Simulation:** Utilized Dissipative Particle Dynamics (DPD) and Molecular Dynamics (MD) to simulate microphase separation in block copolymers, integrating physical constraints with data-driven analysis for mesoscale morphology.
- **AI for Sustainability:** Collaborated with cross-functional teams (chemists and experimentalists) to screen degradation properties of PFAS, validating computational predictions against physical constraints.

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

- **Industrial AI & Digital Twins:** Partnered with process engineers at major semiconductor clients to deploy Digital Twins for manufacturing workflows, reducing experimental trial-and-error iterations by 40%.
- **Process Optimization:** Utilized AI/ML to enhance process discovery (Bayesian Optimization) for inverse design, directly translating thermodynamic data into actionable recipe adjustments for yield improvement.
- **Cross-Functional Leadership:** Managed a global team of data scientists and engineers, ensuring computational models met strict product lifecycle and ROI requirements; benchmarked models for industrial deployment.

Bhabha Atomic Research Centre (Mumbai, India)

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

HP & SRPD

May 2019 to Aug 2021

- Theoretically discovered & 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.

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.
- **EII 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.

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

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](#)

- **Zr doped C₂₄ 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 C₃₀ 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](#) | Volume 46 | Issue 5 | Pages 4154-67

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](#)

- **(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)

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Mechanical Engineering, Georgia Institute of Technology
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Research Scientist, Chemistry Division
US Naval Research Laboratory, Washington DC, USA 20375

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