

PRANOY RAY

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PROFESSIONAL SUMMARY

Computational Materials Scientist & AI Researcher with 5+ years of experience integrating **Generative AI** and **Physics-Informed Machine Learning** with multiscale simulations (MD, DFT, DPD). Expert in **Inverse Design** workflows using Bayesian Optimization and developing **Surrogate Models (MLIPs)** for materials discovery. Proven track record in industrial R&D, delivering **Digital Twin** solutions and optimizing manufacturing processes for Fortune 100 clients. Proficient in bridging HPC-driven atomistic modeling with scalable data-driven frameworks.

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"
- 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

- Generative AI & Machine Learning:** PyTorch, Geometric Deep Learning, GNN, CNN, Autoencoders, Normalizing Flows, Scikit-learn.
- 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 a **Bayesian Optimization** framework to refine Coarse-Grained (CG) topologies, performing inverse design for polymer miscibility (R_g, ρ) in data-scarce regimes.
- 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:** Led computational research on PFAS (forever chemicals), employing statistical mechanics and ML workflows to unravel helical structures and degradation mechanisms, directly supporting environmental remediation goals.

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:** Directed AI/ML strategies for semiconductor and chemical manufacturing clients (Fortune 100), developing **Digital Twins** that reduced experimental trial-and-error iterations by 40%.
- Process Optimization** Deployed **physics-informed ML models** to solve inverse problems in manufacturing, translating complex thermodynamic data into actionable engineering solutions 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)

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.

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.

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
- **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. Brahmananda Chakraborty (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) Research Scientist, Chemistry Division US Naval Research Laboratory, Washington DC, USA 20375	Dr. Andrew J. Medford (ajm@gatech.edu) Associate Professor, Georgia Institute of Technology Atlanta, GA, USA 30332