

PRANOY RAY

Postdoctoral Researcher @ Argonne & UChicago • pranoy@uchicago.edu • <https://pranoy-ray.github.io> • [📄/pranoy-ray](https://github.com/pranoy-ray)

Computational Materials researcher & Data Scientist specializing in molecular structure screening using spatial statistics. Expertise includes developing feature engineering workflows to inform robust material process-structure-property relationships across chemical processes. Experienced in integrating physics-based constraints with data-driven physics models on HPC systems. Innovative R&D professional with a track record of driving technical deliverables (for chemical/semiconductor/federal labs) and leading diverse teams in fast-paced research environments.

EDUCATION

- Ph.D: Mechanical Engineering, Georgia Institute of Technology - Atlanta, USA (08/2021 - 05/2026)
 - Advisor: [Dr. Surya R. Kalidindi](#)
 - Thesis Title: "On efficient screening strategies for molecular structures"
- MS: Computational Science and Engineering, Georgia Institute of Technology - Atlanta, USA (08/2022 - 05/2025)
- B.Tech: Metallurgical & Materials Engineering, National Institute of Technology - Durgapur, India (07/2016 - 07/2020)

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)

SELECTED AWARDS & ACCOLADES

- **William H. Glenn Sr. Fellow** (2026): George W. Woodruff School of Mechanical Engineering, GeorgiaTech (Atlanta, GA, USA)
- **Woodruff School Fellow** (2025): Research Excellence, 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](#) based on the scholarship awarded by [Novelis Inc.](#) (worlds's largest aluminium rolling & recycling) as a top scholar conducting research in aspects of sustainability (de-carbonization), techno-economics of circularity, high-throughput materials discovery, & AI/data science in materials/manufacturing/supply chains.
- **EIIF Fellow** (2022): TokyoTech & Strategic Energy Institute @GT (Honolulu, HI, USA)
 - Invited Scholar: [GT Strategic Energy Institute](#) covering us at 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): Journal article on Lean CNNs highlighted by TMS Editors as a standout article for 2025.
- **The Telegraph (India)** (2018): Featured in "Backyard Startups" regarding the launch of #JustHashtags without VC assistance.

RESEARCH

JOURNAL PUBLICATIONS

- **Unraveling the PFAS helix: A statistical approach**
P. Ray, H. Cavalli, G. Bizana, A. Castillo, S. Vyas, R. Siefert, S.R. Kalidindi, M. Kolel-Veetil | June 2026
ACS Journal of Chemical Information and Modeling (Under Review)
- **Optimal mixture designs for alloy compositions**
P. Ray, W. Yang, V.R. Joseph, S.R. Kalidindi | May 2026
Journal of Materials (Under Review)
- **Spatial statistics for screening molecular structures**
P. Ray, S.R. Kalidindi | May 2026
arXiv preprint | Small (Under Review)
- **Assessing the accuracy of Bayesian-optimized CGMD in predicting polymer miscibility**
P. Ray, Y. Asoma, M. Buzzy, N. Vankireddy, A. P. Generale, M. Nakauchi, H. Lee, K. Yoshida, S.R. Kalidindi, Y. Okuno | May 2026
ChemRxiv preprint | IMMI (Under Review)
- **Electronic manifolds for extrapolative alloy discovery**
P. Ray, S. Bhowmik, P. Suryanarayana, S.R. Kalidindi, A.J. Medford | Mar 2026
arXiv preprint | RSC Digital Discovery (Under Review) | [Code](#)
- **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](#)
- **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

PROFESSIONAL EXPERIENCES

Multiscale Technologies Inc (Seattle, USA)

Data Science Manager & Materials Scientist Intern

R&D Team

Jan 2024 to Aug 2024

> Designed and deployed active learning workflows to accelerate process optimization, effectively minimizing experimental trial-and-error loops for semiconductor, chemical and US national lab partners.

> Supervised and led a team of Data Scientists and engineers across the USA, France, India, and Pakistan to deliver exploratory materials design solutions for multiple Fortune 100 clients.

> Architected the integration of physics-based material simulations into the MIND ecosystem, creating unified pipelines that link disparate engineering APIs for automated analysis. Implemented and developed impactful integration workflows between product, solutions, and engineering teams adapted to MOT/Root Cause Analysis protocols.

Bhabha Atomic Research Centre (Mumbai, India)

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

HP & SRPD

May 2019 to Aug 2021

Established theoretical design principles for solid-state hydrogen storage using DFT and AIMD. Published multiple papers.

Hindustan Aeronautics Limited (Bangalore, India)

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

Foundry & Forge Division

May 2018 to July 2018

Accomplished projects: (1) Conducted root cause analysis on manufacturing defects in investment casting, applying process control measures relevant to yield improvement. (2) Developed preventive measures for quality control using Lean management

SERVICES TO THE SCIENTIFIC COMMUNITY

Academic:

- Reviewer & Committee Member: SciPy Conference (2023, 2024, 2025)
- Peer Reviewer (AI4Mat): NeurIPS 2025, CVPR 2025, PEARC 2025, ICLR 2026
- Peer Reviewer: Springer Nature, Journal of Materials, Chemical Papers, Artificial Intelligence Review, npj Computational Mat.
- Session Chair & Reviewer: GT Undergraduate Research Symposium (2025)

Leadership:

- Board Member: Emerging Leaders Advisory Board @GT (2025-2026)
- Internal VP: Mechanical Engg Grad Association (MEGA) @GT (2023-2024)
- President: Entrepreneurship Development Cell, NIT Durgapur, India (2016-2020)
- Treasurer: Strokes (Art & Photography Club), NIT Durgapur, India (2017-2020)

TECHNICAL SKILLS

- **Machine Learning/AI:** Neural Networks, Gaussian Process Regression, Normalizing Flows, Autoencoder, Convolutions
- **Programming & Data Science:** Python (with key libraries like PyTorch, GPyTorch, BOPorch, Pyvista, SciPy, scikit-learn), R, Java, C
- **Computational Materials Science:** VASP, LAMMPS, GROMACS, DFT, Molecular Dynamics, CG-Martini3, ORCA
- **HPC/Cloud Platforms:** MPI, AWS, GCP, Azure, Shell Scripting (SLURM/PBS), Flask, Firebase, Hadoop, BigData
- **Advanced Graduate Courses:** Parallel Computing (HPC), Density Functional Theory, Materials Informatics, DoE, ML, DL
- **Autonomous Design & Decision Making:** Bayesian Optimization, Active Learning/Sequential Decision Making, Pareto Frontier Analysis, Design of Experiments (DoE)

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