PRANOY RAY

pranoy@gatech.edu • https://pranoy-ray.github.io • +1 (404) 918-8682 • /pranoy-ray

OVERVIEW

Computational Materials Scientist and AI/ML Engineer with a dual background in Mechanical Engineering and Computational Science. Specialized in benchmarking and optimizing MLIPs and Bayesian frameworks for materials discovery, while deploying AI workflows (Lean CNNs) on HPC infrastructure. Proven leader of multidisciplinary teams in high-profile RD projects, driving timelines and deliverables within fast-paced startup and academic environments. Experienced in building diverse teams, resolving root causes, and communicating complex milestones. Innovator with expertise in materials chemistry, molecular simulations, and feature engineering within product-driven Materials Informatics and ICME workflows.

EDUCATION

- Ph.D: Mechanical Engineering, Georgia Institute of Technology - Atlanta, USA (exp-2026)
- 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)

INDUSTRY EXPERIENCES

Multiscale Technologies Inc (Seattle, USA) **R&D Team**
Data Science Manager *April 2024 to Aug 2024*
- Commercialized optimized manufacturing solutions for Fortune 100, cutting production costs. Led interdisciplinary teams.

Materials Scientist Intern *Jan 2024 to April 2024*
- Deployed AI workflows that accelerated time-to-market for newer materials, cutting R&D cycle time by 80% for federal labs.

Bhabha Atomic Research Centre (Mumbai, India) **HP & SRPD**
Research Assistant (Advisor: Dr. Srikumar Banerjee & Dr. Brahmananda Chakraborty) *May 2019 to Aug 2021*
- Theoretically discovered 3 distinct novel material systems for alternative fuels (Hydrogen Storage) using DFT & MD

Hindustan Aeronautics Limited (Bangalore, India) **Foundry & Forge Division**
Project & Industrial Intern (Advisor: Soumya Mandi) *May 2018 to July 2018*
- Deployed two projects: (1) ID of Post Investment Casting Defects (2) Preventive Measures for QC using Lean Management

ACADEMIC EXPERIENCES

George W. Woodruff School of Mechanical Engineering (Atlanta, USA) **MINED Group @ GT**
Graduate Research Assistant (Advisor: Dr. Surya R. Kalidindi) *Aug 2021 to Present*
- Formulating efficient spatial featurization protocols for lower-order ML models, promoting accelerated materials design and UQ

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)

Indian Institute of Technology (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 (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)

GRANTS & ACCOLADES

- Woodruff School Fellow (2025): GWW School of Mechanical Engineering, GeorgiaTech (Atlanta, GA, USA)
- Novelis Graduate Scholar (2024): Novelis Innovation Hub & Novelis Inc (Kennesaw, GA, USA)
- EIIF Fellow (2022): TokyoTech & Strategic Energy Institute @GT (Honolulu, HI, USA)
- CMS3 Fellow (2022): NSF + Texas A&M University (College Station, TX, USA)
- Best Poster Award: TEQIP III Grant (NIT Durgapur) @ DAE-CCS 2019 (Mumbai, MH, India)

TECHNICAL SKILLS

- **Machine Learning/AI:** Neural Networks, Gaussian Process Regression, Bayesian Optimization, Normalizing Flows, Autoencoder
- **Programming & Data Science:** Python (with key libraries like PyTorch, GPyTorch, BOTorch, 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, Flask, Firebase, Hadoop, BigData
- **Advanced Graduate Courses:** Parallel Computing (HPC), Density Functional Theory, Materials Informatics, DOX, ML, DL

MEDIA MENTIONS

- **TMS Standout Article** - Pittsburgh (USA) - 30th November 2025: Journal article on Lean CNNs for S-P linkages (see section below) highlighted by **TMS** Editors as a standout article for 2025 (pseudo cover article).

- **Novelis Graduate Scholar** - Georgia (USA) - 12th January 2024: 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.
- **2nd EIIF TokyoTech** - Hawaii (USA) - 13th January 2023: based on an invited talk at the 2nd Energy & Informatics Forum @ Oahu in December 2022 supported by the Strategic Energy Institute (SEI) at GeorgiaTech
- **Backyard Startups** - The Telegraph (India) - 1st August 2018: based on #JustHashtags (a startup that Ray co-founded) which was launched in the city of Calcutta, India without the assistance of investors.

RESEARCH WORK

JOURNAL PUBLICATIONS [Google Scholar]

- **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
  RSC Chemical Science | Under Review
- **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
- **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
  ACS Journal of Chemical Information and Modeling | 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
- **Zr doped C_{24} 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 C_{30} 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 (Elsevier) | Volume 46 | Issue 5 | Pages 4154-67

ORAL PRESENTATIONS/TALKS (CONFERENCES)

- **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**

PROFESSIONAL SERVICES/RESPONSIBILITIES

Academic:

- Reviewer & Committee Member: SciPy Conference (2023, 2024, 2025)
- Peer Reviewer (AI4Mat): NeurIPS 2025, CVPR 2025
- Peer Reviewer: PEARC25, Springer Nature Journal of Materials (2023–Present)
- 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)

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. Manoj Kolel-Veetil (manoj.k.kolel-veetil.civ@us.navy.mil)
Research Scientist, Chemistry Division
US Naval Research Laboratory, Washington DC, USA 20375

Dr. Brahmananda Chakraborty (brahma@barc.gov)
Scientist G, HP&SRPD, Bhabha Atomic Research Center
Associate Professor, Homi Bhabha National Institute
Mumbai, MH, India 400085