PRANOY RAY

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OVERVIEW

Computational Materials Scientist Data Scientist specializing in Materials Informatics and ICME. Expertise includes feature engineering, molecular simulations, and optimizing MLIPs via Bayesian frameworks on HPC systems. Innovative R&D professional with a track record of driving technical deliverables and leading diverse teams in fast-paced research environments.

EDUCATION

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

PROFESSIONAL EXPERIENCES

Multiscale Technologies Inc (Seattle, USA) **R&D Team**

Data Science Manager *April 2024 to Aug 2024*

- Supervised and led a team of Data Scientists and engineers across the USA, France, India, and Pakistan to deliver materials design solutions for multiple Fortune 100 clients.
- Part-time Solution Architect (SA) for the Product Team with a focus on seamless linking various materials science and engineering APIs into the MIND ecosystem
- Implemented and developed impactful integration workflows between product, solutions, and engineering teams adapted to MOT (Management of Technology) protocols.

Materials Scientist Intern *Jan 2024 to April 2024*

- Successfully developed AI-based Materials Design workflows for transnational industry-based clients and US national labs.
- Successfully integrated valuable workflows and features in the pursuit of accelerated materials discovery.

Bhabha Atomic Research Centre (Mumbai, India) **HP & SRPD**

Research Assistant (Advisor: Dr. Srikumar Banerjee & Dr. Brahmananda Chakraborty) *May 2019 to Aug 2021*

- Accomplished multiple projects on materials design for solid-state Hydrogen Storage with the application of DFT and AIMD simulations. 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

SELECTED 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)

RESEARCH

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**

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.

SERVICES TO THE SCIENTIFIC COMMUNITY

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)

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 (SLURM/PBS), Flask, Firebase, Hadoop, BigData
- **Advanced Graduate Courses:** Parallel Computing (HPC), Density Functional Theory, Materials Informatics, DOX, ML, DL

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
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Dr. Andrew J. Medford (ajm@gatech.edu)
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