PRANOY RAY

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Computational Materials & Data Scientist specializing in Materials Informatics using Bayesian statistics for multiscale modeling. Expertise includes developing efficient feature engineering methods for robust materials process-structure-property relationships, process optimization, and integrating physics-based constraints with data-driven AI/ML 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. Presently a final year PhD candidate, graduating in May 2026 (Spring).

EDUCATION

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

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*
  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 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 | 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 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**

SELECTED AWARDS & 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)

- *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.

PROFESSIONAL EXPERIENCES

Multiscale Technologies Inc (Seattle, USA) **R&D Team**
Data Science Manager & Materials Scientist Intern *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) **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. Established design principles for solid-state hydrogen storage using DFT and ab initio MD, identifying three novel candidate material systems with high reversible capacity.

Hindustan Aeronautics Limited (Bangalore, India) **Foundry & Forge Division**
Project & Industrial Intern (Advisor: Soumya Mandi) *May 2018 to July 2018*

- Deployed 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 (since 2023)
- 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, 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, 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