PRANOY RAY

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

PROFESSIONAL SUMMARY

Computational Materials Scientist with 5+ years of experience in **Multiscale Modeling (DFT, MD, Phase Field)** and **Physics-Informed AI** for materials discovery. Expert in **High-Throughput Screening** and **Inverse Design** workflows, utilizing Bayesian Optimization to accelerate the development of energy storage and structural materials. Proven track record in industrial R&D, delivering **Digital Twin** solutions and optimizing manufacturing processes for Fortune 100 clients. Proficient in bridging **HPC-driven electronic structure theory** with scalable data-driven frameworks (PyTorch) to solve complex structure-property relationships.

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

•**Multiscale Modeling & Simulation:** DFT (VASP, QuantumExpresso), Molecular Dynamics (LAMMPS, GROMACS), **Phase Field Modeling**, Ab Initio MD (AIMD), Dissipative Particle Dynamics (DPD), Finite Element Analysis (FEA concepts).
•**Generative AI & Machine Learning:** PyTorch, Geometric Deep Learning, GNN, CNN, Autoencoders, Scikit-learn.
•**Process Informatics & Inverse Design:** Bayesian Optimization, Gaussian Processes (BoTorch), Active Learning, Uncertainty Quantification (UQ), Pareto Frontier Analysis, Design of Experiments (DoE), **Physics-Informed Machine Learning**.
•**HPC & Programming:** Python (Advanced), MATLAB, C, MPI, CUDA, AWS/GCP, SLURM, Shell Scripting, Git, Workflow Automation.

RESEARCH & INTERNSHIP EXPERIENCES

George W. Woodruff School of Mechanical Engineering (Atlanta, USA) **MINED Group @ GT**
Graduate Research Assistant (see Google Scholar & LinkedIn) *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) **R&D Team**
Data Science Manager & Materials Scientist Intern *Jan 2024 to Sep 2024*

- **Industrial AI & Digital Twins:** Directed AI/ML strategies for semiconductor and chemical manufacturing clients, developing **Digital Twins** that modeled complex process parameters, reducing experimental trial-and-error iterations by ~40%.
- **Process Optimization:** Deployed **physics-informed ML models** to solve inverse problems in manufacturing, translating thermodynamic and kinetic data into actionable engineering solutions for yield improvement.
- **Cross-Functional Collaboration:** Led a global team of data scientists and engineers, collaborating with experimental counterparts to benchmark computational models for industrial deployment and ROI validation.

Bhabha Atomic Research Centre (Mumbai, India) **HP & SRPD**
Research Assistant (Advisor: Dr. Srikumar Banerjee & Dr. Brahmananda Chakraborty) *May 2019 to Aug 2021*

- Conducted high-throughput **DFT & AIMD simulations** to screen and discover 3 novel material systems for **advanced energy storage applications** (Hydrogen), focusing on phase stability and electronic properties.

Indian Institute of Technology (IIT Bombay, India) **IMaGen Lab**
Research Intern (Advisor: Dr. Alankar Alankar) *July 2020 to Nov 2020*

Indian Institute of Technology (IIT Kharagpur, India) **SRMSC Lab**
Research Intern (Advisor: Dr. Shibayan Roy) *June 2020 to Oct 2020*

- **Phase Field Modeling:** Contributed to a computational study involving Phase-Field Modeling coupled with DFT & MD simulations to predict microstructure evolution and phase transformations (collab with Washington University at St. Louis).

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

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