Ankit Kumar Gautam

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STEM-OPT: Eligible to work in the U.S. without employer sponsorship until April 2029. H-1B $100K rule does NOT apply

Summary

PhD Computational Scientist | 7+ Years Integrating Predictive Modeling (Quantum Chemistry & Machine Learning) for Materials Design | 5+ Publications, 8+ Conference Talks | Mentored 5+ Students | Best Oral Presentation Award

Skills

DFT & MD Simulations (VASP, ORCA, CP2K, Q-Chem) | **ML & Data Science** (Python, PyTorch, Scikit-Learn, RDKit)
Drug Design (Schrödinger Suite, Molecular Docking, Virtual Screening) | **HPC** (SLURM, Parallel Computing)

Education

Ph.D., Chemical Engineering, **GPA: 4.0/4,** University of Illinois Urbana-Champaign (Urbana, IL) *Apr 2026

M.S., Chemical Engineering, **GPA: 3.97/4,** Carnegie Mellon University (Pittsburgh, PA) Dec 2020

B.Tech., Chemical Engineering, **GPA: 8.1/10,** Indian Institute of Technology Bombay (India) Jul 2018

Predictive Modeling and Simulations Experience

Graduate Research Assistant, Guide: Prof. Alex Mironenko, UIUC Jan 2021 - Mar 2025

- Developed a predictive *ab initio* electrooxidation stability model for metal carbide catalysts, enabling sub-0.1 V agreement with experiments and guiding catalyst design for durable materials
- Applied DFT and energy decomposition to redox-mediated metallocene separation, uncovering ~70% electrostatic interactions and enabling targeted molecular design strategies
- Developed an interpretable, physics-informed model of solvated La^{3+} molecular dynamics that runs 500x faster than DFT and outperforms ML in transferability

Machine Learning Experience

Graduate Research Assistant, Guide: Prof. John Kitchin, CMU Aug 2019 - Dec 2020

- Performed 4,000+ DFT calculations to train an ML model, enabling Monte Carlo simulations 10^5x faster with 2 meV/atom accuracy for CuAgAu surface segregation
- Generated compositional heat maps from 20,000 fs MC simulations, revealing Au/Ag surface enrichment consistent with theory and experiments

Pharmaceutical Experience

Process Engineer - Formulations, Dr. Reddy's Labs, Hyderabad, India Jul 2018 - May 2019

- Developed a theoretical and CFD-DEM model of a wet drug-coating process, achieving 100x scale-up
- Improved tablet spray quality by 4% through empirical identification of optimal atomization parameters

Publications

- 1 first-authored in *ACS Catalysis* (2025)
- 4 co-authored publications in *JACS* (2025), *JMCA* (2024), *Nano Letters* (2023), *Surface Science* (2025)

Leadership and Volunteer Experience

Outreach Lead, Mironenko Research Group, UIUC Jul 2022, '23, '24

- Designed and led hands-on modeling workshop for 20+ high school students, promoting STEM engagement
- Developed and managed the group's wiki page, offering support to beginners with useful code, scripts, and tips