ANKIT KUMAR GAUTAM

PHD CANDIDATE AT UIUC

gautam6@illinois.edu
Urbana, IL 61801
linkedin.com/in/ankitkgautam
gautamankitkumar.github.io

Summary

Chemical engineer specializing in computational chemistry, atomistic simulations, and electro-catalysis with experience in process modeling, optimization, and machine learning

Education

- **Ph.D.** in **Chemical Engineering**, University of Illinois Urbana-Champaign — Urbana, IL
  GPA: 4.0/4.0 — Expected Dec 2025
- **M.S.** in **Chemical Engineering,** Carnegie Mellon University — Pittsburgh, PA
  GPA: 3.97/4.0 — Dec 2020
- **B.Tech.** in **Chemical Engineering,** Institute of Technology (IIT) Bombay — Mumbai, India
  GPA: 8.1/10.0 — Jun 2018

Professional Experience

Process Engineer, Dr. Reddy's Labs, Hyderabad, India — Jul 2018 - May 2019
- Achieved 100x scale-up of a drug-coating process by developing its theoretical and CFD-DEM model
- Enhanced the consistency of tablet spray atomization by 4% by developing correlations among parameters

Summer Intern, Dr. Reddy's Labs, Hyderabad, India — May 2017 - Jul 2017
- Awarded pre-placement offer (1 out of 24 people) for excellent work employing continuous flow chemistry
- Proposed 3 end-to-end pilot scale plants with an average 25% reduction in operating costs than batch mode

Summer Intern, Oil and Natural Gas Corp., Uran, India — May 2016 - Jun 2016
- Increased heat exchanger thermal effectiveness by 4.4% by proposing a switch from Shell & Tube to Plate-type

Research Experience

Graduate Research Assistant, Advisor: Prof. Alex Mironenko, UIUC — Jan 2021 - Dec 2025*
- Investigated molybdenum carbide as an cost-effective (1000x cheaper than Pt) electrocatalyst for fuel cells
- Developed minimally-empirical tight-binding based methods (500-1000x faster than DFT) for transition metals in catalysis and non-covalent interactions

Graduate Research Assistant, Advisor: Prof. John Kitchin, CMU — Aug 2019 - Dec 2020
- Performed 4000+ DFT calculations studying surface segregation to assist CuAgAu catalyst design
- Implemented a neural network trained on DFT energies to accelerate (10^5x faster) Monte Carlo simulations

Undergraduate Research Assistant, Advisor: Prof. Abhijit Chatterjee, IIT Bombay — Aug 2016 - Jul 2018
- Conceptualized, established experimental setup and synthesized ~4 nm diameter bimetallic AuAg nanoparticles
- Developed semi-automatic code that identified key 26 neighboring atoms for adatom surface diffusion

Skills

- **Programming**: Python (numpy, scipy, pandas, matplotlib, scikit-learn, tkinter), C++, MATLAB, GAMS
- **Atomic Simulation & Modeling**: Density Functional Theory (DFT) calculations in VASP, QChem, CP2K, ORCA
- **Data Science & Machine Learning**: Skilled in applying data science methods and machine learning algorithms
- **Process Modeling & Optimization:** Experience in MATLAB, COMSOL, and Aspen Plus

Leadership and Volunteer Experience

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

- Led outreach efforts for 20+ high school students over multiple years with activities such as experimental demonstration, hands-on lessons on modeling software
- Designed and managed the group's Wiki page, offering support to beginners with important code/scripts/tips

Volunteer Work, Training and Development Center, Dr. Reddy's Labs — Jul 2018 - May 2019

- Raised awareness for the center by extensive on the road social outreach throughout the city
- Conducted multiple (20+) mock interviews and provided feedback to improve candidates' job prospects

Publications and Conferences

Presented work at AIChE 2024, AIChE 2023, ACS MWGRLM 2023, NAM 2023, ACS Fall 2022

1. Developing minimally-empirical tight-binding model for transition metals to accelerate catalysis and non-covalent interaction studies. Ankit Kumar Gautam et al. *in preparation*
2. Elucidating the electronic effects of substituent on N-Heterocyclic carbene stability on gold nanoclusters. Ankit Kumar Gautam et al. *in preparation*
3. Planar chiral metallopolymers for electrochemically-mediated enantioselective separations. Jemin Jeon, Fabio Galetto, Ankit Kumar Gautam et al. *submitted*
4. Role of surface oxygen in α-MoC catalyst stability and activity under electrooxidation conditions. Ankit Kumar Gautam et al. *in revision*, doi:10.26434/chemrxiv-2024-xwh17
5. Implication of surface oxidation of nanoscale molybdenum carbide on electrocatalytic activity. Siying Yu, Ankit Kumar Gautam et al. *Journal of Materials Chemistry A*, 2024, doi: 10.1039/D4TA01746C
6. Defect engineering of WO_3 by rapid flame reduction for efficient photoelectrochemical conversion of methane into liquid oxygenates. Ho Kun Woo, Ankit Kumar Gautam et al. *Nano Letters,* 2023, doi: 10.1021/acs.nanolett.3c03131
7. Inferring layer-by-layer composition in Au-Ag nanoparticles using a combination of X-ray Photoelectron Spectroscopy and Monte Carlo simulations. Irfan Arif, Gargi Agrahari, Ankit Kumar Gautam et al. *Surface Science*, 2020, doi: 10.1016/j.susc.2019.121503

Selected Awards

- Received Hanratty travel award to present research work in NAM 2023, Providence, RI — Apr 2023
- Awarded undergraduate research awards URA01 and URA02 for exceptional work — Jul 2018
- Selected as best senior-year research project by a committee of external industry experts — Apr 2018
- Received hostel sports color for distinguished athletic contribution representing the hostel — Apr 2018
- Won second place in soccer at the inter-collegiate sports meet, IIT Kanpur — Dec 2016