Ankit Kumar Gautam

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Summary

- PhD Computational Chemist with experience in catalysis, reaction engineering and process development
- Proven ability to integrate modeling with experiments with 7+ years of experience in heterogeneous catalysis and 1+ year in pharma. 5+ publications across interdisciplinary collaborations (ChemE, Chem, MatSE, MechE)

Skills

- **Reaction and Materials Modeling**: Density Functional Theory in VASP, ORCA, QChem, CP2K, QE
- **Multiphysics Process Modeling:** Python, MATLAB, COMSOL, ANSYS Fluent, CFD-DEM
- **Programming**: Python (NumPy, SciPy, Pandas, Matplotlib, Scikit-Learn, PyTorch, RDKit), C++, Bash, GAMS
- **In Silico Design:** Molecular Dynamics, Machine Learning, High-Throughput Screening, Molecular Docking
- **Surface Kinetics Modeling:** Ab initio thermodynamics, Microkinetic Modeling, Surface Science

Professional Experience

Process Engineer - Formulations, 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
- Improved tablet spray quality by 4% through empirical identification of optimal atomization 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

Summer Intern, Oil and Natural Gas Corporation, Uran, India — May 2016 - Jul 2016

Academic Experience

Graduate Research Assistant, Advisor: Prof. Alex Mironenko, UIUC — Jan 2021 - Dec 2025*

- Built a sub-0.1 V accuracy model by coupling thermodynamics and kinetics to quantify electrooxidation stability on Mo_xC_y and reveal key catalyst deactivation pathways
- Developed a 500x faster than DFT physics-informed model of solvated La^{3+} to enable efficient MD simulations
- Identified >2x lower OH* generation on WO_3, reducing CH_4 overoxidation and attaining 69.4% catalyst selectivity
- Revealed a dominant (70%) role of electrostatics for redox-selectivity using DFT and energy decomposition, enabling atomic-level tuning of reaction mechanisms

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

- Performed 4000+ DFT calculations to study CuAgAu alloy catalyst surface segregation to guide its optimal design
- Developed a machine learning model with 2 meV/atom accuracy, enabling 10^5x faster Monte Carlo simulations, enabling high-throughput atomistic catalyst screening

Capstone Research Project - Process Design, Group Project**,** IITB — Jan 2018 - May 2018

- Designed a 416 ton/day Fischer-Tropsch biodiesel plant using Aspen Plus and MATLAB, along with its economics, parametric analysis and heat-integration
- Applied advanced reactor modeling to optimize water-gas shift performance, achieving a targeted 39% conversion and precise 2:1 H_2:CO ratio for downstream synthesis process

Undergraduate Research Assistant, Advisor: Prof. Abhijit Chatterjee, IITB — Aug 2016 - May 2018

- Led the design and synthesis of ~4 nm diameter bimetallic AgAu nanoparticles for enhanced CO oxidation
- Integrated XPS, TEM, EDS results and modeling to map 3 to 5 surface atomic layers post 400°C reduction

Selected Awards

- 4th place at poster presentation Young Scientist Symposium at the Catalysis Club of Chicago — Jan 2024
- Received Hanratty travel award to present research work in NAM 2023, Providence, RI — Apr 2023
- Awarded 1st prize among undergraduate class by external industry members at convocation — Jul 2018
- Awarded undergraduate research awards URA01 and URA02 for exceptional work — Jul 2018

Leadership and Volunteer Experience

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

- Designed and led workshop for 20+ high school students with hands-on modeling lessons in catalysis, promoting STEM engagement and fostering early exposure to computational catalysis
- Developed and managed the group's wiki page, offering support to beginners with important code, scripts and tips. Link: mironenkogroup.web.illinois.edu/wiki
- Mentored 3+ graduate and 2+ undergraduate students guiding project execution in catalysis and modeling

Education

Key Coursework: Advanced Reaction Kinetics, Data Science and Machine Learning in ChemE, Multiscale Modeling, Material Science, Process Systems Engineering, Process Plant Simulation

- **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, **Indian Institute of Technology (IIT) Bombay** — Mumbai, India
  GPA: 8.1/10.0 — Jun 2018

Publications and Conferences

1. **Gautam**, **A. K.** et al., Minimally empirical, interpretable interatomic potentials for atomistic simulations of rare-earth electroseparations, (*in preparation)*
2. Kim, H., **Gautam**, **A. K.** et al., Continuous Electrochemical Liquid-Liquid Extraction for Selective PGM Recovery. (*in preparation)*
3. Jeon, J., Kappenberg, Y., **Gautam**, **A. K.** et al., Planar chiral metallopolymers for electrochemically-mediated enantioselective separations. *Journal of the American Chemical Society*, 2025, doi: 10.1021/jacs.5c01571
4. **Gautam**, **A. K.** et al., Role of surface oxygen in *α*-MoC catalyst stability and activity under electrooxidation conditions. *ACS Catalysis*, 2025, doi: 10.1021/acscatal.4c06544
5. Yu, S., **Gautam**, **A. K.** et al., Implication of surface oxidation of nanoscale molybdenum carbide on electrocatalytic activity. *Journal of Materials Chemistry A*, 2024, doi: 10.1039/D4TA01746C
6. Woo, H., **Gautam**, **A. K.** et al., Defect engineering of WO_3 by rapid flame reduction for efficient photoelectrochemical conversion of methane. *Nano Letters*, 2023, doi: 10.1021/acs.nanolett.3c03131
7. Arif, I., Agrahari, G., **Gautam**, **A. K.** et al., Inferring layer-by-layer composition in Au-Ag nanoparticles using a combination of XPS & Monte Carlo simulations. *Surface Science*, 2020, doi: 10.1016/j.susc.2019.121503

Full list available at https://scholar.google.com/citations?user=XGt8R-MAAAAJ&hl=en

Conferences:

- American Institute of Chemical Engineers Annual Meeting *2025 (Boston), 2024 (San Diego), 2023 (Orlando)
- American Chemical Society Fall *2025 (Washington DC), 2022 (Chicago)
- ChBE Graduate Symposium 2024, UIUC, IL
- North American Catalysis Society Meeting 2023, Providence, RI