ANKIT MATHANKER

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Summary

Ph.D. Candidate in Chemical Engineering with research experience in atomistic modeling, reaction kinetics, and machine learning for applications in material science and catalysis.

Education

- **Doctoral of Philosophy Candidate (Chemical Engineering)** Aug 2021–Present
  University of Michigan, USA GPA: 4.0/4.0
- **Master of Science (Chemical Engineering)** Jan 2018–Jan 2020
  University of Alberta, Canada GPA: 3.8/4.0
- **Bachelor of Technology (Chemical Engineering)** Jul 2013–May 2017
  IIT (ISM) Dhanbad, India GPA: 8.9/10.0

Skills

- **Atomistic Modeling:** Atomic Simulation Environment, Pymatgen, VASP, JDFTx, GROMACS, MACE, DeePMD-kit, Microkinetic modeling
- **High-throughput Computing:** Slurm, PBS, LSF
- **Data Science/Machine Learning:** Python (Pandas, NumPy, SciPy, scikit-learn), MATLAB

Research Experiences

- **Graduate Research Assistant**, University of Michigan, USA Aug 2021–Present
  - Understanding the effect of electrode potential, electrolyte species, and co-reactants on the electrocatalytic hydrogenation of organics using density functional theory, molecular dynamics, and machine learning. (Ongoing)
- **Graduate Intern**, Lawrence Livermore National Laboratory, USA Jun–Aug 2024
  - Estimating potential-dependent physicochemical properties at metal–electrolyte interfaces using machine learning interatomic potentials developed using MACE architecture. (Ongoing)
- **Graduate Research Assistant/Research Assistant**, University of Alberta, Canada Jan 2018–Jan 2021
  - Investigate the synergistic impact of agricultural and forest residue on hydrothermal liquefaction using supercritical water medium in an autoclave reactor.
- **Research Assistant (Indian Academy of Science Fellow)**, IIT Guwahati, India May–Jul 2016
  - Investigate the synthesis of low-cost tubular ceramic membrane (TCM) via the extrusion process. Experimentally and analytically measure water flux and porosity.
- **Undergraduate Dissertation**, IIT (ISM) Dhanbad, India May 2016–Apr 2017
  - Synthesize PEI-impregnated adsorbents for CO_2 capture and simulate adsorbent packed bed for CO_2 adsorption on Aspen Adsorption.

Publications

1. Mathanker, A.; Sharma, G.; Tran, B.; Singh, N.; Goldsmith, B. R. Effect of ions on the aqueous-phase adsorption of small aromatic organics on silver. *J. Phys. Chem. C* 2025, 129, 29, 13433-13444.

2. Mathanker, A.; Halarnkar, S.; Tran, B.; Singh, N.; Goldsmith, B. R. Synergistic effects in organic mixtures for enhanced catalytic hydrogenation and hydrodeoxygenation. *Chem Catalysis* 2024, 4, 101135.
3. Mathanker, A.; Yu, W.; Singh, N.; Goldsmith, B.R. Effects of ions on electrocatalytic hydrogenation and oxidation of organics in aqueous phase. *Curr. Opin. Electrochem.* 40, 101347 (2023).
4. Das, S.; Mathanker, A.; Pudasainee, D.; Khan M.; Kumar, A.; Gupta, R. Synergistic effect of water and co-solvents on the hydrothermal liquefaction of agricultural biomass to produce heavy oil. *International Journal of Energy for a Clean Environment* 2022, 23(4):31-45.
5. Mathanker, A.; Das, S.; Pudasainee, D.; Khan, M.; Gupta, R. A review on hydrothermal liquefaction of biomass for biofuels production with special focus on the effect of process parameters, co-solvents and extraction solvents. *Energies* 2021, 14, 4916.
6. Mathanker, A.; Pudasainee, D.; Kumar, A.; Gupta, R. Hydrothermal liquefaction of lignocellulosic biomass feedstock to produce biofuels: Parameter study and products characterization. *Fuel* 2020, 271, 117534.
7. Mathanker, A. Hydrothermal liquefaction of lignocellulosic biomass to produce biofuels. *Thesis* 2020.

Upcoming Publications

1. Mathanker, A.; Guo, J.; Goldsmith, B. R.; Varley, J.; Govindarajan, N. Estimating potential-dependent physicochemical properties at metal–electrolyte interfaces using machine learning interatomic potentials. *ACS Electrochemistry (In review 2025-2026).*
2. de Kam, L. B. T.; Zhu, J. X.; Mathanker, A.; Doblhoff-Dier, K.; Govindarajan, N. Benchmarking short-range machine learning potentials for atomistic simulations of metal-electrolyte interfaces. *(to be submitted Winter 2026).*

Conference Talks and Posters (most recent)

- Mathanker, A. "Estimating potential-dependent physicochemical properties at metal–electrolyte interface using machine learning interatomic potentials" Gordon Research Conference - AI for Materials, Energy, and Chemical Science, 2026. Texas, USA.
- Mathanker, A.; Guo, J.; Goldsmith, B. R.; Varley, J. B.; Govindarajan, N. "Estimating Water Coverage and Adsorption Isotherms at Electrolyte/Metal Interfaces Using Machine Learning Potentials". AIChE Annual Meeting: Catalysis and Reaction Engineering Division, 2025. Boston, Massachusetts, USA.
- Mathanker, A.; Sharma, G.; Tran, B.; Singh, N.; Goldsmith, B. R. "Effect of ions on the aqueous-phase adsorption of small aromatic organics on silver". AIChE Annual Meeting: Catalysis and Reaction Engineering Division, 2025. Boston, Massachusetts, USA.
- Mathanker, A. "Can aqueous ions modify the adsorption of organics on Ag?" The Student and Postdoc Summer Seminar Series, CSiDIR, 2025, University of Michigan, Ann Arbor, MI, USA.
- Mathanker, A.; Sharma, G.; Tran, B.; Singh, N.; Goldsmith, B. R. "Effect of ions on the aqueous-phase adsorption of small aromatic organics on Ag". The 46th Michigan Catalysis Society Symposium, 2025. Warren, Michigan, USA.

Teaching Experiences

- **Graduate Teaching Assistant**, University of Michigan, USA 2023
  - CHE 538: Statistical thermodynamics
  - Managed a class of 57 students, facilitated collaborative learning via Piazza discussions and office hours, and developed additional resources to address common challenges faced by students from diverse departments.

  - Applied pedagogical training in course material development, student engagement, and feedback integration, leading to increased student collaboration and engagement throughout the semester.
- **Graduate Teaching Assistant**, University of Alberta, Canada 2019
  - CHE 316: Equilibrium stage processes, Spring and Fall terms.
  - Developed course tutorials and delivered over 40 hours of seminars to a class of 42 students and incorporated classroom engagement techniques such as role reversal for active and collaborative learning.
- **Graduate Teaching and Learning (Foundation and Practicum)**, University of Alberta, Canada 2018–2019
  - Advanced foundational teaching skills and strategies for effective classroom engagement through workshops on course design and pedagogy.
  - Gained hands-on experience in the advanced teaching practices, learning objectives, micro teaching skills and lesson planning strategies.

Awards

- LLM Hackathon for Applications in Materials and Chemistry–Visionary Awards for RedoxFlow
  - Awarded to top 25 teams for outstanding vision for the use of Agentic-AI in field of material science.
- CRE Division Travel Award-AIChE AIChE Annual Meeting, USA
  - CRE Travel Award is presented by the AIChE's Catalysis and Reaction Engineering Division in recognition of exceptional individuals who have made significant advancements in the field.
- Rackham Travel Award (2022,2023,2024) University of Michigan, USA
  - Awarded to present research at national and international conferences.
- Captain Thomas Farrell Greenhalgh Memorial Graduate Scholarship University of Alberta, Canada
  - Awarded for the excellent academic achievements to top 5 percent of incoming cohort.
- Mary Louise Imrie Graduate Student Award University of Alberta, Canada
  - Awarded to present extraordinary research work in prestigious conferences across the globe.
- Graduate Student Association Travel Award University of Alberta, Canada
  - Awarded to present graduate research in international conferences.
- Summer Research Fellowship Programme Scholarship Indian Academy of Science, Bengaluru, India
  - Awarded to top 10 percent applicants through Indian Academy of Sciences to conduct academic research internship in top programs over summer.

Industrial Work Experience

- **Management trainee**, Polyplex Corporation Ltd., India Jul–Sept 2017
  - Trained in end-to-end production process handling, quality assurance for PET and PE polymer chips and packaging film manufacturing.

Academic/ Non-academic Community services

- Graduate Student Director, AIChE Catalysis and Reaction Engineering Division, 2025-2026
  - Lead the management of the social media team with Prof. Omar Abdelrahman and spearheaded initiatives to enhance graduate student engagement and participation in division events.
- Graduate Student Representative, Michigan Chapter of North American Catalysis Society, 2022-2024
  - Promoted graduate student perspectives, facilitating greater involvement and collaboration within the society.
- Graduate Recruitment Planning Member, Department of Chemical Engineering, University of Michigan, 2022-2024

  - Organized and coordinated recruitment activities, including technical sessions and social events, for incoming graduate students.
- Core Team Member, Chemical Engineering Society (ChEGs), University of Michigan, 2022-2023
  - Helped in organization of various academic and social events for graduate students, fostering a strong community within the department.
- Vice President, Toastmasters International, University of Alberta, Canada, 2018-2019
  - Directed membership management, public relations efforts, and organized public speaking competitions to enhance communication skills within the university community.
- Volunteer, UNITEA – Community Social Work Team, University of Alberta, Canada, 2018-2019
  - Collaborated with the community welfare team to promote mental health and well-being initiatives among graduate students.
- Volunteer, Kartavya – Non-Governmental Organization, IIT (ISM) Dhanbad, India, 2015-2017
  - Tutored approximately 20 underprivileged students weekly, providing over 200 hours of academic support while leading a team of 50 undergraduate students to manage their school responsibilities.
- President, Chemical Engineering Society, IIT (ISM) Dhanbad, India, 2015-2016
  - Organized various academic and social events, including leading a team for the department's annual symposium, which brought together undergraduate and graduate students.