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 electrocatalysis.

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 Experience

- **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.
- **Graduate Intern**, Lawrence Livermore National Laboratory, USA Jun–Aug 2024
  - Estimating potential-dependent water adsorption isotherms and the nature of O–H bond characteristics at electrolyte-metal interfaces on using MACE-trained machine learning interatomic potentials.(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
  - Investigated the synthesis of low-cost tubular ceramic membrane (TCM) via the extrusion process. Experimentally and analytically measured water flux and porosity.
- **Undergraduate Dissertation**, IIT (ISM) Dhanbad, India May 2016–Apr 2017
  - Synthesized PEI-impregnated adsorbents for CO_2 capture and simulated 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.

Seminar Talks

1. 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.

Conference Talks and Posters

- 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.; 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.
- Mathanker, A.; Sharma, G.; Tran, B.; Singh, N.; Goldsmith, B. R. "Effect of ions on the aqueous-phase adsorption of organics on Ag". The 29th North American Catalysis Society Meeting, 2025. Atlanta, Georgia, USA.
- Mathanker, A.; Tran, B.; Goldsmith, B. R. "Modeling the effect of electrolyte composition on the aqueous-phase adsorption of phenol, catechol, and benzene on Ag(111)". AIChE Annual Meeting: Catalysis and Reaction Engineering Division, 2024. San Diego, California, USA.
- Mathanker, A.; Halarnkar, S.; Sharma, G; Tran, B.; Singh, N.; Goldsmith, B. R. "Understanding the aqueous-phase adsorption of organics in the presence of electrolytes". 12th Annual Chemical Engineering Graduate Symposium. Ann Arbor, MI, USA.
- Mathanker, A.; Yu, W.; Tran, B.; Singh, N.; Goldsmith, B. "The impact of electrolytes on the adsorption of phenol on a platinum electrode". AIChE Annual Meeting: Catalysis and Reaction Engineering Division, 2023. Orlando, Florida, USA.
- Mathanker, A.; Yu, W.; Barth, I.; Akinola, J.; Singh, N.; Goldsmith, B. "Aqueous-phase heats of adsorption of phenolics in mixed electrolytes". AIChE Annual Meeting: Catalysis and Reaction Engineering Division, 2022. Phoenix, Arizona, USA.
- Mathanker, A.; Yu, W.; Barth, I.; Singh, N.; Goldsmith, B. "Estimating aqueous-phase heats of adsorption of phenolics". 43rd Michigan Catalysis Society Symposium, 2022. Ann Arbor, Michigan, USA.

- Mathanker, A.; Pudasainee, D.; Kumar, A.; Gupta, R. "Parametric study on hydrothermal treatment of biomass to produce biofuels". Clearwater Clean Energy Conference:44th International Conference on Clean Energy, 2019. Tampa, Florida, USA.
- Mathanker, A.; Kumar, M.; Kumar, V.; Pugazhenthi, G. "Effect of sintering temperature on characteristics of low-cost tubular ceramic support manufactured from Indian raw materials for membrane applications". 69th Annual Session of Indian Institute of Chemical Engineers, 2016. Chennai, Tamil Nadu, India.
- Mathanker, A.; Dey, R.; Samanta, A. "Simulation of CO2 adsorption in a packed bed column using Aspen adsorption". 68th Annual Session of Indian Institute of Chemical Engineers, 2015. Guwahati, Assam, India.
- Mathanker, A.; Javed, K.; Pudasainee, D.; Kumar, A.; Gupta, R. "Study of hydrothermal treatment of corn stover to produce biofuels". Faculty of Engineering Graduate Research Symposium, 2018. Edmonton, Alberta, Canada.
- Vaezi, M.; Javed, K.; Pudasainee, D.; Mathanker, A.; Kumar, A.; Gupta, R. "Integration of pipeline hydro-transport and hydrothermal conversion technologies to produce biofuels. Future Energy System". Open House Symposium, 2018. Edmonton, Alberta, Canada.
- Mathanker, A. "Breaking the wall of energy crisis and pollution". Falling Wall Lab, 5th Annual Event, 2018. Edmonton, Alberta, Canada.
- Mathanker, A. "Fueling the future". 3 Minute Thesis. 2018. University of Alberta, Canada.

Teaching Experience

- **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, microteaching 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.