ANKIT MATHANKER

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Summary

Ph.D. Candidate in Chemical Engineering with extensive research experience in atomistic modeling, machine learning applications in catalysis, and biomass conversion technologies. Specialized in electrocatalytic hydrogenation and hydrothermal liquefaction processes.

Education

Doctoral of Philosophy Candidate (Chemical Engineering)

 University of Michigan, USA
 Master of Science (Chemical Engineering)
 University of Alberta, Canada
 Bachelor of Technology (Chemical Engineering)
 IIT (ISM) Dhanbad, India

 Aug 2021-Present

 GPA: 4.0/4.0

 Jan 2018-Jan 2020

 GPA: 3.8/4.0

 Jul 2013-May 2017

 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
 - Predicting electrocatalytic hydrogenation of organic mixture using density functional theory to understand the synergistic or antagonistic effects of organics on each other in a biooil mixture. (Ongoing)
 - Utilized classical molecular dynamics and quantum mechanical modeling to study the effect of electrolytes on organic adsorption at the liquid/solid interfaces.
- Graduate Intern, Lawrance Livermore National Laboratory, USA Jun-Aug 2024
 - Currently training machine learning interatomic potentials using MACE toolkit for understanding water properties and its effect on organic adsorption at 27 different electrified electrocatalyst interfaces. (Ongoing)
 - Predicting the water coverage and adsorption of reactant on electrodes for different surface charging.
- Research Assistant, University of Alberta, Canada Oct 2020–Mar 2021
 - Optimized process parameters to investigate the synergistic impact of agricultural and forest residue on hydrothermal liquefaction. Implemented regression models to establish correlations.
- Graduate Research Assistant, University of Alberta, Canada Jan 2018–Jan 2020
 - Initiated the first biofuels project within the coal technology group, focusing on hydrothermal liquefaction of biomass. Conducted independent troubleshooting, optimized process parameters, and established operational procedures, including SOPs and safety inspections.
- 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 prepared adsorbents for CO2 capture by preparing fly ash and SBA-15 based adsorbents in laboratory, followed by activation and impregnation process.
- Modelled and simulated adsorbent packed bed for CO2 adsorption and compared different breakthrough curves on Aspen Adsorption v8.6.

Publications

- 1. Mathanker, A.; Sharma, G.; Tran, B.; Singh, N.; Goldsmith, B. R. Effect of ions on the aqueous-phase adsorption of organics on silver. (In publication process).
- 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.; 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.

- <u>Mathanker, A.</u>; 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.
- <u>Mathanker, A.</u>; 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.; <u>Mathanker, A.</u>; 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

• 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

 $Jul\text{--}Sept\ 2017$

 Trained in end-to-end production process handling, quality assurance for PET and PE polymer chips and packaging film manufacturing.

Community Volunteer Experience

• Graduate student director, AIChE Catalysis and Reaction Engineering Division

2025

- Graduate student representative, Michigan Chapter of North American Catalysis Society 2022–2024
- Graduate recruitment planning member in Chemical Engineering, University of Michigan, USA 2022–2024
- Core team member, Chemical Engineering Society ChEGs, University of Michigan, USA 2022–2023
- Vice President, Toastmasters International, University of Alberta, Canada 2018–2019

 Managed memberships, public relations and conducted public speaking competitions.
- Volunteer, UNITEA, Community Social Work Team, University of Alberta, Canada 2018–2019
- Volunteer, Kartavya Non-governmental Organization, IIT (ISM) Dhanbad, India 2015–2017
- President, Chemical Engineering Society, IIT (ISM) Dhanbad, India 2015–2016