



**Summary:** A detail-oriented chemical engineer with hands-on background in **materials science**, **computational modeling**, **machine learning** and **scientific software development**, supported by academic research and professional work experience in **interdisciplinary settings**.



## Education



**Doctor of Philosophy in Chemical Engineering** (May 2023)

**Master of Science in Chemical Engineering** (Oct 2021)

University of Rochester, Rochester, NY

Thesis: "Applications of Physics-informed Machine Learning in Chemical Engineering". Advisor: [Andrew D White](#)

**Master of Science in Environmental Engineering** (May 2018)

Missouri University of Science and Technology (UMR), Rolla, MO

Thesis: "Numerical Modeling of Capillary-driven Flow in Open Microchannels: An Implication of Optimized Wicking Fabric Design"

**Bachelor of Science in Chemical Engineering** (July 2015)

University of Tehran, Iran

Thesis: "Experimental Setup and Optimization for Electro-catalytical Generation of Hydroxyl Radicals in Wastewater Treatment"



## Work Experience



**Staff Scientist** (Jan 2024 - present)

**Acceleration Consortium Research Fellow**

Acceleration Consortium, Toronto, ON

(June 2023 – Dec 2023)

- Facilitating AI & Automation (representation learning, Bayesian opt, physics-informed ML and AI-agents) across various self-driving chemistry labs
- Incorporating built-in domain knowledge in self-driving chemistry lab workflows, materials inverse design problem and hit-to-lead optimization
- Developed [chemistry-informed AI agents](#) within Slack API
- Developed [agent-based chemistry plugins](#) via large language models to accelerate design of materials for CO<sub>2</sub> reduction

**Research Assistant** (2019 - 2023)

University of Rochester, Rochester, NY

- Developed a [HuggingFace app](#) that answers questions from scientific papers using OpenAI's large language models
- Developed a [edge-computing cheminformatics tool](#) for semi-supervised classification of the activity of antimicrobial peptides via positive-unlabeled learning using recurrent neural networks
- Developed a [disease modeling tool](#) to predict future disease spreads and infer location of patient-zero
- Developed an [automated tool](#) in CFD modeling that reduces the number of simulations using active learning and generates a symbolic equation for the system of interest via symbolic regression
- Contributed to development of a [simulation-based inference tool](#) via maximum entropy reweighting
- Contributed to development of a plugin with TensorFlow GPU-accelerated operations combined with HOOMD-Blue molecular dynamics simulation engine ([HOOMD-TF](#))
- Developed a [web-app](#) for peptide-based gelator transparency classification using Kernel ridge regression
- Developed an [automated tool](#) on a Raspberry-Pi for real-time monitoring of HPC using Python, JS and HTML
- Implemented finite difference analysis in Python to study [2D shallow water dynamics](#)
- Implemented Monte Carlo simulations in MATLAB to study evolution of spin configurations of a ferromagnet using the Ising model

**Energy & Materials Intern and Research Engineer** (May 2022 - Mar 2023)

Toyota Research Institute, Los Altos, CA

- Developed a deep learning software to predict degradation of used Li-ion batteries with unknown cycling histories (**US Patent pending**).

**Teaching Assistant of "Advanced Transport Phenomena"** (Jan - Dec 2020)

University of Rochester, Rochester, NY

- Tutored students on homework related problems and organized laboratory experiments

**Lead CFD Analyst at Missouri S&T Solar Car Design Team** (2016 - 2018)

Missouri University of Science and Technology, Rolla, MO

- Developed validated wind tunnel simulations in STAR-CCM+ for aerodynamic optimization of the solar car
- Improved aerodynamic design efficiency prior to manufacturing

**Manufacturing Process Modeling Intern** (May-Dec 2017)

The Goodyear Tire & Rubber Company, Akron, OH

- Phase-change heat transfer modeling and optimization of tire vulcanization process in ANSYS
- Model verification based on plant data and analytical solution
- Utilized assets more efficiently through MATLAB post processing and automating the simulation process using OPTIMUS
- Provided faster simulation results using Adaptive Mesh Refinement and High-Performance Computing
- GUI development and coupling ANSYS with MATLAB for time-effective post processing

**Teaching Assistant of "Applied Numerical Methods in CFD"** (Jan-May 2017)

Missouri University of Science and Technology, Rolla, MO

- Organized CFD and programming workshops for ANSYS and Star-CCM +

**Research Assistant** (2016 - 2018)

Missouri University of Science and Technology, Rolla, MO

- Numerical modeling of multiphase flow in open microfluidics using ANSYS and STAR-CCM +
- Reduced simulation run-time by developing an algorithm for adaptive mesh refinement (AMR)



## Work Experience



### Engineering Intern

Emden-Leer University of Applied Sciences, Emden, Germany

(July-Sept 2014)

- Design of experiments in advanced oxidation process (AOP) for wastewater treatment



## Computer Skills



### Scientific Softwares Developed:

- [MaxEnt](#)
- [PyQ](#)
- [HOOMD-TF](#)
- [Decode-ELM](#)
- [Eunomia](#)
- [AL-CFD](#)
- [Peptide.bio](#)
- [dZiner](#)
- [Bye-Cycle](#)
- [Heisenberg](#)

Other tools: AWS, TensorFlow, PyTorch, Scikit-learn, JAX, LangChain

Languages: Python, JavaScript, HTML, CSS



## Honors and Awards



- 3<sup>rd</sup> Place Radical AI Winner at the [2024 LLM Hackathon - Materials and Chemistry](#) (May 2024)  
Toronto, ON
- 2<sup>nd</sup> Place Winner Team at the [Bayesian Optimization Hackathon for Chemistry and Materials](#) (Apr 2024)  
Toronto, ON
- Acceleration Consortium Research Fellowship (May 2023)  
University of Toronto, Toronto
- 1<sup>st</sup> place winner at the [Battery Informatics & ML Kaggle Competition](#) (Dec 2022)  
Materials Research Society, Boston, MA
- Kwang-Yu and Lee-Chien Wang Fellowship (Nov 2021)  
Department of Chemical Engineering, University of Rochester
- Earl W. Costich Graduate Fellowship (May 2020)  
Department of Chemical Engineering, University of Rochester
- 1<sup>st</sup> place winner: 2017 Mike Alizadeh Scholarship (Aug 2017)  
American Society of Civil Engineers (ASCE)
- Recognized reviewer: *Journal of Environmental Chemical Engineering* (May 2016)



## Selected Publications and Patents ([Google Scholar](#))



- [dZiner: Rational Inverse Design of Materials with AI Agents](#) (Oct 2024)  
AI4Mat-NeurIPS 2024 (Accepted)  
M Ansari, J Watchorn, CE Brown, JS Brown
- [Agent-based Learning of Materials Datasets from Scientific Literature](#) (Oct 2024)  
Digital Discovery (Accepted)  
M Ansari, SM Moosavi
- [Learning Peptide Properties with Positive Examples Only](#) (Mar 2024)  
Digital Discovery  
M Ansari, AD White
- [History-agnostic Battery Degradation Inference](#) and **US Patent Pending** (Mar 2024)  
Journal of Energy Storage  
M Ansari, S Torrisi, A Trewartha, S Sun
- [Serverless Prediction of Peptide Properties with Recurrent Neural Networks](#) (Apr 2023)  
Journal of Chemical Information and Modeling  
M Ansari, AD White
- [Assessment of Chemistry Knowledge in Large Language Models that Generate Code](#) (Jan 2023)  
Digital Discovery  
AD White, GM Hocky, HA Gandhi, M Ansari, S Cox, GP Wellawatte, S Sasmal, Z Yang, K Liu, Y Singh, WJ Peña Ccoo
- [Book chapter: Hyper-parameter Optimization in Deep Learning](#) (July 2022)  
Deep Learning for Molecules and Materials, Living Journal of Computational Molecular Science  
M Ansari, AD White
- [Inferring Spatial Source of Disease Outbreaks using Maximum Entropy](#) (July 2022)  
American Physical Society, Physical Review E  
M Ansari, D Soriano-Paños, G Ghoshal, AD White
- [Iterative Symbolic Regression for Learning Transport Equations](#) (Mar 2022)  
AIChE Journal, Special Edition for AI  
M Ansari, HA Gandhi, DG Foster, AD White
- [Simulation-based Inference with Approximately Correct Parameters via Maximum Entropy](#) (Apr 2022)  
Machine Learning in Science and Technology  
R Barrett, M Ansari, G Ghoshal, AD White



## Presentations and Talks



- Multi-modal AI Agents in Materials Discovery (Aug 2024)  
Accelerate 24, Vancouver, BC
- Materials Inverse Design with AI Agents (**Invited talk**) (June 2024)  
Trillion Parameter Consortium, Barcelona, Spain
- AI That Probably Wouldn't Kill You (**Invited talk**) (May 2024)  
2024 LLM Hackathon - Materials and Chemistry, Toronto, ON
- Flexible Automation of Self-driving Labs with Built-in Domain Knowledge (**Invited talk**) (Mar 2024)  
Toyota Research Institute, Los Altos, CA
- Positive Unlabeled Learning of Peptide Properties (Aug 2023)  
Accelerate23 Conference, Toronto, ON
- Maximum Entropy Inference in Chemical Reaction Networks with Unknown Kinetic Parameters (Nov 2022)  
AIChE, Phoenix, AZ
- Rescuing Physics-based Models with Maximum Entropy Reweighting (Sept 2022)  
Wang Lecture, University of Rochester, NY
- Serverless Prediction of Peptide Properties with Recurrent Neural Networks (June 2022)  
Middle Atlantic Regional Meeting of the American Chemical Society, Ewing Township, NJ
- [Simulation-based Inference with Approximately Correct Parameters via Maximum Entropy](#) (Dec 2020)  
Advances in Neural Information Processing Systems 33: Workshop on Machine Learning for Structural Biology