# Mehrad Ansari

**Personal website:** https://mehradans92.github.io          **Email:** mehrad.ansari@utoronto.ca

**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**                                  (June 2023 – Dec 2023)
*Acceleration Consortium, Toronto, ON*

- ➤ 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 $CO_2$ 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)

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## Work Experience

**Engineering Intern**                                                                                                (July-Sept 2014)
*Emden-Leer University of Applied Sciences, Emden, Germany*

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

## Computer Skills

**Scientific Softwares Developed:**
- *MaxEnt*
- *AL-CFD*
- *Py0*
- *Peptide.bio*
- *HOOMD-TF*
- *GTP*
- *Decode-ELM*
- *Bye-Cycle*
- *Eunomia*
- *Heisenberg*

**Other tools:** AWS, TensorFlow, PyTorch, Scikit-learn, JAX, LangChain
**Languages:** Python, JavaScript, HTML, CSS

## Honors and Awards

3rd Place Radical AI Winner at the 2024 LLM Hackathon - Materials and Chemistry                         (May 2024)
*Toronto, ON*

2nd 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*

1st 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*

1st 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)

1. dZiner: Rational Inverse Design of Materials with AI Agents                                           (Sep 2024)
   *AI4Mat-NeurIPS 2024 (Under review)*
   **M Ansari**, J Watchorn, J Brown

2. Agent-based Learning of Materials Datasets from Scientific Literature                                 (Dec 2023)
   *Digital Discovery (Pending review)*
   **M Ansari**, SM Moosavi

3. Learning Peptide Properties with Positive Examples Only                                               (Mar 2024)
   *Digital Discovery*
   **M Ansari**, AD White

4. History-agnostic Battery Degradation Inference and **US Patent Pending**                              (Dec 2023)
   *Journal of Energy Storage*
   **M Ansari**, S Torrisi, A Trewartha, S Sun

5. Serverless Prediction of Peptide Properties with Recurrent Neural Networks                            (Apr 2023)
   *Journal of Chemical Information and Modeling*
   **M Ansari**, AD White

6. 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 Ccoa

7. 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

8. 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

9. Iterative Symbolic Regression for Learning Transport Equations                                        (Mar 2022)
   *AIChE Journal, Special Edition for AI*
   **M Ansari**, HA Gandhi, DG Foster, AD White

10. 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

1. Multi-modal AI Agents in Materials Discovery                                                          (Aug 2024)
   *Accelerate 24, Vancouver, BC*

2. Materials Inverse Design with AI Agents **(Invited talk)**                                            (June 2024)
   *Trillion Parameter Consortium, Barcelona, Spain*

3. AI That Probably Wouldn't Kill You **(Invited talk)**                                                 (May 2024)
   *2024 LLM Hackathon - Materials and Chemistry, Toronto, ON*

4. Flexible Automation of Self-driving Labs with Built-in Domain Knowledge **(Invited talk)**            (Mar 2024)
   *Toyota Research Institute, Los Altos, CA*

5. Positive Unlabeled Learning of Peptide Properties                                                     (Aug 2023)
   *Accelerate23 Conference, Toronto, ON*

6. Maximum Entropy Inference in Chemical Reaction Networks with Unknown Kinetic Parameters               (Nov 2022)
   *AIChE, Phoenix, AZ*

7. Rescuing Physics-based Models with Maximum Entropy Reweighting                                        (Sept 2022)
   *Wang Lecture, University of Rochester, NY*

8. Serverless Prediction of Peptide Properties with Recurrent Neural Networks                            (June 2022)
   *Middle Atlantic Regional Meeting of the American Chemical Society, Ewing Township, NJ*

9. 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*