Mehrad Ansari

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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
- Pyθ
- Peptide.bio
- HOOMD-TF
- dZiner
- 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 (Oct 2024)
   Spotlight AI4Mat-NeurIPS 2024
   ***M Ansari**, J Watchorn, CE Brown, JS Brown*
2. Agent-based Learning of Materials Datasets from Scientific Literature (Oct 2024)
   Digital Discovery
   ***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** (Mar 2024)
   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)
    NeurIPS 2020, Machine Learning in Science and Technology
    *R Barrett, **M Ansari**, G Ghoshal, AD White*

Presentations and Talks

1. Live Demo: Rational Inverse Design of Materials with Chemist AI Agents (Dec 2024)
   Spotlight AI4Mat-NeurIPS 2024, Vancouver, BC
2. Multi-modal AI Agents in Materials Discovery (Aug 2024)
   Accelerate 24, Vancouver, BC
3. Materials Inverse Design with AI Agents **(Invited talk)** (June 2024)
   Trillion Parameter Consortium, Barcelona, Spain
4. AI That Probably Wouldn't Kill You **(Invited talk)** (May 2024)
   2024 LLM Hackathon - Materials and Chemistry, Toronto, ON
5. Flexible Automation of Self-driving Labs with Built-in Domain Knowledge **(Invited talk)** (Mar 2024)
   Toyota Research Institute, Los Altos, CA
6. Positive Unlabeled Learning of Peptide Properties (Aug 2023)
   Accelerate23 Conference, Toronto, ON
7. Maximum Entropy Inference in Chemical Reaction Networks with Unknown Kinetic Parameters (Nov 2022)
   AIChE, Phoenix, AZ
8. Rescuing Physics-based Models with Maximum Entropy Reweighting (Sept 2022)
   Wang Lecture, University of Rochester, NY
9. Serverless Prediction of Peptide Properties with Recurrent Neural Networks (June 2022)
   Middle Atlantic Regional Meeting of the American Chemical Society, Ewing Township, NJ
10. 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