Samuel C. Hoover

samuelhoover@umass.edu • samuelhoover.github.io • linkedin.com/in/samuel-hoover/

Skills

Languages: Python, C, MATLAB, Bash, SQL, HTML, Markdown, LaTeX, Mathematica
Methods: Machine learning, regression, computer vision, Monte Carlo, Langevin dynamics, numerical analysis
Software: PyTorch, scikit-learn, XGBoost, pandas, NumPy/SciPy, Matplotlib, seaborn, COMSOL, GROMACS, LAMMPS, Schrödinger
Development: Git/GitHub/GitLab, Visual Studio Code, Jupyter Notebook, Vim, Anaconda

Education

University of Massachusetts Amherst | PhD, Chemical Engineering, 3.6/4.0 GPA **Sept 2018 – May 2024**
- PhD Thesis: "Study of Charged Macromolecule Phase Behavior using Conventional and Modern Modeling Methods"
- Graduate level coursework in machine learning, deep learning, AI, computer vision, data science, thermodynamics, probability & statistics, variational calculus, computational material science, and transport phenomena

Clarkson University | BS, Chemical Engineering, 3.6/4.0 GPA **May 2018**
- Minors in Mathematics and International & Cross-Cultural Perspectives

Experience

Graduate Research Assistant | University of Massachusetts Amherst **Jan 2019 – Present**

Using Explainable AI to Predict Order-Disorder Transition of Charged Heteropolymers (Prof. M. Muthukumar)
- Combining gradient boosted decision trees and explainable AI methods to investigate the effect of monomer sequence in charged heteropolymer assemblies
- Accurately predicted (RMSE ~ 1%) the order-disorder transition point of charged heteropolymers using a large (>260K rows) dataset of nine hand-engineered features while accounting for solution conditions
- Implemented SHAP values to evaluate each feature's importance for individual predictions, early findings suggest complex interplay with solution conditions
- Compiled multitype dataset from multiple sources into single pandas DataFrame, cleaned 3% of original dataset based on physics-informed filtering and checking for null solutions from calculations
- Ongoing work, manuscript in preparation

Theory of Polyzwitterion-Polyelectrolyte Complex Coacervation (Prof. M. Muthukumar)
- Developed mean field theory for polyzwitterion-polyelectrolyte complex (pZC) phase behavior as a function of pH
- Modeled polyzwitterion as a chain of dipolar, anionic, cationic, and uncharged monomers whose composition is a function of relevant chemical and physical parameters and solution conditions
- Found dipolar electrostatic interactions can trigger formation or dissolution of pZC coacervates
- Investigated all chemical and physical parameters to develop molecular design strategy for desired pZC phase stability
- Rewrote group's legacy multidimensional free energy minimization script to achieve 10x runtime speedup
- Manuscript to be submitted

Convolutional Neural Networks for Nanoporous Zeolite Adsorption Property Prediction (Prof. Peng Bai)
- Trained convolutional neural networks on volumetric and geometric data for nanoporous material property prediction
- Extracted, loaded, and transformed large (>1 GB files) volumetric data of zeolite pore structure
- Wrote custom PyTorch Datasets and Transforms to handle multimodal data loading and scaling
- Found zeolite pore geometry data alone are cannot reliably predict adsorption properties, volumetric data are needed
- Developed command-line interfacing pipeline for data loading and preprocessing, experiment logging, training/inference, hyperparameter tuning, and model performance analysis
- Published in 2023 in Journal of Materials Chemistry A (https://doi.org/10.1039/D3TA01911J)

Sensing and Separations Technologies Intern | Triton Systems, Inc. **Jun 2023 – Aug 2023**

Breathalyzer Detection Platform for Presence of Viral Infections
- Developed parameterized electromagnetic heating model in COMSOL for $1M Phase II SBIR project for the DHS
- Optimized induction heating coil design to desorb volatile organic compounds sequentially and selectively
- Led initial stages of signal processing design; created circuit element model for molecular sensing device and provided recommendations for data acquisition

- Conducted literature review for use of machine learning in breath volatile organic compounds analysis

Global Manufacturing Technology Intern | SI Group **May 2017 – Aug 2017**

- Collaborated on designing and implementing a real-time monitoring and controls system of chemical manufacturing processes in PI Asset Framework
- Collaborated with Environment, Health & Safety Department to aggregate and analyze company loss events from domestic and international locations and compiled findings to assist in future risk analysis
- Managed group intern project to standardize and update the Block Flow Diagrams of 18 key company processes

Publications

- Liu, Y.; Perez, G.; Cheng, Z.; Sun, A.; **Hoover, S. C.**; Fan, W.; Maji, S. & Bai, P. ZeoNet: 3D Convolutional Neural Networks for Predicting Adsorption in Nanoporous Zeolites. *Journal of Materials Chemistry A* **2023**. DOI: https://doi.org/10.1039/D3TA01911J.
- **Hoover, S. C.**; Margossian, K. O. & M. Muthukumar. Theory and Quantitative Assessment of pH-response Polyzwitterion-Polyelectrolyte Complexation. *In preparation.*
- **Hoover, S. C.**; Li, S.-F. & M. Muthukumar. Using Explainable AI to Predict the Order-Disorder Transition of Sequence-Defined Charged Heteropolymers in Concentrated Solutions. *In preparation.*

Presentations & Conferences

- UMass Amherst Chemical Engineering Graduate Open House Poster Session — Spring 2023
- Center for UMass / Industry Research on Polymers Event Poster Session — Spring 2022, Fall 2022, Fall 2023
- Nanopore Sequencing: From Genomes to Proteomes Poster Session — Summer 2022
- NHGRI Advances in Genomic Technology Development Virtual Meeting — Spring 2021

Awards

- Best Teaching Assistant Award — Fall 2022