Samuel C. Hoover

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Expected chemical engineering Ph.D. with 5+ years of lab experience in simulation and modeling and 4+ years of lab experience applying machine learning to the natural sciences. Experience with free energy minimization, molecular dynamics, and machine learning to study coacervation, adsorption processes, and polymer dynamics and to build computational tools for modeling and data analysis.

EDUCATION

University of Massachusetts Amherst, Amherst, MA 2018 – Expected May 2024
Ph.D., Chemical Engineering – GPA: 3.6/4.0
M.S. coursework, Chemical Engineering

Clarkson University, Potsdam, NY May 2018
B.S., Chemical Engineering (minors: Mathematics and International & Cross-Cultural Perspectives) – GPA: 3.6/4.0

ACADEMIC EXPERIENCE

University of Massachusetts Amherst 2018 – Present

Graduate Research Assistant, Polymer Simulation Laboratory – Dr. Murugappan Muthukumar
Proposed Dissertation Title: Study of Charged Macromolecule Phase Behavior using Conventional and Modern Modeling Methods

- Utilizing model systems to study the fundamental physics that govern charged macromolecule phase behavior and self-assembly
- Developing theory to understand the effects of pH on electrostatic interactions in polyzwitterion-polyelectrolyte complex coacervation
- Creating physics-informed, hand-engineered features for machine learning studies of polymeric systems
- Using machine learning to accurately predict the phase behavior of sequence-defined polymers
- Studying the impact of precise monomer sequence of charged macromolecules on their self-assembly behavior using explainable machine learning methods
- Managing group high-performance GPU computing cluster
- Maintaining group website

Graduate Research Assistant, Bai Research Group – Dr. Peng Bai

- Applied convolutional neural networks to volumetric and geometric data for material property prediction for long chain hydrocarbons in nanoporous materials
- Computed liquid-vapor coexistence curves of small organic molecules using Gibbs ensemble Monte Carlo simulations and Schrödinger suite
- Developed command-line interface for end-to-end deep learning with PyTorch

Teaching Assistant

- Senior Laboratory (400 level); Separation Processes (300 level); Process Controls (400 level)

Clarkson University 2016 – 2018

Undergraduate Research Assistant, Multicomponent Mass Transfer Laboratory – Dr. Ross Taylor

- Performed reliability testing for a process simulator
- Optimized performance using thermodynamic calculations to improve initial guesses and efficiency of numerical analysis

Extended Day STEM Peer Educator

- STEM outreach program for local elementary and middle school students
- Organized and led educational tutorials and games to introduce math and engineering concepts

Tutor

- Transfer Process Fundamentals (300 level); Probability and Statistics (300 level)

Teaching Assistant

- Intro to Engineering Use of Computers (100 level); Transfer Process Fundamentals (300 level)
- Filled in when necessary for professor for Transfer Process Fundamentals lectures

INDUSTRIAL EXPERIENCE

SI Group, Schenectady, NY 2017

Global Manufacturing Technology Intern

- 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

SKILLS

Computational Methods:

- Machine learning, deep learning, explainable artificial intelligence, Langevin dynamics simulations, Monte Carlo simulations, scientific computing, high performance computing, data analysis, numerical analysis, regression analysis

Programming Languages and Operating Systems:

- Python, C, MATLAB, Simulink, Bash shell scripting, SQL, macOS, Linux, Windows

Software Packages:

- LAMMPS, Schrödinger suite, PyTorch, TensorFlow, NumPy, SciPy, Matplotlib, seaborn, pandas, scikit-learn, XGBoost, Jupyter Notebook, Adobe Illustrator, Microsoft Office

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

- UMass Amherst Chemical Engineering Graduate Open House Poster Session — Spring 2023
- Center for UMass / Industry Research on Polymers Event Poster Session — Spring, Fall 2022
- Nanopore Sequencing: From Genomes to Proteomes Poster Session — Summer 2022

AWARDS

- Best Teaching Assistant Award — Fall 2022

RELEVANT COURSEWORK

- Machine Learning (500 level)
  - Regression, classification, kernels, Bayesian methods, unsupervised learning
- Neural Networks: A Modern Introduction (600 level)
  - Classification, natural language processing, generative models, adversarial examples
- Intro to Computational Materials Science (600 level)
  - Ising model, Monte Carlo methods, molecular dynamics, lattice statics
- Polymer Dynamics (700 level)
  - Zimm model, Rouse model, entanglement effects