Samuel C. Hoover

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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

SKILLS & RELEVANT COURSEWORK

Languages: Python, C, MATLAB, Bash, SQL, HTML, LaTeX, Mathematica
Simulation Methods/Software: LAMMPS, Schrödinger, Monte Carlo simulations, Langevin dynamics
Libraries/Frameworks: PyTorch, TensorFlow, scikit-learn, XGBoost, pandas, NumPy, SciPy, Matplotlib, seaborn
Development: GitHub, GitLab, Docker, Visual Studio Code, Jupyter Notebook, Vim, Anaconda
Relevant Coursework: Machine Learning, Neural Networks, Thermodynamics, Fourier Series, Probability & Statistics, Mathematical Modeling, Numerical & Engineering Computing, Computational Material Science, Transport Processes

RESEARCH EXPERIENCE

University of Massachusetts Amherst — 2018 – Present
Graduate Research Assistant, Dr. Murugappan Muthukumar
Dissertation Title: Study of Charged Macromolecule Phase Behavior using Conventional and Modern Modeling Methods

- Studying the impact of precise monomer sequence of charged macromolecules on their self-assembly behavior using explainable machine learning methods
- Using gradient boosted decision trees to accurately predict the phase behavior of sequence-defined polymers
- Creating physics-informed, hand-engineered features for machine learning studies of polymeric systems
- Developing theory to understand the effects of pH on electrostatic interactions in complex coacervation
- Developing model to represent the charged states of polyzwitterions in a dynamic pH environment
- Performing free energy minimization calculations to study the role of dipolar interactions during complexation
- Managing group high-performance GPU computing cluster and group website

Graduate Research Assistant, Dr. Peng Bai

- Applied convolutional neural networks to volumetric and geometric data for material property prediction for long chain hydrocarbons in zeolites, found simple geometric descriptors were not enough to make reliable predictions
- Extracted, loaded, and transformed datasets of large volumetric data
- Constructed liquid-vapor coexistence curves of small organic molecules (THMs) using Gibbs ensemble Monte Carlo simulations and torsional parameters from forcefield development using Schrödinger suite
- Developed command-line interface for end-to-end deep learning

Clarkson University — 2017 – 2018
Undergraduate Research Assistant, Dr. Ross Taylor

- Analyzed process simulation software for reliability
- Optimized performance using thermodynamics to improve initial guesses and efficiency of numerical analysis

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
- Aggregated and analyzed company loss events 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.*