Samuel C. Hoover

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Education

University of Massachusetts Amherst **May 2024**
Ph.D., Chemical Engineering, **3.6/4.0 GPA**
- Thesis: "Study of Charged Macromolecule Phase Behavior using Conventional and Modern Modeling Methods"
- Committee: M. Muthukumar, Sarah Perry, David Hoagland, Peng Bai

Clarkson University **2018**
B.S., Chemical Engineering, **3.6/4.0 GPA** (Distinction)
- Minors in Mathematics and International & Cross-Cultural Perspectives

Skills

Methods: molecular dynamics; AI/ML/DL; polymer physics; computational biology; genomic sequencing
Programming Languages: Python; C; Bash; MATLAB; SQL; HTML; LaTeX; Markdown
Software: PyTorch; scikit-learn; pandas; NumPy/SciPy; COMSOL; GROMACS; LAMMPS; PyMOL; Git; AWS

Research Experience

Graduate Research Assistant; Prof. M. Muthukumar, University of Massachusetts Amherst **2021 – Present**
- Studying fundamental polymer physics underpinning polymer aggregation in synthetic and biological systems
- Using machine learning to learn microphase separation of sequence-defined charged heteropolymers
  - Applied **gradient-boosted decision trees** to accurately predict (RMSE ~1%) microphase separation transition using a large (>260k rows) hand-curated data set with hand-engineered features
  - Implementing **SHAP** values to extract learned monomer sequence effects on microphase separation
  - Compiled multitype data set into single **pandas** DataFrame, cleaned using physics-informed filtering
- Developed theory to probe pH effects on polyzwitterion-polyelectrolyte complex coacervates (pZCs)
  - Created design rules for pZCs with an exploitable pH sensitivity relevant to encapsulation and drug delivery
  - Performed **free energy minimization** calculations to construct experimentally-relevant phase diagrams
  - Rewrote group's legacy free energy minimization script to achieve **10x** execution time speedup
- Managing group high-performance GPU computing cluster and website

Graduate Research Assistant; Prof. Peng Bai, University of Massachusetts Amherst **2019 – 2020**
- Studied small molecule and hydrocarbon phase behavior in confined nanoporous zeolite materials
- Using convolutional neural networks to virtually screen nanoporous materials for optimal adsorption properties
  - Extracted, loaded, and transformed large (>1 GB) volumetric data using **HDF5** wrapper for Python
  - Wrote custom **PyTorch** Datasets and Transforms to handle multimodal data loading and scaling
  - Developed pipeline for data loading and preprocessing, training, logging, and model performance analysis
- Computed force field parameters for organic small molecules using the Schrödinger suite

Undergraduate Research Assistant; Prof. Ross Taylor, Clarkson University **2017 – 2018**
- Optimized, tested, and assisted in pushing an update for a separation processes modeling software (ChemSep)

Industrial Experience

Sensing & Separations Technologies Intern; Triton Systems, Inc. **2023**
- Developed parameterized induction heating model in **COMSOL** for $1M Phase II SBIR project for the DHS
  - Optimized induction heating coil to sequentially and selectively desorb 5+ organic compounds
- Created circuit element model for molecular sensing device and provided recommendations for data acquisition
- Conducted literature survey to determine and analyze signal processing methods for breath volatile analysis

Global Manufacturing Technology Intern; SI Group **2017**

- Implemented **PI Asset Framework**, analyzed and compiled company loss events, and led group intern project

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.

Ongoing Work

- **Hoover, S. C.**; Margossian, K. O.; M. Muthukumar. Theory and Quantitative Assessment of pH-responsive Polyzwitterion-Polyelectrolyte Complexation. **In preparation.**
- **Hoover, S. C.**; Li, S.-F.; M. Muthukumar. Using Machine Learning to Predict the Microphase Separation Transition of Sequence-Defined Charged Heteropolymers in Concentrated Solutions. **In preparation.**

Presentations

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

Awards

- **PPG Fellowship**; PPG Industries, Inc. **2024**
- **Best Teaching Assistant Award**; University of Massachusetts Amherst Chemical Engineering Dept. **2022**
- **Clarkson Scholarship**; Clarkson University **2014 – 2018**
- **Dean's List**; Clarkson University **2014 – 2017**

Academic Services

- **Teaching Assistant**; Senior Laboratory (ChE 401), University of Massachusetts Amherst **2023**
- **Teaching Assistant**; Senior Laboratory (ChE 401), University of Massachusetts Amherst **2022**
- **Teaching Assistant**; Separation Processes (ChE 338), University of Massachusetts Amherst **2022**
- **Teaching Assistant**; Process Control (ChE 446), University of Massachusetts Amherst **2021**
- **Extended Day STEM Peer Educator**, Clarkson University **2017 – 2018**
- **Tutor**; Probability & Statistics (STAT 383), Clarkson University **2018**
- **Tutor**; Transfer Process Fundamentals (ChE 330), Clarkson University **2017**
- **Teaching Assistant**; Transfer Process Fundamentals (ChE 330), Clarkson University **2017**
- **Senior Teaching Assistant**; Intro to Engineering Use of Computers (ES 100), Clarkson University **2017**
- **Teaching Assistant**; Intro to Engineering Use of Computers (ES 100), Clarkson University **2016**

Other Services

- **Senator**; University of Massachusetts Amherst Graduate Student Senate **2020 – 2022**
- **Volunteer**; AIChE Northeast Regional Meeting Jeopardy Competition **2019**
- **President**; Delta Chapter, Omega Chi Epsilon **2017 – 2018**
- **Treasurer**; WTSC 91.1FM **2017 – 2018**
- **Radio Show Host & DJ**; WTSC 91.1FM **2014 – 2018**
- **President**; Clarkson University ChemE Car **2016 – 2017**
- **Treasurer**; Clarkson University ChemE Car **2015 – 2016**