Samuel C. Hoover

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I am a PPG Fellow and Ph.D. candidate in Chemical Engineering at University of Massachusetts Amherst studying the phase behavior of complex and multicomponent polymer systems in the Muthukumar Group. My work focuses on using theory, simulation, and machine learning techniques to investigate the fundamental physics underlying polymer aggregates and self-assemblies in synthetic and biological systems.

Education

University of Massachusetts Amherst **May 2024**
Ph.D., Chemical Engineering
- 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 (with distinction)
- Minors in Mathematics and International & Cross-Cultural Perspectives

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
- Applied explainable machine learning to predict microphase separation transition of charged heteropolymers
  - Quantitated effects of monomer sequence on microphase separation transition using SHAP values
  - Created a >260k row dataset with hand-engineered features and cleaned 3% using physics-informed filtering
  - Deployed model can estimate theoretical calculations ($R^2 > 0.9$) in a fraction of the time (>10x speedup)
- Developed theory to probe pH effects on polyzwitterion-polyelectrolyte complex coacervates (pZCs)
  - Identified three physicochemical handles for designing pZCs with pH-sensitivities relevant to encapsulation
  - Performed multidimensional free energy minimization 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
- High-throughput hit identification via computer vision-augmented virtual screening of nanoporous materials
  - 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 framework for data loading, 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 ChemSep – a separation processes modeling software

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 RLC circuit element model for ultra-low (< 1 ppm) molecular sensing device
- Surveyed literature to recommend signal processing and data acquisition 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 & Conferences

UMass Amherst Chemical Engineering Graduate Research Assistant Student Seminar	**2023**
SIGGRAPH	**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**
NHGRI Advanced Genomic Technology Development Virtual Meeting	**2021**

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**

Extracurricular Activities

Volunteer; League of Women Voters of Amherst Book Sale	**2022**
Senator; University of Massachusetts Amherst Graduate Student Senate	**2020 – 2022**
Volunteer; AIChE Northeast Regional Meeting	**2019**
Organizer & Co-director; Clarkson University Fashion Show	**2018**
President; Delta Chapter, Omega Chi Epsilon	**2017 – 2018**
Treasurer; WTSC 91.1FM	**2017 – 2018**
Radio Show Host & DJ; WTSC 91.1FM	**2014 – 2018**

- **Senior Advisor**; Clarkson University ChemE Car   **2017 – 2018**
- **President**; Clarkson University ChemE Car   **2016 – 2017**
- **Treasurer**; Clarkson University ChemE Car   **2015 – 2016**

Skills

Computational methods: molecular dynamics; data science; computational biology; computational chemistry; free energy calculations; cheminformatics; genomic sequencing analysis; numerical analysis; high performance computing; molecular modeling; Monte Carlo simulations; statistical modeling; computational materials science

Machine learning: regression; computer vision; convolutional neural networks; recurrent neural networks; Transformers; ensemble methods; classification; feature selection; dimensionality reduction; clustering; data curation

Programming languages: Python; C; shell scripting; MATLAB; SQL; HTML; LaTeX; Markdown

Software: PyTorch; scikit-learn; pandas; NumPy; SciPy; XGBoost; SHAP; COMSOL; GROMACS; LAMMPS; PyMOL; RDKit; AWS; Matplotlib; seaborn; Schrödinger suite

Development: Git/GitHub/GitLab; Docker; Anaconda; Jupyter Notebook; Vim; Visual Studio Code; Linux; macOS; Windows

Other: polymer physics; biophysics; scientific software development; Slurm; Adobe Illustrator; Microsoft Office