Samuel C. Hoover

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Ph.D. graduate in Chemical Engineering at University of Massachusetts Amherst with over five years of experience applying machine learning to the physical and biological sciences. Applied theory and machine learning to investigate the physics underlying polymer aggregates in synthetic and biological systems in the Muthukumar Group. Awarded the prestigious PPG Fellowship for my work on machine learning of microphase separation of charged heteropolymers – relevant to intrinsically disordered proteins and biomolecular condensates. Theory- and data-driven modeler with experience developing scientific software tools and visualizations.

Education

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

Clarkson University   **May 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   **Jan 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
  - Quantified 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   **Jan 2019 – Dec 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   **Sep 2017 – May 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.   **Jun 2023 – Sep 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   **May 2017 – Aug 2017**
- Implemented PI Asset Framework, analyzed and compiled company loss events, and led group intern project

Publications
- **Hoover, S. C.**; Margossian, K. O.; M. Muthukumar. Theory and Quantitative Assessment of pH-responsive Polyzwitterion-Polyelectrolyte Complexation. **Accepted** (2024).
- 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* **11**, 17570–17580. doi: 10.1039/D3TA01911J (2023).

Ongoing Work
- **Hoover, S. C.**; Margossian, K. O.; M. Muthukumar. Theory and Quantitative Assessment of pH-responsive Polyzwitterion-Polyelectrolyte Complexation. **In submission.**
- **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	**Oct 2023**
SIGGRAPH	**Aug 2023**
Center for UMass / Industry Research on Polymers Fall Event Poster Session	**Oct 2023**
Center for UMass / Industry Research on Polymers Spring Event Poster Session	**May 2023**
UMass Amherst Chemical Engineering Graduate Open House Poster Session	**Mar 2023**
Nanopore Sequencing: From Genomes to Proteomes Poster Session	**May 2022**
Center for UMass / Industry Research on Polymers Spring Event Poster Session	**May 2022**
NHGRI Advanced Genomic Technology Development Virtual Meeting	**May 2021**

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

Selected Academic Services
Teaching Assistant; Senior Laboratory, University of Massachusetts Amherst	**Fall 2023**
Teaching Assistant; Senior Laboratory, University of Massachusetts Amherst	**Fall 2022**
Teaching Assistant; Separation Processes, University of Massachusetts Amherst	**Spring 2022**
Teaching Assistant; Process Control, University of Massachusetts Amherst	**Fall 2021**
Extended Day STEM Peer Educator, Clarkson University	**Sep 2017 – May 2018**
Tutor; Probability & Statistics, Clarkson University	**Fall 2018**
Tutor; Transfer Process Fundamentals, Clarkson University	**Fall 2017**
Teaching Assistant; Transfer Process Fundamentals, Clarkson University	**Fall 2017**
Senior Teaching Assistant; Intro to Engineering Use of Computers, Clarkson University	**Spring 2017**
Teaching Assistant; Intro to Engineering Use of Computers, Clarkson University	**Spring 2016**

Selected Extracurricular Activities
Senator; University of Massachusetts Amherst Graduate Student Senate	**Sep 2019 – May 2021**
Volunteer; AIChE Northeast Regional Meeting	**May 2019**
Organizer & Co-director; Clarkson University Fashion Show	**Sep 2017 – May 2018**
President; Delta Chapter, Omega Chi Epsilon	**Sep 2017 – May 2018**

- **Treasurer**; WTSC 91.1FM   **Sep 2017 – May 2018**
- **Radio Show Host & DJ**; WTSC 91.1FM   **Sep 2014 – May 2018**
- **Senior Advisor**; Clarkson University ChemE Car   **Sep 2017 – May 2018**
- **President**; Clarkson University ChemE Car   **Sep 2016 – May 2017**
- **Treasurer**; Clarkson University ChemE Car   **Sep 2015 – May 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; Polars; NumPy; SciPy; XGBoost; SHAP; COMSOL; GROMACS; LAMMPS; PyMOL; RDKit; Matplotlib; seaborn; Schrödinger suite

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

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