Samuel C. Hoover

CONTACT INFORMATION

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EDUCATION

Ph.D., Chemical Engineering, UMass Amherst, Amherst, MA, USA **August 2024**

Dissertation Advisor: Prof. Murugappan Muthukumar

Dissertation Title: *Study of charged macromolecule phase behavior using conventional and modern modeling methods*

B.S., Chemical Engineering, Clarkson University, Potsdam, NY, USA **May 2018**

Degree conferred with distinction.

Minors: Mathematics and International & Cross-Cultural Perspectives

EMPLOYMENT

Research Assistant, UMass Amherst, Amherst, MA, USA **January 2019–Present**

Lab of Prof. Murugappan Muthukumar

The overarching goal of my current doctoral research is to use simpler synthetic analogs to uncover the fundamental physics that govern biological self-assemblies like biomolecular condensates (**Project 2**) and protein aggregations (**Projects 1 & 3**). Additionally managed group high-performance GPU computing cluster and static HTML webpage.

Project 1 – Learning the sequence effects of microphase separation transition

- Created a >260k row dataset from theoretical calculations and cleaned 3% using physics-informed filtering
- Developed novel molecular modeling method that uniquely captured the sequence-specificity of each macromolecule
- Trained a gradient-boosted decision trees model to accurately predict microphase separation transition ($R^2 > 0.9$)
- Quantified the effects of sequence on self-assembly, found second-order salt-dependent interactions on self-assembly using SHAP values

Project 2 – Theory of polyzwitterion-polyelectrolyte complexation

- Generalized theory to account for the dynamic phase stability of polyzwitterion-polyelectrolyte complexes
- Performed a quantitative assessment of phase stability of complexes with varying molecular structures, chemistries, and solution conditions
- Refactored group legacy free energy minimization script to achieve a 10x execution time speedup

Project 3 – Phase behavior of polydipoles

- Computed phase diagrams of complexation between polymers that contain an electric dipole on each monomer
- Determined salt sensitivity with varying electrostatic dipolar interaction strengths

Lab of Prof. Peng Bai
The goal of this research was utilize computer vision to aid virtual screening of nanoporous materials like zeolites. Additionally computed phase diagrams and forcefield parameters for small organic molecules.

Project 1 – Convolutional neural networks for virtual screening

- Extracted, loaded, and transformed volumetric data ($>$ 1 GB) using HDF5 wrapper for Python and custom PyTorch classes
- Developed deep learning pipeline with experiment logging and analysis
- Found simple geometric descriptors for zeolites do not provide reliable predictions for their adsorption properties

DTMD Intern, Triton Systems, Inc., Chelmsford, MA, USA **June–September 2023**
In the Disruptive Technology & Materials Design (DTMD) group, performed electromagnetic modeling on COMSOL for a Phase II SBIR project for the DHS.

- Optimized induction heating coil to selectively desorb 5+ volatile organic compounds
- Developed RLC circuit model for sensitive ($<$ 1 ppm) molecular sensing device
- Determined state-of-the-art breath volatile organic compounds analysis from literature, provided recommendations for signal acquisition and processing

Research Assistant, Clarkson University, Potsdam, NY, USA **September 2017–May 2018**

STEM Educator, Clarkson University, Potsdam, NY, USA **September 2017–May 2017**

Global Manufacturing Tech. Intern, SI Group, Schenectady, NY, USA **May–August 2017**

Research Interests

Computational studies (machine learning, simulation, theory) of synthetic and biological polymeric systems. One major theme is to elucidate the physical mechanisms underpinning protein aggregations and self-assemblies that give rise to neurodegeneration. Another theme is to use complex coacervates as models for biomolecular condensates to further understand the spatiotemporal organization within the cell.

Honors and Awards

PPG Fellowship, PPG Industries, Inc. **2024**

Teaching Assistant Award, University of Massachusetts Amherst **Fall 2022**

Clarkson Scholarship, Clarkson University **Fall 2014–Spring 2018**

Dean's List, Clarkson University **Fall 2014–Fall 2017**

Teaching Experience

Teaching Assistant, University of Massachusetts Amherst

CHEM-ENG 401, Senior laboratory **Falls 2022–2023**
CHEM-ENG 338, Separation processes **Spring 2022**
CHEM-ENG 446, Process control **Fall 2021**

Tutor, Clarkson University

STAT 383, Probability and statistics **Spring 2018**
CH 370, Transfer process fundamentals **Fall 2017**

Teaching Assistant, Clarkson University

CH 370, Transfer process fundamentals **Fall 2017**

ES 100, Intro to engineering use of computers **Spring 2016**

Senior Teaching Assistant, Clarkson University

ES 100, Intro to engineering use of computers **Spring 2017**

Professional Membership, Activities, Outreach, and Service

University of Massachusetts Graduate Student Senate

Senator **September 2019–May 2021**

Order of the Engineer

Member **2018–Present**

Omega Chi Epsilon

Delta Chapter President **2017–2018**

Member **2016–Present**

American Institute of Chemical Engineers

Clarkson University ChemE Car Senior Advisor **2017–2018**

Clarkson University ChemE Car President **2016–2017**

Clarkson University ChemE Car Treasurer **2015–2016**

Member **2014–Present**

Outreach

AIChE Eckhardt Northeast Student Regional Conference volunteer **March 30, 2019**
Hosted ChemE Jeopardy Competition

Extended Day STEM Peer Educator **September 2017–May 2018**
After school activities to teach STEM to local middle school students on a weekly basis

Skills

Proficient in Python, Bash, MATLAB. Experience in C. Proficient at *nix and HPC. Markup languages: LaTeX, HTML, CSS, Markdown.

Methods—Polymer physics, biophysics, molecular dynamics, machine learning, statistical modeling, data engineering, explainable machine learning, deep learning, and computational biology.

Software—Most contributions can be found at https://github.com/samuelhoover. Proficient in machine learning and numerical toolkits like PyTorch, scikit-learn, NumPy, SciPy, pandas, PostgreSQL, XGBoost, and SHAP. Experience with coarse-grained and atomistic molecular dynamics packages like GROMACS, LAMMPS, PyMOL, Avogadro, Schrödinger, and VMD. Experience with development tools like Git, Docker, and AWS. Experience developing machine learning and deep learning pipelines for physical science research. Experience with finite element analysis with COMSOL. Proficient with visualization tools like Matplotlib, seaborn, and Inkscape.

Publications in Progress

3. **Hoover, S. C.**, Li, S. -F., Muthukumar, M. (2024) *Learning the sequence effect on the microphase separation transition of charged heteropolymers.*

Refereed Publications

2. **Hoover, S. C.**, Margossian, K. O., Muthukumar, M. (2024) *Theory and quantitative assessment of pH-responsive polyzwitterion-polyelectrolyte complexation*, Soft Matter **20**, 7199-7213.
1. Liu, Y., Perez, G., Cheng, Z., Sun, A., **Hoover, S. C.**, Fan, W., Maji, S., Bai, P. (2023) *ZeoNet: 3D convolutional neural networks for predicting adsorption in nanoporous zeolites*, J. Mater. Chem. A **11**, 17570-17580.

Presentations and Conferences

7.	UMass Amherst Chemical Engineering G.R.A.S.S. talk	October 2023
6.	Center for UMass / Industry Research on Polymers poster session	October 2023
5.	Center for UMass / Industry Research on Polymers poster session	May 2023
4.	UMass Amherst Chemical Engineering Graduate Open House poster session	March 2023
3.	Nanopore Sequencing: From Genomes to Proteomes poster session	May 2022
2.	Center for UMass / Industry Research on Polymers poster session	May 2022
1.	NHGRI Advanced Genomic Technology Development virtual meeting	May 2021

References

Available upon request.