

# Samuel C. Hoover

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## CONTACT INFORMATION

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## EDUCATION

**Ph.D., Chemical Engineering**, UMass Amherst, Amherst, MA, USA **February 2025**

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 polyelectrolyte-polyelectrolyte complexation**

- Generalized theory to account for the dynamic phase stability of polyelectrolyte-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:  $\text{\LaTeX}$ , 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

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| 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.