Samuel C. Hoover

CONTACT INFORMATION

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Summary

I am a research scientist, PPG Fellow, and Chemical Engineering Ph.D. with 6 years of experience building data-driven models and computational tools to answer complex problems in the natural sciences. Proven track record of success through peer-reviewed publications, interdisciplinary internships, and open-source projects. Adept at wearing many hats, working in fast-paced cross-functional teams, and effectively communicating difficult subjects. Seeking to applying my experience in computational roles.

EDUCATION

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

Committee: Murugappan Muthukumar (Chair), Peng Bai, David Hoagland, Sarah Perry

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

Relevant coursework: Neural Networks, Machine Learning, Computational Materials Science, Statistical Mechanics, Advanced Mathematical Analysis, Transfer Process Fundamentals, Polymer Dynamics

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

Degree conferred with distinction.

Minors: Mathematics and International & Cross-Cultural Perspectives

Relevant coursework: Mathematical Modeling, Boundary Value Problems & Fourier Series, Probability & Statistics

EXPERIENCE

Research Assistant, UMass Amherst, Amherst, MA, USA **January 2019–December 2024**

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 real-world data and improved data quality by identifying 5% of sample as unreliable using physics-informed filtering
- Developed novel molecular modeling method that uniquely captured the sequence-specificity of each macromolecule
- Trained gradient-boosted decision trees to accurately predict microphase separation transition ($R^2 > 0.9$), 90x faster than traditional methods
- 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, allowing for design of cargo-releasing materials
- 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, resulted in 20,000x quicker materials property predictions than traditional methods. Additionally computed phase diagrams and forcefield parameters for small organic molecules.

Project 1 – Convolutional neural networks for virtual screening

- Created an automated pipeline to process, analyze, and visualize over 100,000 materials in HDF5 format using MATLAB
- Built custom PyTorch framework for processing large datasets (>1 GB/sample), training, model analysis, and experiment logging; ensured reproducibility and reliability for 8 person research team
- 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**
Technology & Signal Processing Intern in the Disruptive Technology & Materials Design (DTMD) group, performed electromagnetic modeling on COMSOL for a Phase II SBIR project for the DHS.

- Optimized design of electromagnetic components for a handheld viral detection device in collaboration with engineers
- Developed an easy-to-use application for product testing, enabled non-technical users to perform complex finite element methods calculations and estimate performance on-the-fly
- Supported design best practices by reviewing current literature on data acquisition and signal processing for breath volatile organic compound analysis
- Worked with key stakeholders, meeting monthly to present research updates and respond to questions from financial sponsors

Research Assistant, Clarkson University, Potsdam, NY, USA **September 2017–May 2018**
Performed stability testing for a process simulator for Prof. Ross Taylor.

- Improved numerical analysis convergence by using more reliable initial conditions calculations
- Collected data on simulation performance and troubleshot diverged calculations

Global Manufacturing Tech. Intern, SI Group, Schenectady, NY, USA **May–August 2017**
Worked with the Global Manufacturing Technology and Global EH&S departments across multiple projects.

- Strengthed institutional knowledge by identifying root causes of company loss events and determining impact on revenue and production
- Led group intern project to standardize the block flow diagram of 19 key assets, reduced potential errors by improving consistency and clarity
- Implemented PI Asset Framework for real-time processing monitoring, enabled quick decisions and eliminated guesswork

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, Rust, C/C++, Bash, MATLAB, and SQL. Proficient at *nix and Windows based systems and cloud-based high-performance computing. Markup languages: LaTeX, HTML, CSS.

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, scikit-image, 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.