# Samuel C. Hoover

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# Experience

#### Muthu Polymer Group (Graduate Research Assistant) UMass Amherst, Amherst, MA

Jan 2021 - Aug 2024

- Created a >260k row dataset and applied learning to predict conformations of sequence-defined polymers
- Quantified effects of monomer sequence on self-assembly using SHAP values
- Developed theory to model pH effects on polymer self-assemblies relevant to biological systems
- Rewrote group legacy free energy minimization script to achieve 10x execution time speedup

#### Triton Systems, Inc. (Sensing & Separations Technologies Intern) Chelmsford, MA

Jun 2023 - Sep 2023

- Designed induction heating coil to selectively desorb VOCs for ultra-low (< 1 ppm) molecular sensing device</li>
- Surveyed literature to recommend signal processing and data acquisition methods for breath VOCs analysis

#### **Bai Research Group** (Graduate Research Assistant) *UMass Amherst, Amherst, MA*

Jan 2019 - Dec 2020

- · High-throughput virtual screening of nanoporous materials utilizing convolutional neural networks
- Wrote deep learning pipeline using custom PyTorch modules to handle 3D volumetric data

SI Group (Global Manufacturing Technology Intern) Schenectady, NY

May 2017 - Aug 2017

### Selected Presentations

## UMass Amherst Chemical Engineering G.R.A.S.S. Talk Amherst, MA

Oct 2023

Using machine learning to predict microphase separation transition of charged heteropolymers

#### **Nanopore Sequencing: From Genomes to Proteomes** *Boston, MA*

Apr 2022

Computational design engine for accurate and efficient sequencing of DNA and RNA

# Education

### University of Massachusetts Amherst Amherst, MA

Sep 2018 - Aug 2024

Ph.D. in Chemical Engineering

Thesis: "Study of Charged Macromolecule Phase Behavior using Conventional and Modern Modeling Methods"

Awards: PPG Fellowship (Spring 2024), Teaching Assistant Award (Fall 2022)

#### Clarkson University Potsdam, NY

Aug 2014 - May 2018

B.S. in Chemical Engineering; Minors in Mathematics and Cross-Cultural & International Perspectives

#### Skills

- Languages: Python, C, Bash, MATLAB, HTML, LaTeX
- · Tools: machine learning, polymer physics, molecular dynamics, PyTorch, scikit-learn, GROMACS, PyMOL, Git, AWS

# Publications & Ongoing Work

- **Hoover, S. C.**, Li, S.-F. & Muthukumar, M. Learning the sequence effects on the microphase separation transition of charged heteropolymers. **In preparation**.
- **Hoover**, **S. C.**, Margossian, K. O. & Muthukumar, M. Theory and quantitative assessment of pH-responsive polyzwitterion-polyelectrolyte complexation. *Soft Matter* (2024) doi: 10.1039/D4SM00575A.
- 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. *J. Mater. Chem. A* 11, 17570-17580. (2023) doi: 10.1039/D3TA01911J.