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
- 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* April 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.