

Samuel C. Hoover

samuelhoover@umass.edu • samuelhoover.github.io • LinkedIn

EDUCATION

University of Massachusetts Amherst

May 2024

Ph.D., *Chemical Engineering*, **3.6/4.0 GPA**

- Thesis: “Study of Charged Macromolecule Phase Behavior using Conventional and Modern Modeling Methods”

Clarkson University

May 2018

B.S., *Chemical Engineering*, **3.6/4.0 GPA (Distinction)**

- Minors in Mathematics and International & Cross-Cultural Perspectives
- Dean’s List (F2014-F2017); ChemE Car President; Chemical Engineering Honors Society President

SKILLS & INTERESTS

- **Methods:** molecular dynamics; numerical analysis; machine learning; computer vision; Monte Carlo; cheminformatics
- **Programming Languages:** Python, C, Bash, MATLAB, SQL, HTML, LaTeX, Markdown
- **Software:** PyTorch, scikit-learn, pandas, NumPy/SciPy, COMSOL, GROMACS, LAMMPS, Schrödinger, PyMOL, Git
- **Interests:** computational biology; AI/ML/DL; polymer science; Seinfeld; Twin Peaks; Sopranos; cooking; baking

WORK EXPERIENCE

Graduate Research Assistant, *University of Massachusetts Amherst*

Jan. 2021 – Present

- Studying fundamental polymer physics underpinning polymer aggregation in synthetic and biological systems
- Using machine learning to learn microphase separation of sequence-defined charged heteropolymers
 - Applied **gradient-boosted decision trees** to accurately predict (RMSE ~1%) microphase separation transition using a large (>260k rows) hand-curated data set with hand-engineered features
 - Implementing **SHAP** values to extract learned monomer sequence effects on microphase separation
 - Compiled multitype data set into single **pandas** DataFrame, cleaned using physics-informed filtering
- Developed theory to probe pH effects on polyelectrolyte complex coacervates (pZCs)
 - Created design rules for pZCs with an exploitable pH sensitivity relevant to encapsulation and delivery
 - Performed **free energy minimization** calculations to construct experimentally-relevant phase diagrams
 - Rewrote group’s legacy free energy minimization script to achieve **10x** execution time speedup
- Managing group high-performance GPU computing cluster and website

Sensing & Separations Technologies Intern, *Triton Systems, Inc.*

June 2023 – Sep. 2023

- Developed parameterized induction heating model in **COMSOL** for [\\$1M Phase II SBIR project for the DHS](#)
 - Optimized induction heating coil to sequentially and selectively desorb 5+ organic compounds
- Created circuit element model for molecular sensing device and provided recommendations for data acquisition
- Conducted literature review for use of machine learning in breath volatile organic compounds analysis

Graduate Research Assistant, *University of Massachusetts Amherst*

Jan. 2019 – Nov. 2020

- Studied small molecule and hydrocarbon phase behavior in confined nanoporous zeolite materials
- Using convolutional neural networks to virtually screen nanoporous materials for optimal adsorption properties
 - Published in Journal of Materials Chemistry A: <https://doi.org/10.1039/D3TA01911J>
 - Extracted, loaded, and transformed large (>1 GB) volumetric data using **HDF5** wrapper for Python
 - Wrote custom **PyTorch** Datasets and Transforms to handle multimodal data loading and scaling
 - Developed pipeline for data loading and preprocessing, training, logging, and model performance analysis

Global Manufacturing Technology Intern, *SI Group*

May 2017 – Aug. 2017

- Designed implementation of **PI Asset Framework**, created slide deck of company loss events with root cause analysis, and led group intern project to standardize 18 key company chemical manufacturing processes