Samuel C. Hoover

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Ph.D. graduate with over five years of experience applying machine learning to the physical and biological sciences. Applied theory and machine learning to investigate the physics underlying polymer aggregates in synthetic and biological systems. Awarded the prestigious PPG Fellowship for my work on machine learning of microphase separation of charged heteropolymers – relevant to intrinsically disordered proteins and biomolecular condensates. Theory- and data-driven modeler with experience developing scientific software tools and visualizations.

Education

Ph.D., Chemical Engineering; University of Massachusetts Amherst **Aug 2024**
- Thesis: "Study of Charged Macromolecule Phase Behavior using Conventional and Modern Modeling Methods"

B.S., Chemical Engineering; Clarkson University **May 2018**
- Minors in Mathematics and International & Cross-Cultural Perspectives

Skills

Methods: machine learning; polymer physics; molecular dynamics; data engineering; statistical modeling
Programming languages: Python; C; Bash; MATLAB; SQL; HTML
Frameworks: PyTorch; scikit-learn; pandas; Polars; NumPy; SciPy; Matplotlib; SHAP; RDKit; Git; AWS

Experience

Graduate Research Assistant; Prof. M. Muthukumar, University of Massachusetts Amherst **Jan 2021 – Aug 2024**
- Applied explainable machine learning to predict microphase separation transition of charged heteropolymers
  - Quantified effects of monomer sequence on microphase separation transition using SHAP values
  - Created a >260k row dataset with hand-engineered features and cleaned 3% using physics-informed filtering
  - Deployed model can make accurate predictions ($R^2 > 0.9$) in a fraction of the time (>10x speedup)
- Developed theory to model pH effects on polyzwitterion-polyelectrolyte complex coacervates (pZCs)
  - Identified three physicochemical handles for designing pZCs with pH-sensitivities relevant to encapsulation
  - Rewrote group's legacy free energy minimization script to achieve 10x execution time speedup

Sensing & Separations Technologies Intern; Triton Systems, Inc. **Jun 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 RLC circuit element model for ultra-low (< 1 ppm) molecular sensing device
- Surveyed literature to recommend signal processing and data acquisition methods for breath volatile analysis

Graduate Research Assistant; Prof. Peng Bai, University of Massachusetts Amherst **Jan 2019 – Dec 2020**
- High-throughput hit identification via computer vision-augmented virtual screening of nanoporous materials
  - Handled large (>1 GB) volumetric data using HDF5 wrapper and custom PyTorch modules
  - Developed command line interfacing end-to-end deep learning framework with experiment logging

Global Manufacturing Technology Intern; SI Group **May 2017 – Aug 2017**
- Implemented PI Asset Framework, analyzed and compiled company loss events, and led group intern project

Publications & Ongoing Work

- 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).
- **Hoover, S. C.**; Margossian, K. O.; M. Muthukumar. Theory and Quantitative Assessment of pH-responsive Polyzwitterion-Polyelectrolyte Complexation. **Accepted** (2024).
- **Hoover, S. C.**; Li, S.-F.; M. Muthukumar. Using Machine Learning to Predict the Microphase Separation Transition of Sequence-Defined Charged Heteropolymers in Concentrated Solutions. **In preparation.**