Samuel C. Hoover

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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"
- Committee: M. Muthukumar, Sarah Perry, David Hoagland, Peng Bai
- PPG Fellow; Graduate Student Senate Senator

Clarkson University   **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 Honor Society President

Skills

Methods: molecular dynamics; AI/ML/DL; polymer physics; computational biology; genomic sequencing
Programming Languages: Python; C; Bash; MATLAB; SQL; HTML; LaTeX; Markdown
Software: PyTorch; scikit-learn; pandas; NumPy/SciPy; COMSOL; GROMACS; LAMMPS; PyMOL; Git; AWS

Experience

Graduate Research Assistant; Prof. M. Muthukumar, University of Massachusetts Amherst   **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 polyzwitterion-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.   **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 survey to determine and analyze signal processing methods for breath volatile analysis

Graduate Research Assistant; Prof. Peng Bai, University of Massachusetts Amherst   **2019 – 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
- Computed force field parameters for organic small molecules using the Schrödinger suite

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