

SAMUEL J. DAWLEY

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SUMMARY

Ph.D. candidate in computational chemistry (B.A. Applied Mathematics & Statistics and Chemistry, GPA 3.87) working on inverse statistical mechanics, large-scale GPU simulation, statistical inference and uncertainty quantification, and deep learning for inverse problems. First-author *Phys. Rev. E*. Expected graduation May 2029.

EDUCATION

Princeton University 2023 – May 2029 (expected)
Ph.D. Candidate in Chemistry; Graduate Certificate in Computational Science & Engineering *Princeton, NJ*

Johns Hopkins University 2019 – 2023
B.A. in Applied Mathematics & Statistics and Chemistry (Departmental Honors); GPA 3.87 *Baltimore, MD*

- Minor in Mathematics. **Coursework:** Probability, Statistics, Bayesian Statistics, Optimization, Linear Algebra, Differential Equations, Topology, Statistical Mechanics. **Honors:** ACS Undergraduate Award (2023); General Honors; Dean's List every semester

RESEARCH EXPERIENCE

Graduate Research Assistant, Princeton University 2023 – Present
Complex Materials Theory Group | Advisor: Prof. Salvatore Torquato *Princeton, NJ*

- Advance theory and computational methods in inverse statistical mechanics for targeted materials design; model how disordered many-particle systems relax to equilibrium and to stealthy hyperuniform ground states with large-scale Monte Carlo and molecular dynamics on multi-GPU clusters (first-author *Phys. Rev. E*; second manuscript in preparation).
- Designed and implemented scalable CPU- and GPU-parallel many-body simulation algorithms in HPC environments (C/C++ with OpenMP and SIMD, CUDA, JAX).
- Built a bootstrap uncertainty-quantification pipeline for relaxation times from noisy simulation time series, cutting data volume and runtime by orders of magnitude while reproducing the original estimates exactly; diagnosed and corrected estimator bias and sampling artifacts.
- Implemented GPU-accelerated mutual-information estimators in JAX to detect directional dependence in 100s of GB of stochastic trajectories.
- Developed and benchmarked deep-learning models (neural operators, diffusion models, equivariant graph networks) in PyTorch to infer interaction potentials from structural data across hundreds of tracked GPU experiments.

Research Intern, PARADIM (NSF Materials Innovation Platform) Summer 2022
Advisors: Dr. David Elbert, Prof. Tyrel McQueen, Dr. Apurva Mehta *Baltimore, MD*

- Designed a statistical-learning method for automated signal detection in streaming X-ray diffraction data and built the live data-streaming pipeline (Apache Kafka) toward autonomous, real-time experimental control; presented at Cornell University.

Undergraduate Research Assistant, Johns Hopkins University 2020 – 2023
Advisors: Prof. Lan Cheng, Prof. J. D. Tovar *Baltimore, MD*

- Modeled vibrational lifetimes of optically trapped molecules with coupled-cluster theory in collaboration with Harvard experimentalists (co-author, *Phys. Rev. A*; ACS National Meeting talk); developed a Python package quantifying electron delocalization from DFT data run on HPC clusters.

PUBLICATIONS

- [1] **S. J. Dawley** and S. Torquato. Quantification of the relaxation of nonequilibrium initial conditions of many-particle systems to their equilibrium states. *In preparation* (2026).
- [2] **S. J. Dawley** and S. Torquato. Evolution of various initial many-particle configurations to disordered stealthy hyperuniform ground states. *Phys. Rev. E* **112**, 045310 (2025).
- [3] N. B. Vilas, C. Hallas, L. Anderegg, P. Robichaud, C. Zhang, **S. Dawley**, L. Cheng, and J. M. Doyle. Blackbody thermalization and vibrational lifetimes of trapped polyatomic molecules. *Phys. Rev. A* **107**, 062802 (2023).

TECHNICAL SKILLS

Programming & systems: Python (NumPy, SciPy), C/C++ (OpenMP, SIMD), CUDA, MATLAB, Mathematica; Git, pytest, Kafka, SLURM, multi-GPU clusters

Statistics & methods: probability, statistical inference, Bayesian statistics, Monte Carlo, stochastic processes, time series, uncertainty quantification, numerical optimization

Machine learning: PyTorch, JAX, deep learning (neural operators, diffusion models, graph networks), experiment tracking (Weights & Biases)

COMMUNICATION, TEACHING & LEADERSHIP

Presentations: Princeton Materials Institute Symposium (2025); ACS National Meeting (2023); Cornell University (2022). **Teaching Assistant (7 courses):** graduate Statistical Mechanics, Software Engineering for Scientific Computing, Computational Molecular Medicine (ML, hypothesis testing); Calculus; Organic Chemistry.

Leadership: Head PILOT Leader, JHU (2020–23) – led weekly peer-learning sessions and co-wrote the problem sets used by the whole course; First-Year Mentor (2020–21); Best Buddies volunteer and fundraiser (2019–present).