

SAMUEL J. DAWLEY

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EDUCATION

Princeton University

Sept. 2023 – May 2029 (expected)

Ph.D. in Chemistry | Advisor: Prof. Salvatore Torquato

Princeton, NJ

- Ph.D. candidate – General Examination passed May 31, 2025. Graduate Certificate in Computational Science & Engineering.

Johns Hopkins University

Sept. 2019 – May 2023

B.A. in Chemistry (Departmental Honors) and Applied Mathematics & Statistics; Minor in Mathematics

Baltimore, MD

- GPA 3.87/4.00. Graduated with General Honors; Dean's List every semester.

RESEARCH EXPERIENCE

Graduate Research Assistant, Princeton University

Sept. 2023 – Present

Complex Materials Theory Group | Advisor: Prof. Salvatore Torquato

Princeton, NJ

- Advance theory and computational methods in inverse statistical mechanics for the targeted design of materials with prescribed structure, with emphasis on disordered stealthy hyperuniform ground states.
- Quantified how diverse initial many-particle configurations evolve to hyperuniform ground states and, separately, how nonequilibrium initial conditions relax to equilibrium, using large-scale Monte Carlo and molecular dynamics simulations on multi-GPU clusters; first-author paper in *Phys. Rev. E* and a second first-author manuscript in preparation.
- Designed and implemented scalable CPU- and GPU-parallel algorithms for many-body simulation in HPC environments (C/C++ with OpenMP and SIMD, CUDA, JAX).
- Built a bootstrap uncertainty-quantification pipeline for relaxation times estimated from noisy simulation time series, reducing data volume and runtime by orders of magnitude while reproducing the original estimates exactly.
- Diagnosed estimator bias and sampling artifacts in simulation output that would otherwise have distorted published results, and designed corrected analysis protocols.
- Implemented GPU-accelerated mutual-information estimators in JAX to analyze hundreds of gigabytes of stochastic trajectory data.
- Developed deep-learning models (neural operators, diffusion models, equivariant graph networks) in PyTorch to infer interaction potentials from structural data, benchmarking architectures across hundreds of tracked GPU runs.

Research Intern, PARADIM (NSF Materials Innovation Platform), Johns Hopkins University

Summer 2022

Advisors: Dr. David Elbert, Prof. Tyrel McQueen, Dr. Apurva Mehta

Baltimore, MD

- Advanced strategies for real-time data analysis and autonomous experimental control with machine learning, toward accelerated discovery of inorganic materials.
- Developed a statistical-learning algorithm and its implementation for automatic signal-structure and spectral-peak detection in X-ray diffraction data.
- Implemented live streaming of experimental data and online analysis with Apache Kafka; gained hands-on experience in inorganic synthesis and X-ray diffraction characterization.

Undergraduate Research Assistant, Johns Hopkins University

Jan. 2020 – May 2023

Department of Chemistry | Advisor: Prof. Lan Cheng (Jan. 2022 – May 2023)

Baltimore, MD

- Studied relativistic effects in light- and heavy-atom molecules with coupled-cluster theory, aiming at quantitative descriptions of laser-cooled molecular and heavy-element ionic diatoms; computed vibrational lifetimes and polarizabilities.
- Modeled blackbody-driven vibrational lifetimes of optically trapped polyatomic molecules in collaboration with the Doyle experimental group (Harvard); co-authored the resulting *Phys. Rev. A* paper and presented the work at the ACS National Meeting.
- Produced benchmark calculations assessing perturbative versus variational treatments of spin-orbit coupling in heavy-element molecules.

Department of Chemistry | Advisor: Prof. J. D. Tovar (Jan. 2020 – May 2023)

- Investigated non-planar, hybrid radial-linear conjugation pathways in cycloparaphenylenes and their derivatives.
- Computed optimized geometries and molecular-orbital energies with density-functional theory on HPC clusters; developed a Python package computing nucleus-independent chemical shifts to quantify electron delocalization, and automated Gaussian16 geometry optimizations on the Maryland Advanced Research Computing Center.
- Synthesized novel organic compounds for cycloparaphenylene modeling and characterized them by NMR and mass spectrometry.

Research Intern, Massachusetts General Hospital

Summer 2021

Division of Pulmonary and Critical Care Medicine | Advisors: Dr. Tristan Kooistra, Dr. Benjamin Medoff

Boston, MA

- Studied the response of airway epithelial cells to lung inflammation and scarring toward an improved understanding of idiopathic pulmonary fibrosis.
- Created, maintained, and monitored tissue co-cultures grown from basal and immune cells of murine samples.
- Developed a Python algorithm based on Delaunay triangulation to parse the spatial distribution of cultured cells and visualize inflammation patterning.

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).

PRESENTATIONS

- [1] **S. J. Dawley** and S. Torquato. “Evolution of various initial many-particle configurations to disordered stealthy hyperuniform ground states.” Princeton Materials Institute Symposium, Princeton, NJ (2025).
- [2] **S. J. Dawley**, C. Zhang, X. Zheng, and L. Cheng. “Blackbody thermalization and vibrational lifetimes of trapped polyatomic molecules.” Talk, ACS Spring National Meeting, Indianapolis, IN (2023).
- [3] **S. J. Dawley**, D. Elbert, T. McQueen, and A. Mehta. “Streaming by design for materials characterization.” Talk, Cornell University, Ithaca, NY (2022).

GRANTS & FUNDING

Life Design Lab Grant, Johns Hopkins University (Spring 2021) – funded summer research at Massachusetts General Hospital on idiopathic pulmonary fibrosis.

HONORS & AWARDS

American Chemical Society Undergraduate Award, Maryland Section of the ACS (2023) – recognizes outstanding achievement by chemistry students across universities in the Maryland Section.

Departmental Honors in Chemistry, Johns Hopkins University (2023) – awarded for exceptional performance in both coursework and research.

General Honors, Johns Hopkins University (2023); **Dean’s List**, all semesters (2019–2023).

Loneragan Award, Dover-Sherborn High School (2019) – the school’s highest award, given to the two graduating seniors who best exemplify altruism, character, dignity, integrity, and loyalty.

TEACHING EXPERIENCE

Teaching Assistant, Princeton University Fall 2025

Department of Chemistry; Program in Applied & Computational Mathematics

Princeton, NJ

- **Statistical Mechanics** (graduate) – equilibrium and nonequilibrium thermodynamics, classical and quantum statistics, critical phenomena, and computational techniques for simulating physical systems.
- **Software Engineering for Scientific Computing** (graduate) – best practices for writing portable, robust code in high-performance computing environments.
- **Calculus I** (undergraduate).

Teaching Assistant, Johns Hopkins University

Spring 2022 – Summer 2023

Department of Applied Mathematics & Statistics; Department of Chemistry

Baltimore, MD

- **Computational Molecular Medicine** (EN.553.450/650, graduate; Spring 2023) – machine learning, statistical inference, and multiple hypothesis testing for high-dimensional data in computational systems biology.
- **Organic Chemistry I & II** (AS.030.205/206) – fundamentals of organic reactions and mechanisms with emphasis on structure, bonding, and reactivity.
- **Intermediate Organic Chemistry Laboratory** (AS.030.228) – advanced synthesis and characterization, emphasizing independent hypothesis development and testing.
- **Introductory Organic Chemistry Laboratory** (AS.030.227) – synthesis techniques and instrumentation: NMR, IR, UV-Vis, mass spectrometry, gas chromatography.

Peer Tutor, Johns Hopkins University

Fall 2020 – Spring 2023

Office of Academic Advising

Baltimore, MD

- **Head PILOT Leader** – organized and led weekly peer-led team-learning sessions in multivariable calculus and organic chemistry; co-wrote with the course instructor the problem sets and answer keys used by all students in the course; ran midterm and final review sessions.
- **Private Tutor** – one-on-one tutoring in linear algebra, multivariable calculus, organic chemistry, and physical chemistry.
- **Tutorial Project** – individualized tutoring in math, reading, and writing for Baltimore public elementary-school students, in collaboration with their parents.

MENTORING & LEADERSHIP

First-Year Mentor, Johns Hopkins University (Summer 2020 – Spring 2021) – oriented and mentored a cohort of incoming students through their first year with year-round peer-to-peer support.

Chemistry Student Safety Committee, Johns Hopkins University (Fall 2021 – Spring 2023) – addressed safety hazards across departmental facilities and individual labs; trained in laboratory safety, management, and conduct.

Best Buddies Club, Johns Hopkins University (Fall 2019 – Spring 2023) – organized the weekly transport of the student volunteer team to the Claremont School, which serves students with moderate to profound intellectual and developmental disabilities; built friendships between Claremont and Hopkins students through sports, arts, and gardening.

COMMUNITY SERVICE

Best Buddies International (Spring 2019 – Present) – volunteer with people with intellectual and developmental disabilities at community events; fundraising through auctions, road races, and bike rides.

Exceptional Citizens' Week, Pembroke, MA (Summer 2015 – Present) – one-on-one support counselor at a week-long camp for people with intellectual and developmental disabilities; member of the team organizing meals and activities (arts and crafts, fairs, parades, theater) for the entire camp; year-round fundraising.

TECHNICAL SKILLS

Programming: Python (NumPy, SciPy, PyTorch, JAX), C/C++ (OpenMP, SIMD), CUDA, Mathematica, MATLAB, R (basic), LaTeX

High-performance computing: SLURM, multi-GPU clusters, FFTW, FINUFFT, Git, pytest, Weights & Biases, Apache Kafka

Methods: Monte Carlo and molecular dynamics simulation, inverse statistical mechanics, numerical optimization, statistical inference and uncertainty quantification, time-series analysis, deep learning; electronic structure (coupled cluster with CFOUR, DFT with Gaussian16)

Laboratory: organic synthesis; NMR, IR, UV-Vis, mass spectrometry, gas chromatography, X-ray diffraction; mammalian tissue co-culture