# Daniel J. Staros, Ph.D.

*Postdoctoral Research Associate, Quantum and Condensed Matter Physics Group*

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## Education

**Brown University,** Providence, RI — *Ph.D. in Electronic Structure Theory* 2024
Thesis: *"Determining the structure, exciton binding energies, and proximity effects of monolayer $CrI_3$ from first principles"*
Advisor: Dr. Brenda Rubenstein

**Brown University,** Providence, RI — *M.A. in Physical Chemistry* 2020

**Bloomsburg University,** Bloomsburg, PA — *B.S. in Chemistry* 2019
Research advisors: Dr. Gregory Zimmerman, Dr. Kristen Lewis

## Appointments

**Los Alamos National Laboratory,** Los Alamos, NM — *Postdoctoral Research Associate* August 2024 — Present
Supervisors: Dr. Roxanne Tutchton, Dr. Jian-Xin Zhu
Primary Staff Collaborators: Dr. Beth Lindquist, Dr. Ryan Jadrich, Dr. Christopher Lane, Dr. Ivana Gonzales

**Lawrence Livermore National Laboratory,** Livermore, CA — *High Energy Density Physics Intern* 2019
Mentor: Dr. Caleb Mattoon

**Oak Ridge National Laboratory,** Oak Ridge, TN — *Nuclear Engineering Intern* 2018
Mentor: Dr. Ashley Shields

## Research Experience

**Los Alamos National Laboratory,** Los Alamos, NM — *Postdoctoral Research* August 2024 — Present
Worked independently to derive and program a novel lattice model, establishing that strong magnetic fields combined with strong correlation can degrade the integer quantum Hall effect. Collaboratively automated and calculated high-quality DFT data for a database of energy/volume curves and vibrational spectra to improving equations of state. Gained design physics training in collaboration with Beth Lindquist and Ryan Jadrich of X division.

**Brown University,** Providence, RI — *Doctoral Research* August 2019 — May 2024
Contributed to multi-university/lab effort to settle structural, magnetic and optical properties of ML $CrI_3$. I used QMC to predict a crystal structure later confirmed to be within 0.5% of experiment, compared to 10% across the DFT literature. Additionally collaborated with experimental groups to explain the origin of anomalies in X-ray scattering of thin $NiPS_3$ samples using DFT and cluster models, finding that Ni-S orbital hybridization changes in reduced dimensions.

**Lawrence Livermore National Laboratory,** Livermore, CA — *HEDP Research* May 2019 — August 2019
Worked within the Nuclear Data and Theory Group to support code development for propagating errors through nuclear covariance matrices in the LLNL nuclear data code FUDGE, improving FUGDE's handling of uncertainties in various data formats. Presented findings in summer student research seminar.

**Oak Ridge National Laboratory,** Oak Ridge, TN — *NESLS Research* May 2018 — August 2018
Worked within the Nuclear Security Advanced Technologies group to identify new stable/metastable uranium fluoride compounds using a high-throughput evolutionary algorithm/DFT workflow. We characterized correlations between coordination number/phonon spectra and stability to help characterize amorphous nuclear fuel materials.

**Bloomsburg University,** Bloomsburg, PA — *Undergraduate Research* May 2017 — May 2019
Worked with Gregory Zimmerman to predict the ionic mobility of aqueous alkali chloride ions under hydrothermal conditions. We developed a few-parameter model that fit data over a wider temperature range than previously possible. Also worked with Kristen Lewis, using molecular dynamics to show that sucralose can potentially inhibit uptake of sucrose by human salivary amylase.

## Research Funding and Computer Time (total research funding: $79,000)

**Center for Integrated Nanotechnologies Allocation,** CINT — July 2025
*PI, "Identifying Electrical Transport Signatures of Topology in 2D Correlated-Electron Materials"*

**Office of Science Graduate Student Research Fellowship,** Department of Energy ($50,000) — Aug. 2021
*Team Lead, "Unraveling magnetic and vdW physics in 2D $CrI_3$ materials using Diffusion Monte Carlo"*

**NASA Rhode Island Space Grant,** NASA RISG Consortium ($14,000) — April 2021
*Team Lead, "Unraveling magnetic and vdW physics in 2D $CrI_3$ materials using Diffusion Monte Carlo"*

**Duane and Susan Greenly Professional Experience Research Grant,** Bloomsburg University ($3,000) — Feb. 2019
*Team Lead, "Using molecular dynamics to model binding of human salivary amylase to sucralose in artifical sweetener metabolism"*

**Duane and Susan Greenly Professional Experience Research Grant,** Bloomsburg University ($3,000) — Feb. 2018
*Team Member, "Development of an Engineer Friendly Equation for Conductivity Measurements of KCl (aq)"*

**Duane and Susan Greenly Professional Experience Research Grant,** Bloomsburg University ($3,000) — Aug. 2017
*Team Member, "Nonlinear Regression of Conductivity Measurements"*

**Undergraduate Research URSCA Grant,** Bloomsburg University ($6,000) — May 2017
*Team Member, "Using Nonlinear Regression to Develop an Equation for [Calculating the Ionic Mobility of Hydrothermal KCl"]*

## Honors and Awards

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| LANL Spot Award for Theoretical Lightning Talk Judging Contributions | 2025 |
| National Research Council Postdoctoral Fellowship *(declined)* | 2024 |
| William R. Potter Conference Travel Award | 2024 |
| Brown Department of Chemistry Graduate Ambassador Program Award | 2022 |
| Department of Defense SMART Semi-Finalist Award | 2021 |
| Second Prize Chemistry Poster Award, Bloomsburg STEM Symposium | 2019 |
| American Chemical Society Undergraduate Award in Physical Chemistry | 2019 |

## Teaching Experience

**Independent Work,** Remote — *Organic Chemistry Tutoring* — January 2024 – April 2024
Performed individualized tutoring online for an undergraduate organic chemistry student at Binghamton University. During tutoring, the student's exam score rose 10% consecutively for the next 3 exams, resulting in a change from failing to passing.

**Brown University,** Providence, RI — *Research Mentor* — August 2021 – May 2022
Coached one graduate student and one undergraduate international student, guiding them through details of crystal structure files, how to do Density Functional Theory, and best practices/tips for supercomputing and data management. Received acknowledgement in the graduate student's first publication due to my coaching role.

**Brown University,** Providence, RI — *CHEM 0330 Laboratory Teaching Assistant* — August 2020 – May 2021
Worked as a teaching assistant with Li-Qiong Wang in the Department of Chemistry. Led weekly pre-lab lectures for between 10 and 20 students, performed grading, and collaborated with other TAs and the course instructor to mold pedagogy of key concepts. Received overwhelmingly positive student evaluations.

**Bloomsburg University,** Bloomsburg, PA — *Volunteer Chemistry Tutor* — August 2018 – May 2019
Volunteered countless hours in the chemistry department common room, helping students understand and solve general chemistry, organic chemistry, and physical chemistry problems.

## Professional Activities and Affiliations

### Society Affiliations

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| Member, American Chemical Society | 2018-Present |
| Member, American Physical Society | 2021-Present |

### Specialist Workshops Attended

"Quantum Matters in Materials Science (QMMS) Workshop" — January 2023
National Institute for Standards and Technology, VIRTUAL

"Crash Course in Supercomputing" — June 2022
National Energy Research Scientific Computing Center, VIRTUAL

"Molecular Dynamics/Theoretical Chemistry Program" — June 2020
Air Force Office of Science Research, VIRTUAL

## Service Activities

### Volunteer Work

Judge, LANL Summer Student Research Symposium — July 2025

Judge, LANL Theoretical Division Lightning Talks — July 2025

Organizer, QMCPACK Users Workshop — Dec. 2023

Tutor, Bloomsburg Chemistry Club — 2018 – 2019

### Outreach

Panel Member, Brown Graduate School Accepted Students Day — April 2022

Participant, Brown STEM Day 2020 Science Outreach Program — January 2020

Judge, Brown Times$^2$ STEM Academy Science Fair — Sept. 2019

## Developed Codes

**STARLIGHT: Sigma TrAnsveRse in LattIces with Gutzwiller-renormalized Hopping Terms** — 2024 – Present
**Role:** Author
**Language:** Python
**GitHub Repository:** https://github.com/dstaros-t4/STARLIGHT
**Description:** STARLIGHT is a tight-binding code developed to aid in discovery of novel quantum phases of 2D materials. It introduces a symmetrized treatment of electron correlation in the magnetized lattice, allowing for investigation into the correlation-induced renormalization of topological band structures for much lower field strengths than previously possible.

## Publications (total publications: 7, h-index: 5, total citations: 99, Google Scholar Link)

7. **Staros, D.**; Gasperich, K.; Annaberdiyev, A.; Benali, A.; Ganesh, P.; Rubenstein, B. A many-body characterization of the fundamental gap in monolayer $CrI_3$. *npj 2D Mater. Appl.*, 2025.

6. **Staros, D.**; Rubenstein, B.; Ganesh, P. A first-principles study of bilayer 1T'-$WTe_2$/$CrI_3$ as a topological spin filter candidate. *npj Spintronics,* 2 (4), 2024.

5. Sahoo, S.; Xub, Q.; Leic, X.; **Staros, D.**; Iyer, G.; Rubenstein, B.; Suryanarayanae, P.; Medford, A. Self-consistent convolutional density functional approximations: Formulation and application to adsorption at metal surfaces. *Chem. Phys. Chem.*, 202300688, 2024.

4. DiScala, M.; **Staros, D.**; de la Torre, A.; Lopez, A.; Wong, D.; Bartkowiak, M.; Schulz, C.; Rubenstein, B.; Plumb, K. Dimensionality dependent electronic structure in exfoliated van der Waals antiferromagnet $NiPS_3$. *Adv. Phys. Res.*, 202300096, 2024.

3. **Staros, D.**; Hu, G.; Tiihonen, J.; Nanguneri, R.; Krogel, J.; Bennett, M. C.; Heinonen, O.; Ganesh, P.; Rubenstein, B. A Combined First-Principles Study of the Electronic, Magnetic, and Phonon Properties of Monolayer $CrI_3$. *J. Chem. Phys.*, 156, 014707, 2022.

2. Zimmerman, G.; **Staros, D.**; Arcis, H. Critical Review of Transport and Equilibrium Properties of Potassium Chloride in High Temperature Water. *J. Chem. Eng. Data*, 67 (3), 533-544, 2022.

1. Shields, A.; Miskowiec, A.; Maheshwari, K.; Kirkegaard, M.; **Staros, D.**; Niedziela, J.; Kapsimalis, R.; Anderson, B. The impact of coordination environment on the thermodynamic stability of uranium oxides. *J. Phys. Chem. C*, 123, 15985-15995, 2019.

## Preprints/In Progress

4. **Staros, D.**; Lane, C.; Zhu, J-X.; Tutchton, R.
STARLIGHT: A Python package for calculating correlation and conductivity in magnetized lattices. *In Preparation (planned for Journal of Open Source Software).,* 2026.

3. **Staros, D.**; Tutchton, R.; Zhu, J-X.
Effect of electronic correlation on the integer quantum Hall effect. *In Preparation (planned for Physical Review Letters).,* 2026.

2. Isbill, S.; Shields, A.; Spano, T.; **Staros, D.**; Niedzala, J.; Miskowiec, A.
The Impact of Coordination Environment on the Structural Properties of Uranium Fluorides from First Principles. *LA-UR-25-30332* 2025.

1. Rubenstein, B.; Annaverdiyev, A.; Ganesh, P.; Gasperich, K.; Iyer, G.; Krogel, J.; Lopez, A.; Melton, C.; Mitas, L.; Nirenberg, S.; Saritas, K.; Shin, H.; **Staros, D.**; Kent, P.
A Practical Guide to Quantum Monte Carlo Calculations Using QMCPACK and Nexus. *In Preparation.,* 2025.

## Professional Presentations (15 total presentations)

### Invited Talks

4. "Guiding 2D Materials Property Prediction using Correlated Methods" — November 2024
BLABS Seminar, Los Alamos, NM

3. "Determining the structure, EBEs, and proximity effects of ML $CrI_3$ from first-principles" — April 2024
University of California Santa Cruz, Santa Cruz, CA

2. "Spin Textures from QMC" — November 2023
Center for Predictive Simulation of Functional Materials, Oak Ridge, TN

1. "From Two-Atom Materials to Two-Dimensional Materials" — May 2022
Graduate Student Ambassador Seminar, Bloomsburg, PA

### Contributed Talks

6. "Towards controlling local excitons with chiral edge states in the terraced BL 1$T'$-$WTe_2/CrI_3$" — March 2024
American Physical Society March Meeting, Minneapolis, MN

5. "Towards controlling local excitons with chiral edge states in the terraced BL 1$T'$-$WTe_2/CrI_3$" — November 2023
SCGSR Career Conversations, Virtual

4. "Exciton binding energies in monolayer $CrI_3$ from Diffusion Monte Carlo" — June 2023
Stochastic Methods in Electronic Structure Theory, Telluride, CO

3. "Unraveling magnetic and vdW physics in 2D $CrI_3$ using Diffusion Monte Carlo" — April 2022
NASA RI Space Grant Symposium, Providence RI, USA

2. "Engineering quantum materials from the bottom-up" — February 2022
*Co-speaker* — Brown Corporation Meeting, Providence RI, USA

1. "Nuclear Energy's Role in the Climate Crisis" — November 2020
Brown Graduate Student Leadership Committee Seminar

### Posters

5. "Correlation Effects on Electrical and Magneto-Transport Properties of Actinides" — July 2025
Conference on Strongly Correlated Electron Systems, Montréal, Quebec, CA

4. "Correlation Effects on Magneto-Transport Properties of Actinides" — March 2025
APS Global Physics Summit, Anaheim, CA

3. "Correlation Effects on Electrical and Magneto-Transport Properties of Actinides" — March 2025
New Mexico Postdoc Research Symposium, Albuquerque, NM

2. "Accurate electronic ground- and excited-state properties of 2D $CrI_3$ and its heterostructures" — March 2023
American Physical Society March Meeting, Las Vegas, NV

1. "Unraveling magnetic physics in monolayer $CrI_3$ using Diffusion Monte Carlo" — August 2021
American Chemical Society Fall 2021 National Meeting, Atlanta GA, USA