Daniel J. Staros

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Education

Doctor Philosophiae in Theoretical Chemistry *Expected* May 2024
Brown University *Providence, RI*

- Graduate Ambassador Program Nomination
- Elected to Sigma Xi Scientific Research Honor Society

Artium Magistri in Chemistry May 2020
Brown University *Providence, RI*

- Completed en route to PhD

Bachelor of Science in Chemistry May 2019
Bloomsburg University of Pennsylvania *Bloomsburg, PA*

- American Chemical Society certification

Experience

Research Assistant January 2023 – Present
Brown University - The Rubenstein Group *Providence, RI*

- Continued bilayer and exciton collaborations with the Center for Predictive Simulation of Functional Materials
- Calculated catalytic Pt-CO adsorption energies for comparison to machine learning functionals
  Methods: Diffusion Monte Carlo (QMCPACK)
  Machines: Perlmutter (NERSC)

DOE Office of Science Graduate Student Research Fellow January 2022 – January 2023
Brown University / Oak Ridge National Laboratory - Center for Nanophase Materials Science *Oak Ridge, TN*

- Led literature review, manuscript writing and submission process for SCGSR-sponsored research.
- Determined theoretical evidence for dissipationless edge conductance of quantum spins in the terraced bilayer 1T'-WTe_2/CrI_3
- Elucidated the atomic properties of local CrI_3 excitons using Quantum Monte Carlo and quantum chemistry.
  Methods: Density functional theory (QE,PySCF), macimally-localized Wannier functions (Wannier90), Chern number calculation (Z2Pack), configuration interaction (Quantum Package), diffusion Monte Carlo (QMCPACK)
  Machines: Perlmutter, Cori (NERSC); Summit, Andes (OLCF); Polaris (ALCF)

NASA Rhode Island Space Grant Graduate Fellow April 2021 – December 2021
Brown University - The Rubenstein Group *Providence, RI*

- Led literature review, manuscript writing and submission process for NASA-sponsored research of monolayer CrI_3.
- Predicted the accurate crystal structure of monolayer CrI_3 using Quantum Monte Carlo; helped develop a new DMC-based structural optimization method; demonstrated larger magnetic moments in monolayer CrI_3 than previously predicted
- Determined energies of strained chromium trihalides to inform machine-learned finite-size corrections
  Methods: Density functional theory (QE, VASP), variational Monte Carlo/diffusion Monte Carlo (QMCPACK)
  Machines: Cori, Perlmutter (NERSC); Oscar (Brown CCV); Andes (OLCF)

High Energy Density Physics Intern May 2019 – August 2019
Lawrence Livermore National Laboratory *Livermore, CA*

- Developed Python code for generation of grouped covariance matrices with nuclear transport applications
  Methods: Nuclear data manipulation (FUDGE), code development (Python)
  Machines: Borax (HPC @ LLNL)

Nuclear Engineering Science Laboratory Synthesis Intern May 2018 – August 2018
Oak Ridge National Laboratory *Oak Ridge, TN*

- Performed high-throughput prediction of new stable UF_x and UO_x crystal structures using evolutionary algorithms
  Methods: Density functional theory (VASP), evolutionary algorithms (USPEX)
  Machines: Metis (OLCF)

Awards

William R. Potter Conference Travel Grant March 2024
Brown Department of Chemistry William R. Potter Fund

Cane-Nambiar Endowment Travel Fund June 2023
Brown University Graduate School

Conference Travel Fund June 2023
Brown University Graduate School

William R. Potter Conference Travel Grant February 2023
Brown Department of Chemistry William R. Potter Fund

Conference Travel Fund January 2023
Brown University Graduate School

William R. Potter Conference Travel Grant August 2021
Brown Department of Chemistry William R. Potter Fund

Department of Defense SMART Semi-Finalist April 2021
DoD SMART Scholarship-for-Service Program

American Chemical Society Undergraduate Award in Physical Chemistry May 2019
ACS Division of Physical Chemistry

Duane and Susan Greenly Professional Experience Research Grant February 2019
Bloomsburg University Department of Chemistry

Junior Chemistry Achievement Award May 2018
Bloomsburg University Department of Chemistry

Duane and Susan Greenly Professional Experience Research Grant February 2018
Bloomsburg University Department of Chemistry

Duane and Susan Greenly Professional Experience Research Grant September 2017
Bloomsburg University Department of Chemistry

Undergraduate Research Scholarhip (URSCA) May 2017
Bloomsburg University Department of Chemistry

Publications

· **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.

· 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.

· 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.

· **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.

· 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.

· 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

· **Staros, D.**; Gasperich, K.; Annaberdiyev, A.; Benali, A.; Ganesh, P.; Rubenstein, B.
A fully many-body characterization of excited states in monolayer CrI_3.
In preparation, 2024.

· Berard, K.; Lopez, A.; Whelpley, N.; Iyer, G.; **Staros, D.**; Krogel, J.; Rubenstein, B.
Making Quantum Monte Carlo More Practical via Surrogate Methods.
In preparation, 2024.

Presentations

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

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

DiScala, M.**, Staros, D.** *et al.* Elucidating the Role of Dimensionality on the Electronic Structure [of $NiPS_3$] — March 2024
Oral — American Physical Society March Meeting, Minneapolis MN

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

Staros, D. Spin Textures from QMC — November 2023
Oral — CPSFM All-Hands Meeting, Oak Ridge TN

Staros, D. Exciton binding energies in monolayer CrI_3 from Diffusion Monte Carlo. — June 2023
Oral — Stochastic Methods in Electronic Structure Theory, Telluride CO

Staros, D. , *et. al.* Accurate electronic ground- and excited-state properties of 2D CrI_3 and its heterostructures. — March 2023
Poster — American Physical Society March Meeting, Las Vegas NV

Staros, D. From Two-Atom Materials to Two-Dimensional Materials. — May 2022
Oral — Graduate Student Ambassador Seminar, Bloomsburg PA

Staros, D. , Rubenstein, B. Unraveling magnetic and vdW physics in 2D CrI_3 using Diffusion Monte Carlo. — April 2022
Poster — NASA RI Space Grant Symposium, Providence RI

Rubenstein, B. M.**, Staros, D. J.**, Engineering quantum materials from the bottom-up. — February 2022
Oral — Brown Corporation Meeting, Providence RI

Staros, D. , Rubenstein, B. Unraveling magnetic physics in monolayer CrI_3 using Diffusion Monte Carlo. — August 2021
Poster — American Chemical Society Fall 2021 National Meeting, Atlanta GA

Staros, D. Rubenstein, B. Characterizing magnetism in monolayer CrI_3 using Quantum Monte Carlo. — July 2021
Poster — Stochastic Methods in Electronic Structure Theory, Telluride (virtual)

Staros, D. QMC Perspective on Magnetic Ordering in CrI_3. — October 2020
Oral — CMS Kickoff Meeting, virtual

Workshops

QMCPACK Users Workshop — December 2023
Organizer — Argonne National Laboratory, Chicago IL

DOE Center for Predictive Simulation of Functional Materials All-Hands Meeting — November 2023
Attendee — Oak Ridge National Laboratory, Oak Ridge TN

Energy Frontier Research Centers Principal Investigators' Meeting — September 2023
Attendee — United States Department of Energy, VIRTUAL

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

DOE Center for Predictive Simulation of Functional Materials All-Hands Meeting — October 2022
Attendee — Argonne National Laboratory, Chicago IL