Kyle Daniel Miller

kyledmiller@duck.com | Website | LinkedIn | GitHub | Google Scholar

Inquisitive graduate fellow & national laboratory intern with 7 publications and 5 years of experience using first-principles calculation, informatics, and machine learning to solve materials science problems. Passionate about sustainability, mentoring, and explainable models. Excels in scientific communication and integrated ML+simulation workflow development.

Education

Ph.D. (Anticipated) | Northwestern University, Evanston, IL   2018-Aug 2024
  Major: Materials Science & Engineering
  Thesis: Informatics and Simulation Toward Functional Materials Design and Discovery
  Advisor: Professor James M. Rondinelli

B.S., *summa cum laude* | University of Puget Sound, Tacoma, WA   2014-2018
  Majors: Physics (with honors), Mathematics (with honors)
  Minor: Computer Science

Honors & Awards

Award	R&D 100 to **Ma**terials **L**earning **A**lgorithms (MALA) Project to which I contributed	2023
Fellowship	National Science Foundation Graduate Research (3 yrs funding)	2020-2023
Fellowship	Integrated Data-Driven Discovery in Earth and Astrophysical Sciences (1 yr funding)	2019-2020
Scholarship	Peter K. Wallerich (for excellence in scientific research)	2016-2018
Scholarship	Puget Sound Trustee (for academic excellence)	2014-2018
Scholarship	Raymond and Olive Seward (for excellence in physics)	2016-2018
Scholarship	McGill Family (for excellence in math)	2016-2018
Scholarship	Thomas Malcolm and Hilda Enden Jack (for excellence in math)	2016-2018

Publications

Machine learning the electronic structure of matter across temperatures. Fiedler, L.; Modine, N. A.; Miller, K. D.; Cangi, A. *Physical Review B* 2023, 108 (12), 125146.

Testing the Limits of the Global Instability Index. Miller, K. D.; Rondinelli, J. M. *Applied Physics Letters Materials* 2023 11 (10) 101108.

Carrier-induced metal-insulator transition in trirutile $MgTa_2O_6$. Miller, K. D.; Rondinelli, J. M. *Physical Review Materials* 2022, 6 (7), 075007.

Database, Features, and Machine Learning Modeling to Identify Thermally Driven Metal-Insulator Transition Compounds. Georgescu, A. B.; Ren, P.; Toland, A. R.; Zhang, S.; Miller, K. D.; Apley, D.; Olivetti, E. A.; Wagner, N.; Rondinelli, J. M. *Chemistry of Materials* 2021, 33 (14), 5591-5605.

AB_2X_6 Compounds and the Stabilization of Trirutile Oxides. Schueller, E. C.; Oey, Y. M.; Miller, K. D.; Wyckoff, K. E.; Zhang, R.; Zhang, W.; Wilson, S. D.; Rondinelli, J. M.; Seshadri, R. *Inorganic Chemistry* 2021. 60 (12), 9224-9232.

Structural signatures of the insulator-to-metal transition in $BaCo_{1-x}Ni_xS_2$. Schueller, E. C.; Miller, K. D.; Zhang, W.; Zuo, J. L.; Rondinelli, J. M.; Wilson, S. D.; Seshadri, R. *Physical Review Materials* 2020, 4 (10), 104401.

Optimization and Validation of Efficient Models for Predicting Polythiophene Self-Assembly. Miller, E. D.; Jones, M. L.; Henry, M. M.; Chery, P.; Miller, K.; Jankowski, E. *Polymers* 2018, 10 (12), 1305.

Research Experience

Research Scientist | Citrine Informatics   Jun 2024-Present

ARPA-E ONWARDS: Optimizing Nuclear Waste and Advanced Reactor Disposal Systems
· Leveraging materials informatics to develop safer, more efficient nuclear waste forms

ARPA-E CHADWICK: Creating Hardened And Durable fusion first Wall Incorporating Centralized Knowledge
· Leveraging materials informatics to develop harder, radiation-resistant fusion alloys

DARPA R^2: Rubble to Rockets
· Using materials informatics to enable recycling of scrap metal into new parts

Graduate R&D Intern | Sandia National Laboratories   Sep 2022-Aug 2024

Accelerating Large-Scale Electronic Structure Predictions with Machine Learning
· Developed memory-constrained data shuffling method for PyTorch-based **Ma**terials **L**earning **A**lgorithms (MALA)
· Designed active sampling algorithm to overcome redundancy in massive data sets and improve edge case learning
   · Maintained $> 95\%$ accuracy on defective semiconductors with 95% reduction in training set size
· Expanded MALA neural network surrogate models from pure elements to binary compounds

Graduate Student Researcher | Northwestern University   Sep 2018-Aug 2024

Screening for Novel Ferroelectric Materials
· Built a high-throughput, closed-loop screening workflow incorporating machine learning and first-principles calculation to identify novel ferroelectric material candidates
· Characterized strain-dependent ferroelectricity in 7 novel candidates

Decoratypes: An Extensible Taxonomic Generalization of Anti-Structures
· Developed a novel classification scheme describing decorations of atomic properties on crystalline structures
· Created an high-throughput identification workflow and classified >38,000 unique structures

Testing the Limits of the Global Instability Index (GII)
· Overhauled understanding of GII as an absolute metric for structural stability, proposing new guidelines for effective use
· Performed large-scale (>20,000 compounds) analysis of GII dependence on structure and chemistry

Carrier-Induced Metal-Insulator Transition in Trirutile $MgTa_2O_6$
· Mapped the electronic and magnetic phases across electron doping in $MgTa_2O_6$
· Investigated coupling between electronic state and established structural indicators

Structural Signatures of the Insulator-to-Metal Transition in $BaCo_{1-x}Ni_xS_2$
· Discovered the origin of structural distortions observed by experimental collaborators using first-principles calculation
· Transformed our understanding of the insulator-to-metal transition by connecting it to the origin of the distortions

Participant | Solid-State Materials Chemistry and Data Science Hackathon @ U. of Utah & Lehigh U.   Jan 2023

Generalized Tolerance Factor for Inorganic Crystals
· Facilitated rapid project progression from infancy to working prototype in 2 days with a 3-person interdisciplinary team
· Created a symbolic learning model to produce cheap, transparent stability predictions for inorganic crystals

Summer Research Intern | Boise State University   May-Aug 2017

High-throughput molecular simulations into the morphology of P3HT:PCBM blends
· Developed coarse-grained molecular dynamics model of self-assembly in conducting polymer blends
· Mapped morphology phase diagram using radial distribution, clustering algorithms, and simulated X-ray scattering

Contributed Presentations

Talk | APS March Meeting | American Physical Society

   Structure Complements (Decoratypes): A New Materials Taxonomy   Mar 2024

   How Global is the Global Instability Index?   Mar 2023

   Insulator-to-metal transition in $BaCoS_2$ via chlorine substitution   Mar 2022

   Structural signatures of the insulator-to-metal transition in $BaCo_{1-x}Ni_xS_2$ Mar 2021

   Electronic and Lattice Dynamical Properties of $MgTa_2O_6$ Mar 2020

Poster & Talk | Joint University Microelectronics Program 2.0 | DARPA+SRC+Cornell University

   Ferroelectric Materials Discovery *via* Hybrid ML-DFT Screening   Aug 2023

Poster | Hands-On DFT and Beyond Workshop | Universitat de Barcelona

   Beyond Binaries: Trirutile oxides as a platform for understanding metal-insulator transitions   Aug 2019

Teaching & Communication

Graduate Student Mentor (2-4 hrs/wk)   Dec 2022 - Present

Northwestern University, Materials Theory and Design Group
· Developed guides for on-boarding and tutorials for high-throughput computing and density functional theory
· Met weekly with junior graduate student to work through tutorials and discuss research

Grant Writer Sep 2018 - Present
Northwestern University, Materials Theory and Design Group
· Independently acquired 6 computing grants from Northwestern Quest HPCC and Amazon Web Services
· Collaboratively acquired 5 computing grants from the National Science Foundation (XSEDE, ACCESS)
· Independently wrote 3 quarterly and 1 annual research updates for Semiconductor Research Corp. grant

Teaching Assistant for Intro. to Computational Materials Science (10 hrs/wk) Jan-Mar 2021, 2022
Northwestern University, Department of Materials Science & Engineering
· Developed molecular dynamics laboratory assignment

Physics Tutor (7-8 hrs/wk) Sep 2016-May 2018
University of Puget Sound, Center for Writing Learning and Teaching
· Attended summer short courses on pedagogy with a focus on co-learning

Professional Development

Certificate in Management for Scientists and Engineers 2023
Northwestern University, Kellogg School of Management
· 72-hour course covering effective feedback & communication, business ethics, leadership, risk, entrepreneurship, strategy, operations, intellectual property, accounting, finance, negotiation, and marketing

Certificate in Science Communication 2020
Northwestern University, Science Communication Online Programme
· 16-hour course covering audience analysis, storytelling, rhetoric, visual communication, and stage presence

Technical Skills

Languages	Python, Bash, LaTeX, SQL
Python Libs.	PyTorch, scikit-learn, Keras, pandas, Pymatgen, Matminer, Streamlit, Matplotlib/Seaborn/Plotly,
Workflow	Unix shell, Git, high-performance computing (SLURM, PBS/Torque), MySQL
Simulation	VASP (+Wannier90, +Phonopy), Quantum Espresso, HOOMD-blue

Service and Activities

Peer Reviewer | Various academic journals 2022-Present
· *Sci. Rep.* (2025)
· *APL Mach. Learn.* (2024)
· *Comm. Phys.* (2023)
· *Chem. Mater.* (2022)

Curriculum Developer, Mentor for *Coding Club* | Pedersen-McCormick Boys and Girls Club 2020-2022
· [GitHub repository] Developed intermediate and advanced Python lessons and projects for high school-age students
· Tutored/mentored local high school students at weekly code literacy lessons

Mentor for *Junior Science Club* | Pedersen-McCormick Boys and Girls Club 2019-2020
· Engaged young students with weekly educational science sessions
· Developed exciting, hands-on, and informative curricula for weekly science sessions

Student Representative on *Strategic Planning Steering Committee* | University of Puget Sound 2017-2018
· Drafted the university's 10-year vision, goals, and evaluative metrics with a team of 20 faculty, administrators, trustees, and students meeting every 3-4 weeks for a year
· Gathered, condensed, and presented student feedback to steering committee to advocate for student needs

Media Coordinator for *Advocates for Detained Voices* (club) | University of Puget Sound 2015-2018
· Raised $5,000 to help fund cancer treatment for a detained person
· Helped run support stand providing legal resources and humanitarian aid for visitors to detention center

Member/Programmer for *Physics Club* | University of Puget Sound 2014-2016/2016-2018.
· Collaborated in three annual weather balloon launches, collecting pressure, temperature, and magnetic field data
· Organized informational sessions to promote and share advice about undergraduate research opportunities