

Kyle Daniel Miller

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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. , <i>summa cum laude</i> 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 Materials Learning Algorithms (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 $\text{BaCo}_{1-x}\text{Ni}_x\text{S}_2$.** 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
<i>ARPA-E ONWARDS: Optimizing Nuclear Waste and Advanced Reactor Disposal Systems</i>	
· Leveraging materials informatics to develop safer, more efficient nuclear waste forms	
<i>ARPA-E CHADWICK: Creating Hardened And Durable fusion first Wall Incorporating Centralized Knowledge</i>	
· Leveraging materials informatics to develop harder, radiation-resistant fusion alloys	
<i>DARPA R²: Rubble to Rockets</i>	
· Using materials informatics to enable recycling of scrap metal into new parts	

Graduate R&D Intern | Sandia National Laboratories

Sep 2022-Present

Accelerating Large-Scale Electronic Structure Predictions with Machine Learning

- Developed memory-constrained data shuffling method for PyTorch-based **Materials Learning Algorithms (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-Present

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 $\text{BaCo}_{1-x}\text{Ni}_x\text{S}_2$

- 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 $\text{BaCo}_{1-x}\text{Ni}_x\text{S}_2$

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

Reviewer | 4 manuscripts | *Chem. Mater.* (2022) | *Comm. Phys.* (2023) | *APL Mach. Learn.* (2024) | *Sci. Rep.* (2025)
2022-Present

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