Kyle Daniel Miller

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EDUCATION

Ph.D. in Materials Science & Engineering | GPA: 3.89/4 | NORTHWESTERN UNIVERSITY — 2018-APR 2024
    Certificate in Management for Scientists and Engineers | KELLOGG SCHOOL OF MANAGEMENT — 2023
    Certificate in Science Communication | NORTHWESTERN SCIENCE COMMUNICATION ONLINE PROGRAMME — 2020

B.S. in Physics, Mathematics, Computer Science Minor | GPA: 3.99/4 | UNIVERSITY OF PUGET SOUND — 2014-2018

HONORS & AWARDS

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

PUBLICATIONS

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

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

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

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

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

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

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

CONTRIBUTED PRESENTATIONS

TALK | APS March Meeting | AMERICAN PHYSICAL SOCIETY — MAR 2020-2024
    Electronic and Lattice Dynamical Properties of $MgTa_2O_6$
    Structural signatures of the insulator-to-metal transition in $BaCo_{1-x}Ni_xS_2$
    Insulator-to-metal transition in $BaCoS_2$ via chlorine substitution
    How Global is the Global Instability Index?
    (Anticipated) Structure Complements: A New Materials Taxonomy

POSTER & TALK | Joint University Microelectronics Program 2.0 | DARPA+SRC+CORNELL UNIVERSITY — AUG 2023
    Ferroelectric Materials Discovery *via* Hybrid ML-DFT Screening

POSTER | Hands-On DFT and Beyond Workshop | UNIVERSITAT DE BARCELONA — AUG 2019
    Beyond Binaries: Trirutile oxides as a platform for understanding metal-insulator transitions

POSTER | Idaho Conference on Undergraduate Research | BOISE STATE UNIVERSITY — JUL 2017

POSTER | Fall Student Research Symposium | UNIVERSITY OF PUGET SOUND — SEP 2016, 2017

POSTER | Summer Undergraduate Research Expo | UNIVERSITY OF MINNESOTA — AUG 2016

Research Experience

Graduate R&D Intern | Sandia National Laboratories   Sep 2022-Present
Project: Accelerating Large-Scale Electronic Structure Predictions with Machine Learning
· Developed data shuffling method for **Ma**terials **L**earning **A**lgorithms (MALA)
· Expanded MALA neural network surrogate models from pure elements to binary compounds
· Designed active learning 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

Graduate Student Researcher | Northwestern University   Sep 2018-Present
Project: 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

Project: Taxonomy of Structure Complements: Generalized Anti-Structures
· Generalized the concept of anti-structures to include n-ary compounds, termed structure complements (SCs)
· Created an high-throughput identification workflow and screened >80,000 structures to identify and classify SC networks

Project: Testing the Limits of the Global Instability Index (GII)
· Analyzed the effect of various bonding models to construct a more robust GII calculator
· Quantified the sensitivity of the GII metric to chemistry, structure, and data source in small, clustered data sets and large (>20,000 sample) data sets
· Overhauled understanding of GII as an absolute metric for structural stability, proposing new guidelines for effective use

Project: 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
· Assessed the similarities and differences in the transition-driving forces between the trirutile and rutile structures

Project: 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 compatible with anomalous sulfide disorder observed in experiment
· 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
Project: 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
· Attended hands-on workshops to hone my skills in design and tuning of machine learning models and curation of data

Summer Research Intern | Boise State University   May-Aug 2017
Project: 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

Service and Activities

Reviewer for *Chem. Mater.* (2022), *Comm. Phys.* (2023)   2022-Present

Curriculum Developer, Mentor for *Coding Club* | Pedersen-McCormick Boys and Girls Club   2020-Present
· [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 over $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