Kyle Daniel Miller

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

EDUCATION

Ph.D. (Anticipated) | NORTHWESTERN UNIVERSITY, EVANSTON, IL 2018-Apr 2024
    Major: Materials Science & Engineering
    Thesis: Informatics and Simulation Toward the Discovery of Metal-Insulator Transition Materials and Mechanisms
    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

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.

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
· Presented the new ground state structure compatible with previously unexplained 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

Technical Skills

Languages	Python[A], Java[I], Bash[I], MATLAB[I], LaTeX[I], SQL[P], HTML[P]
Python Libs.	PyTorch, scikit-learn, Keras, pandas, Matplotlib, Pymatgen, Matminer, Bokeh (interactive visualization)
Workflow	Unix shell, Git, high-performance computing (SLURM, PBS/Torque)
Simulation	VASP (+Wannier90, +Phonopy), Quantum Espresso, LAMMPS, HOOMD-blue
ML Methods	Neural networks (feedforward & conv.), active learning, decision trees, Bayesian statistics, clustering

[A] *Advanced*, [I] *Intermediate*, [P] *Proficient*

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

Teaching & Mentoring Experience

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

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

Math Tutor and Grader (6 hrs/wk)   Jan-May 2016
University of Puget Sound, Mathematics Department

AP Physics Tutor (2 hrs/wk)   Sep 2015-May 2016
Private Client, High School Student

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

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
· Organized events for awareness and charity to support local immigrants
· Helped run support stand providing legal resources and humanitarian aid for visitors to detention center

Member/Programmer for *Physics Club* | University of Puget Sound   2014/2016-2018.
· 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

REFERENCES

Professor James M. Rondinelli
Walter Dill Scott Professor of Materials Science and Engineering
Northwestern University
jrondinelli@northwestern.edu

Prof. Rondinelli has been my Ph.D. advisor since August 2018.

Doctor Normand Modine
Research Scientist in Computational Materials and Data Science
Sandia National Laboratories
namodin@sandia.gov

Dr. Modine has been my research internship advisor since August 2022.

Professor Ram Seshadri
Fred and Linda R. Wudl Professor of Materials Science
University of California, Santa Barbara
seshadri@mrl.ucsb.edu

Prof. Seshadri is on my dissertation committee and we collaborated on two interdisciplinary publications (listed below).

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.

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