

Kat Nykiel

Computational Materials Scientist

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Research Profile

Computational materials scientist specializing in automated high-throughput workflows and ML-driven materials discovery. Experience in using semi-supervised learning for synthesizability and GNNs for property prediction. Committed to open science and bridging the gap between theory and experiment.

Education

Ph.D. Materials Engineering Aug 2021 – Dec 2025

Purdue University, West Lafayette, IN

Committee: Dr. Alejandro Strachan (advisor), Dr. Arun Mannodi, Dr. Rahim Rahimi, Dr. Babak Anasori

Specialization: Computational Science and Engineering

B.S. Materials Science & Applied Physics Aug 2017 – May 2021

Ohio State University, Columbus, OH

Magna Cum Laude, Honors Research Distinction

Publications

Nykiel, K., Wyatt, B., Anasori, B. & Strachan, A. Exploration of Hexagonal, Layered Carbides and Nitrides as Ultra-High Temperature Ceramics. Preprint at <https://doi.org/10.48550/arXiv.2508.18455> (2025).

Nykiel, K. & Strachan, A. High-throughput density functional theory screening of double transition metal MXene precursors. *Sci Data* 10, 827 (2023).

Chen, C.-C., Appleton, R. J., Mishra, S., **Nykiel, K.** & Strachan, A. Discovery of new high-pressure phases integrating high-throughput DFT simulations, graph neural networks, and active learning. *npj Comput Mater* 11, 191 (2025).

Lee, B. H., **Nykiel, K.**, Hallberg, A. E., Rider, B. & Strachan, A. Thermodynamic fidelity of generative models for Ising system. *Journal of Applied Physics* 137, 124901 (2025).

Chen, C.-C., Appleton, R. J., **Nykiel, K.**, Mishra, S., Yao, S., & Strachan, A. How accurate is density functional theory at high pressures? *Computational Materials Science* 247, 113458 (2025).

Wyatt, B. C., Thakur, A., **Nykiel, K.**, Hood, Z. D., Adhikari, S. P., Pulley, K. K., Highland, W. J., Strachan, A. & Anasori, B. Design of atomic ordering in $\text{Mo}_2\text{Nb}_2\text{C}_3\text{T}_x$ MXenes for hydrogen evolution electrocatalysis. *Nano Lett.* (2023).

Research Experience

Graduate Researcher, Purdue University Aug 2021 – Dec 2025

- Established group infrastructure for high-throughput density functional theory workflows supporting machine-learning driven materials discovery, with over 140,000 completed calculations in the database
- Implemented automated workflows for geometric relaxation, elastic constant, phonons, electronic bandstructure, convex hull stability, FTIR, SQS, equation of state, and MLIP training
- Collaborated with experimental researchers to study stability and synthesizability of 2D MXenes, their precursors, and layered ceramics in computation-guided discovery efforts
- Developed workflows for Quantum ESPRESSO in nanoHUB, with over 200 users and 120,000 simulations
- Applied graph neural networks and active learning for closed-loop discovery of high-entropy carbides

Technical Skills

Electronic Structure	VASP, Q-Chem, Quantum ESPRESSO
Workflow Automation	atomate2, jobflow, FireWorks, pymatgen
Machine Learning	PyTorch, GNNs, semi-supervised learning, MLIPs, local LLMs
Data Infrastructure	high-throughput workflow orchestration, databases, Docker, Kubernetes

Honors and Awards

Fall Symposium Doctoral Talk Award, CIGP, Purdue University	Nov 2025
Best Graduate Student Poster Award, Materials Research Data Alliance	Mar 2023

Presentations

Oral, Accelerated Prediction of Elastic Tensors in High-Entropy Rock-salt Carbides using an Equivariant Graph Neural Network, Materials Research Society, Dec 2025, Boston, MA.

Oral, Exploration of Magnetism in Rare Earth and Mn-doped Double Transition Metal MXenes, Materials Research Society, Dec 2025, Boston, MA.

Oral, Synthesis of Novel Rare-Earth MXenes Using Density Functional Theory and Optimal Experiment Design, Materials Research Society, Apr 2025, Seattle, WA.

Poster, Exploration of Stacked MXenes as Precursors to Ultra-High Temperature Ceramics, EPW School on Electron-Phonon Physics, Jun 2024, Austin, TX.

Oral, Exploration of Stacked MXenes as Precursors to Ultra-High Temperature Ceramics, Materials Research Society, Apr 2024, Seattle, WA.

Oral, Semi-Supervised Prediction of Double-Transition Metal MXene Stability, Materials at Purdue Symposium, May 2023, West Lafayette, IN.

Oral, Semi-Supervised Prediction of Double-Transition Metal MXene Stability, Materials Research Society, Apr 2023, San Francisco, CA.

Oral, Semi-Supervised Prediction of Double-Transition Metal MXene Stability, Materials Research Data Alliance Conference, Mar 2023, Virtual.

Teaching Experience

Graduate Teaching Assistant, MSE 367, Purdue University Jan 2023 – May 2023

- Taught laboratory sessions covering processing of metals, ceramics, and polymers
- Led laboratory instruction and coordinated final design projects

Mentoring Experience

Graduate Student Mentor, MNT Collaborative Undergraduate Research Network May 2023 – Sept 2024

- Mentored three undergraduate researchers in computational analysis projects
- Used statistical natural language processing and LLMs to analyze trends of expert selection in articles

Graduate Student Mentor, nanoHUB, Purdue University May 2022 – Dec 2022

- Mentored a student in simulation of the 2D Ising model using Markov Chain Monte Carlo methods
- Project led to generative model training on Ising trajectories and a co-authored publication