Kat Nykiel

Ph.D. Candidate · Materials Engineering

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Education

Purdue University *West Lafayette, IN*

Ph.D. Materials Engineering (in progress) *Aug. 2021 - present*

- Committee: Dr. Alejandro Strachan (advisor), Dr. Arun Mannodi, Dr. Babak Anasori, Dr. Rahim Rahimi
- Specialization in Computational Science and Engineering

Ohio State University *Columbus, OH*

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

- Magna Cum Laude
- Honors Research Distinction

Research Experience

Graduate Research

Purdue University *West Lafayette, IN*

Advisor: Dr. Alejandro Strachan *Aug. 2021 - present*

- Established group infrastructure for state-of-the-art high-throughput density functional theory workflows, with over 90,000 completed calculations currently stored in the database
- Implemented geometric relaxation, elastic constant, phonons, electronic bandstructure, convex hull stability, FTIR, equation of state, and machine learned interatomic potential training workflows
- Studied stability and synthesizability of MXenes, their precursors, layered and high-entropy carbides
- Developed workflows for Quantum ESPRESSO in nanoHUB, over 200 users and 120,000 simulations performed

Undergraduate Research

Ohio State University *Columbus, OH*

Advisor: Dr. Hamish Fraser *Jan. 2019 - May 2021*

- Developed a MATLAB-based app for stereographic projection and trace analysis
- Performed SEM with OSU's Center for Electron Microscopy and Analysis

Ohio State University *Columbus, OH*

Advisor: Dr. Wolfgang Windl *Jan. 2021 - May 2021*

- Studied goniopolar materials by calculating band structures of TMDs using VASP
- Obtained honors research distinction through undergraduate thesis

Publications

Published

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 Mo2Nb2C3Tx MXenes for Hydrogen Evolution Electrocatalysis. Nano Lett. (2023).

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., **Nykiel, K.**, Mishra, S., Yao, S., Strachan, A. How accurate is density functional theory at high pressures? Computational Materials Science 247, 113458 (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., 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).

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).

Honors and Awards

Mar. 2023 **Best Graduate Student Poster Award**, Materials Research Data Alliance

Presentations

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

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

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

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

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

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

Teaching Experience

Graduate Teaching Assistant *Purdue University*

MSE 367: Materials Processing Laboratory *Jan. 2023 - May 2023*

- Taught Materials Processing Lab, a course covering the processing of metals, ceramics, and polymers
- Led lab sessions and coordinated student final design projects

Mentoring Experience

MNT-CURN Research Program *Virtual*

Graduate Student Mentor *May 2023 - Sept. 2024*

- Mentor three undergraduates through the Micro Nano Technology Collaborative Undergraduate Research Network (MNT-CURN)
- Used statistical natural language processing and large language models to analyze trends of expert selection in news articles

Purdue University, nanoHUB *West Lafayette, IN*

Graduate Student Mentor *May 2022 - Dec. 2022*

- Mentored one high school student / later undergrad through Purdue University
- Simulated 2D ising model of ferromagnetism using markov chain monte carlo, later trained generative models on ising trajectories and published our results