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).

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