# Curriculum Vitae

Kat Nykiel

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### Contact Info

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### Education

**Ph.D. Materials Engineering, Purdue University (in progress)**
Aug. 2021 - Present

- Committee: Dr. Alejandro Strachan, Dr. Arun Mannodi, Dr. Babak Anasori, Dr. Rahim Rahimi
- Concentration in Computational Engineering

**B.S. Materials Science & Applied Physics, Ohio State University**
Aug. 2017 - May 2021

- Magna Cum Laude
- Honors Research Distinction

## Research Experience

**Graduate Research, Purdue University**

Aug. 2021 - Present
Advisor: Dr. Alejandro Strachan

- Implemented high-throughput density functional theory workflows for elastic constants, phonons, electronic bandstructure, convex hull stability, and equations of state
- Studied stability and synthesizability of MXenes, their precursors, and MXene-derived materials
- Developed a set of workflows for Quantum ESPRESSO in nanoHUB

**Undergraduate Research, Ohio State University**

Jan. 2019 – May 2021
Advisor: Dr. Hamish Fraser

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

Jan. 2020 – May 2021
Advisor: Dr. Wolfgang Windl

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

## Teaching Experience

**Graduate Teaching Assistant, Purdue University** Jan. 2023 - May 2023

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

## Mentoring Experience

**Graduate Student Mentor, MNT-CURN** May 2023 - Sept. 2023, May 2024 - Sept. 2024

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

**Graduate Student Mentor, Purdue University** 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

## Honors and Awards

**MaRDA Best Graduate Student Poster Award** Mar. 2023

- Awarded for presenting at the Spring 2023 Materials Research Data Alliance Conference

## Publications

### Journal Publications

- 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) doi:10.1021/acs.nanolett.2c04287.
- **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. Preprint at https://doi.org/10.48550/arXiv.2412.03764 (2024).

## Presentations and Invited Lectures

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.