Kieran Nehil-Puleo

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Summary

Ph.D. in Interdisciplinary Materials Science with expertise in machine learning, molecular simulation, and scientific software development. Experienced in graph neural networks, HPC, and open-source research tools. Strong record of publications, awards, and cross-disciplinary projects.

Experience

Vanderbilt University / Ph.D. Student and Graduate Researcher Aug 2021 – Mar 2026
Nashville, TN

- Performed deep learning with GNN models for ligand-protein binding prediction (multi-egnn).
- Developed software and algorithms for the molecular simulation design framework (mosdef-hub).

Michigan State University / Undergraduate Research Assistant Aug 2017 – Aug 2021
East Lansing, MI

- Applied computer vision algorithms for X-ray diffraction feature detection.
- Conducted computational materials science research using Python, C++, and Bash.
- Developed software to analyze large-scale materials datasets.
- Performed scripting and data analysis on secure Linux shell (ssh).

Textron Bell Flight / Business Analytics Intern Jun 2019 – Aug 2019
Fort Worth, TX

- Automated financial and supply chain processes using Python.
- Analyzed helicopter repair datasets to estimate part consumption for warranty contracts.
- Supported contract proposals and financial reporting with data-driven insights.

Projects

- **Interactional Equivariant Graph Neural Networks (IEGNN)** (First-author) – Designed interpretable GNN with Grad-CAM/feature attribution, pipelines for preprocessing, training, benchmarking; processed millions of atomic structures with PyTorch Geometric.
- **FiberForge: Helical Fibril Simulations** (First-author) – Developed high-throughput pipeline for fibril mechanics; symmetry-based reconstruction, clustering, trajectory analytics, reproducibility analysis. Published with open-source datasets.
- **Robust Areal Diffraction Peak Detection** – Conference presentation.
- **Open-source Powder Dispenser** – CAD + control software.
- **Dynamically Interconnected Microbioreactors** – Patent.
- **Viscosity Prediction via Periodic Perturbation** – Co-author.

Education

Ph.D. Interdisciplinary Materials Science, Vanderbilt University (2021 – 2026)
B.S. Materials Science and Engineering, Michigan State University (2017 – 2021), *Honors*, Minor in Computer Science
B.S. Statistics, Michigan State University (2017 – 2021), *Honors*, Minor in Computational Modeling

Awards

- NSF Graduate Research Fellowship (awarded to ∼2,000 of 12,000+ STEM applicants).
- STATE Scholarship (merit + top 98th percentile ACT).
- Honors in both undergraduate degrees, with minors in Computer Science and Computational Modeling.

Skills

- **Programming:** Python (Adv., 5 yrs), C++ (Adv., 5 yrs), React.js (Fair, 1 yr), Bash (3 yrs), Git (4 yrs).
- **ML/AI:** PyTorch, TensorFlow, PyTorch Geometric (4 yrs).
- **HPC:** SLURM, MPI, OpenMP.
- **DevOps:** GitHub/Git, GitHub Actions (CI), Docker, Linux/Bash.
- **Extensions:** Pybind, CUDA.
- **Scientific Software:** Gromacs, HOOMD, AMBER, Orca.

Hobbies

Weightlifting, Brazilian Jiu Jitsu, Rock Climbing