# **Kirby Broderick**

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## **Professional Summary**

Computational materials and automated design engineer (5 yrs) applying convolutional neural networks and high throughput modeling expertise to high-volume research and manufacturing.

### Skills

Core: Python • PyTorch • Graph/Convolutional NNs • C++ • Slurm • Git Familiar: Rust • Pymatgen • ASE • dask • VASP • ILT • OPC • k8s

# **Experience**

### **Software Research Engineer/Scientist**

Intel Corporation; Hillsboro, OR — Apr 2024–present

- Developed and implemented algorithm to reduce arbitrary-degree mask vertex counts by 30% while preserving manufacturability
- Implemented production-ready inverse lithography curvilinear hotspot repair capability with 100% acceptance rate relative to optical proximity correction on a production layer
- Optimized pytorch training loop to accelerate neural network training speeds by 4x, cutting model development cycle time from 8 to 2 hours on an A100 GPU
- Optimized OPC convolutional neural network to improve edge predictive accuracy by 2x

### **Graduate Student Researcher**

Carnegie Mellon University; Pittsburgh, PA — Aug 2019–Feb 2024

- Designed and developed protocols to combine machine learning and density functional theory for surface property prediction of heterogeneous catalysts for sustainable energy technologies
- Worked with chemists to design and optimize catalysis experiments and interpret results

# **Projects**

### Ternary surface segregation simulations (○ code )

2023

- Worked with vacuum lab chemists to determine the ability of DFT+ML to predict experimental surface expression of noble metal ternary alloys
- Generated 5000 DFT relaxations of 60-atom slabs with disordered compositions
- Trained a DFT surrogate GNN and ran high-throughput Monte-Carlo simulations across composition space to predict atomic surface composition within ~0.1 across 3 systems

### Cleavage energy transfer learning - (Ocode)

2022-202

- Designed and developed transfer learning protocols for predicting intermetallic cleavage energies across functionals, materials, and simulation settings using foundation models
- Improved regression accuracy of facet energy by 52%; termination classification by 2.4x

#### Design of experiments for hydrogen evolution reaction system -

2019-2021

- Designed Bayesian optimization/active learning loops for nanocatalysis experiments
- Used multifidelity modeling to aggregate ML predictions and DFT and experimental data
- Worked with wet lab chemists to understand and interpret experimental results

### **Education**

Carnegie Mellon University | Pittsburgh, PA | PhD Chemical Engineering | Feb 2024 Georgia Inst. of Technology | Atlanta, GA | BS Chemical Engineering. | Apr 2019