Guangchen Liu

PhD, Materials Engineering | Computational Materials Scientist | DFT, MD, ML

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Profiles

My Portfolio | GitHub | Linkedin

Summary

Computational materials scientist with expertise in **first-principles simulations, molecular dynamics, and machine learning** for accelerated materials design. Experienced in developing **automation pipelines** and **predictive ML models** that integrate DFT, thermodynamics, and active learning to optimize alloy, oxide, and interface performance. Proven record of delivering **open-source software tools** (*HEA-ML*, *Interface-Maker*, *LCO-DOPER*, *HEP-Explorer*) and collaborating across disciplines to advance data-driven materials discovery.

Technical Skills

Modeling & Simulation

DFT (VASP), Molecular Dynamics (MD), ML Potentials (Matlantis), ASE, Pymatgen, HPC Workflow

Machine Learning & Data Science

Python (PyTorch; Scikit-learn; Pyro; Optuna), Active Learning, Bayesian Optimization, Muti-Objective Optimization

Materials Informatics & Thermodynamics

Thermo-Calc, PyCalphad, CALPHAD

Programming & Automation

Python, C#, C++, Markdown, Javascript, Git, Linux Shell, API Development, Workflow Automation

Visualization & Analysis

Matplotlib, Seaborn, Plotly, VESTA, Origin, Pandas, Numpy

Tools & Platforms

VS Code, JupyterLab, Github, PyQt5, Streamlit, Slurm, MS Office

Professional Experience

IMPD Group | Advisor: Prof. Yu Zhong — **2021 - Present**
Research Assistant — Worcester Polytechnic Institute, USA

Ph.D. research focuses on integrating first-principles calculations, molecular dynamics, and machine learning to accelerate the design and discovery of complex oxides, interfaces, and high-entropy materials.

- Developed **ML-accelerated atomic simulation frameworks** integrating neural network potentials and active learning to predict formation energies and diffusion coefficients with DFT-level accuracy.
- Automated **Python-based HPC pipelines** (ASE, Pymatgen, Slurm) for large-scale data generation and analysis.
- Authored and co-authored **9 peer-reviewed papers** and contributed to collaborative projects on energy materials and interface design.
- Designed and deployed **4 open-source frameworks**:
  - **HEA-ML** – a framework combining first-principles calculations and machine learning for phase stability and mechanical property prediction in Al–Co–Cr–Fe–Ni high-entropy alloys.
  - **Interface-Maker** – a lattice-matching and interface-generation tool coupling ML potentials with DFT to model $LaCoO_3$/La_2NiO_4 interfaces, achieving over tenfold efficiency improvement in interfacial energy exploration.
  - **LCO-Doper** – an active-learning framework for dopant optimization in $LaCoO_3$ (LCO), revealing composition–structure–property relationships governing lattice distortion and ionic conductivity.
  - **HEP-Explorer** – a multi-target Bayesian neural network platform for investigating substitutional effects in high-entropy perovskites (HEP), incorporating Pareto-front screening for property trade-offs.

Professional Experience

PPM Group | Advisor: Prof. Lijun Zhang **2018 - 2021**
M.S. Researcher Central South University, China

M.S. work centered on coupling computational thermodynamics with machine learning to optimize aluminum-based casting alloys and understand composition–microstructure–property relationships.

- Developed **Alloy-Supermarket**, an open-source platform that couples **Thermo-Calc** and **machine learning** to design Sc-modified A356 Al–Si–Mg alloys.
- Published **2 first-author papers** and received **Best Paper** and **Best Poster Awards** for research on data-driven alloy design.

Selected Projects

HEP-Explorer **2025**
https://github.com/aguang5241/HEP-Explorer

Tech: Python, Optuna, Pyro (Bayesian NN), icet (SQS), Matlantis, EI, HVI, Pareto Optimization, Streamlit

- Built a **multi-target ML platform** to explore the substitutional effects in high-entropy perovskites (HEPs).
- Applied **Bayesian neural networks** and **Pareto-front screening** to balance stability, distortion, and conductivity metrics.
- Delivered a scalable, **open-source tool** for composition–property mapping and multi-objective optimization.

LCO-Doper **2025**
https://github.com/aguang5241/LCO-DOPER

Tech: Python, PyTorch, Pyro (Bayesian NN), Optuna, Matlantis, EI, Streamlit

- Designed an **active-learning framework** for dopant optimization in $LaCoO_3$ (LCO) perovskites.
- Implemented ML models linking dopant composition, lattice distortion, and ionic conductivity.
- Deployed as an **interactive web application**, enabling fast dopant screening and property prediction.

Interface-Maker **2025**
https://github.com/aguang5241/Interface-Maker

Tech: Python, PyTorch, ASE, Matlantis, Streamlit

- Created an **automated interface-generation and lattice-matching tool** coupling ML potentials with DFT to model oxide interfaces.
- Achieved **10× faster interfacial energy prediction** compared to conventional DFT workflows.
- Built modular APIs for seamless integration into **high-throughput materials simulation pipelines**.

HEA-ML **2024**
https://github.com/aguang5241/HEA-ML

Tech: Python, PyTorch, DFT (VASP), ATAT (SQS), PyQt5

- Developed a **machine-learning framework** integrating first-principles to predict phase stability and elastic properties of Al–Co–Cr–Fe–Ni high-entropy alloys (HEAs).
- Released as an **open-source tool** adopted by collaborators for rapid alloy screening and composition optimization.

Education

Worcester Polytechnic Institute, USA **2021 - Present**
Materials Engineering Ph.D.

Central South University, China **2018 - 2021**
Materials Engineering M.S.

Central South University, China **2014 - 2018**
Powder Materials Science & Engineering B.S.

Awards & Honors

National Science Foundation Scholarship 2023
CALPHAD

Golden Egret Scholarship 2020
Xiamen Golden Egret Special Alloy Co., LTD.

Best Paper Award - Grand Prize 2020
Hunan Education Department

Best Poster Award – First Prize 2020
Graduate School of Central South University

Languages

Mandarin - Native

English - Fluent