Guangchen Liu

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

Worcester, MA, USA +1(774)701-9295 gliu4@wpi.edu

Profiles

My Portfolio | GitHub | Linkedin | Google Scholar | ResearchGate | ORCID

Summary

Ph.D. candidate in Materials Engineering at Worcester Polytechnic Institute, specializing in **machine-learning-accelerated first-principles simulations** for advanced materials design. Research integrates **DFT, molecular dynamics, and active learning** to elucidate structure–property relationships in complex oxides, high-entropy materials, and alloy systems. Developer of multiple **open-source frameworks,** including *HEA-ML*, *Interface-Maker*, *LCO-Doper*, *HEP-Explorer,* and *Masgent* for **data-driven discovery and design of novel materials**.

Research Interests

- **Machine-learning-accelerated atomic simulations** for the discovery and design of complex materials.
- **Defect chemistry, doping, and ionic transport** in perovskite oxides and high-entropy materials.
- **Computational frameworks for interface modeling and stability prediction.**
- **Data-driven alloy design** integrating thermodynamics and machine learning.

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.

Research 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 discovery of complex oxides, interfaces, and high-entropy materials.

- Developed several **machine-learning-accelerated atomic simulation frameworks** integrating ML potentials and active learning to predict structural stability and conductivity with DFT-level accuracy.
- Developed an **AI agent for materials simulation**, automating structure handling, VASP input generation, workflow preparation & analysis, and rapid property prediction.
- Designed and deployed multiple **open-source frameworks** including *HEA-ML*, *Interface-Maker*, *LCO-Doper*, *HEP-Explorer*, and *Masgent*.
- Authored and co-authored **7 peer-reviewed papers** in *High Entropy Alloys & Materials, Materials Today Physics, Materials Today Communication, Journal of Alloys and Compounds*, etc.

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

M.S. work focused 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 integrating Thermo-Calc and machine learning to design Sc-modified A356 Al-Si-Mg casting alloys.
- Authored and co-authored **5 peer-reviewed papers** in *Journal of Materials Science & Technology, Materials Today Communications*, *Journal of Materials Informatics, etc.*

Selected Publications

G Liu, S Yang, Y Zhong. Substitutional Effects at A- and B-Sites in High-Entropy ABO3 Perovskites: Insights from Machine Learning-Accelerated Simulations and Active Learning 2025
Chemical Engineering Journal (Submitted)

G Liu, S Yang, Y Zhong. Unraveling Doping Effects in LaCoO3 via Machine Learning-Accelerated Atomic Simulations and Active Learning 2025
Acta Materiala (Submitted)

G Liu, S Yang, Y Zhong. A Computational Framework for Interface Design Using Lattice Matching, Machine Learning Potentials, and Active Learning: A Case Study on LaCoO3/La2NiO4 2025
Materials Today Physics
https://doi.org/10.1016/j.mtphys.2025.101940

G Liu, S Yang, Y Zhong. High-Entropy Materials Design by Integrating the First-Principles Calculations and Machine Learning: A Case Study in the Al-Co-Cr-Fe-Ni System 2024
High Entropy Alloys & Materials
https://doi.org/10.1007/s44210-024-00041-3

W Yi, G Liu, Z Lu, J Gao, L Zhang. Efficient alloy design of Sr-modified A356 alloys driven by computational thermodynamics and machine learning 2022
Journal of Materials Science & Technology
https://doi.org/10.1016/j.jmst.2021.09.061

G Liu, J Gao, C Che, Z Lu, W Yi, L Zhang. Optimization of casting means and heat treatment routines for improving mechanical and corrosion resistance properties of A356-0.54 Sc casting alloy 2020
Materials Today Communications
https://doi.org/10.1016/j.mtcomm.2020.101227

Selected Projects

Masgent 2025
An AI agent for materials simulation that streamlines DFT workflows and analysis, fast machine-learning-potential (MLP) simulations, and lightweight ML modeling for materials science.
https://github.com/aguang5241/Masgent

HEP-Explorer 2025
An application for analyzing substitutional effects in high-entropy perovskites (HEPs), supporting compositional screening, property prediction, and performance optimization.
https://github.com/aguang5241/HEP-Explorer

LCO-Doper 2025
An application for analyzing dopant effects on LaCoO3 (LCO), supporting composition optimization and material performance enhancement.
https://github.com/aguang5241/LCO-DOPER

Interface-Maker 2025
An application for generating customizable slabs and interfaces for first-principles simulations.
https://github.com/aguang5241/Interface-Maker

HEA-ML 2024
An application for designing Al-Fe-Co-Cr-Ni high-entropy alloys by combining first-principles calculations and machine learning.
https://github.com/aguang5241/HEA-ML

Alloy-Supermarket 2022
An application that integrates computational thermodynamics and machine learning for Sc-modified Al-Si-Mg alloy design.
https://github.com/aguang5241/Alloy-Supermarket

Awards & Honors

National Science Foundation Scholarship Jun 2023
CALPHAD

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

Best Paper Award - Grand Prize Dec 2020
Hunan Education Department

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

Teaching & Mentoring

Major Qualifying Project (MQP) — **Aug 2024 - Dec 2024**
Research Mentor — Worcester Polytechnic Institute, USA

ME 4875 - Introduction To Nanomaterials And Nanotechnology — **Mar 2024 - May 2024**
Teaching Assistant — Worcester Polytechnic Institute, USA

ME 5385 - Metal Additive Manufacturing — **Jan 2024 - Mar 2024**
Teaching Assistant — Worcester Polytechnic Institute, USA

MTE 594-D01 - ST: Applied Machine Learning — **Mar 2022 - May 2022**
Teaching Assistant — Worcester Polytechnic Institue, USA

Professional Activities

- **Peer Reviewer** for *npj Computational Materials*, *Scientific Reports*, *Computational Condensed Matter*, *The Journal of Physical Chemistry*, and other international journals in computational materials science.
- **Member**, *The Minerals, Metals & Materials Society (TMS)*.
- **Conference Organizer**, edited the Technical Program and coordinated meeting logistics and activities for the international *CALPHAD 2023* conference.
- **Conference Presentations and Posters**
  - Oral Presentation | *MS&T 2025*
  - Poster Presentation | *WPI Graduate Research Innovation Exchange (GRIE) 2025*
  - Oral Presentation | *CALPHAD 2023*
  - Oral Presentation | *3rd World Congress on High-Entropy Alloys 2023*
  - Oral Presentation | *MS&T 2022*
  - Poster Presentation | *Gordon Conference 2022*

Technical Skills

Modeling & Simulation

DFT (VASP), ASE, Pymatgen, Machine-Learning Potentials, HPC & Workflow Automation

Machine Learning & Data Science

Active Learning, Bayesian Optimization, AI Agent Development, Neural Network Potentials

Materials Informatics & Thermodynamics

Thermo-Calc, PyCalphad, CALPHAD

Programming & Automation

Python, C#, C++, Linux, Markdown, Git, API Development

Visualization & Analysis

Matplotlib, Seaborn, Ploty, VESTA, Origin, Pandas, Numpy

Tools & Platforms

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

Languages

Mandarin
Native

English
Fluent