JIAYI HUANG

COMPUTATIONAL MATERIALS SCIENTIST

CONTACT

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CORE COMPETENCY

- Data-driven Materials Discovery
- Quantum Computations
- Machine Learning
- Python

LANGUAGES

Chinese

English

PROFESSIONAL SUMMARY

Ph.D. in Materials Science & Engineering at Carnegie Mellon University (expected 2027) specializing in Crystal Structure Prediction (CSP), Density Functional Theory (DFT), and Machine-Learning Interatomic Potentials (MLIPs). Skilled in developing computational workflows that integrate quantum simulations and machine learning to accelerate materials discovery and property prediction.

RESEARCH EXPERIENCE

Graduate Researcher Sep 2023 - Present
Carnegie Mellon University

- *Supervisor: Prof. Noa Marom (noamarom.com).*
- *Adapted CSP workflows to handle cocrystals and flexible molecular crystals using DFT and ML.*

Undergraduate Researcher Mar 2022 - Jul 2023
State Key Lab of Luminescent Materials, China

- *Built ML regression models for photovoltaic efficiency prediction from DFT-derived molecular descriptors; co-authored publication in MGE Advances.*

Undergraduate Researcher May 2022 - Jul 2023
South China Advanced Institute, China

- *Synthesized and characterized nanocomposites for solid-state proton conductors; published in Small.*

Research Intern Jun 2022 - Sep 2022
Université de Montréal, Canada

- *Synthesized and characterized bimetallic electrocatalysts for HMF oxidation at low potentials*

EDUCATION

Ph.D. Materials Science and Engineering Aug 2023 - Present
Carnegie Mellon University

- In addition to core MSE coursework, completed CMU ML courses including Introduction to ML, Introduction to Deep Learning, and Generative AI.

Bachelor, Materials Science and Engineering Sep 2019 - Jul 2023
South China University of Technology

- *GPA: 3.91/4.0; Rank: 1/34*
- *National Scholarship (Top 0.2%, 2020)*
- *Outstanding Undergraduate Thesis Award, SCUT* , 2023