Jianghai Wang

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ABOUT ME

Computational Materials Science, First principles calculation, crystal structure prediction, Machine learning

EDUCATION AND TRAINING

Master's degree
Beihang University [Sep 2022 – Jan 2025]

City: Beijing | **Country:** China | **Website:** www.buaa.edu.cn | **Field(s) of study:** Computational Materials Science | **Final grade:** 3.55/4.00

Bachelor's degree
Xiamen University [Sep 2018 – Jun 2022]

City: Xiamen | **Country:** China | **Website:** www.xmu.edu.cn | **Field(s) of study:** Material Science and Engineering | **Final grade:** 3.25/4.00

PROJECTS

[Aug 2023 – Aug 2024]
Crystal Structure Prediction of Ge-Sb-Te System Based on Genetic Algorithm Utilizing a combination of genetic algorithms and first-principles methods, I conducted crystal structure prediction studies on the Ge-Sb-Te system, a pivotal phase change material system, to uncover its inherent complexities and expand our knowledge of its configuration space.
The objective was to enhance comprehension of this intriguing system and potentially identify novel structures or compositions conducive to phase-change storage applications.

[Jan 2024 – Sep 2024]
Machine learning potential accelerates crystal structure prediction In this work, I have developed a framework combining genetic algorithm, and pre-trained potential, which can effectively locate the ground-state or meta-stable states of the relatively large/complex systems. Utilizing machine learning potentials (e.g., general pre-training potentials CHGNet, MACE, MEG, etc.) as energy evaluators instead of first principles methods can significantly expedite the process of crystal structure prediction and more effectively probe the potential energy surface.

HONOURS AND AWARDS

[Oct 2023] Beihang University
Excellent Student Cadre

[Aug 2023] Beihang University
Academic scholarship

[Aug 2022] Beihang University
Freshman scholarship

[May 2022] Xiamen University
Academic scholarship

DIGITAL SKILLS

Programming
Python / Bash / LaTeX

DFT
VASP / Materials Studio

MD
LAMMPS / ASE / VMD / OVITO

CSP
USPEX / CALYPSO

Others
ATAT / VESTA / Atomate2 / Origin

RECOMMENDATIONS

Name: Prof. Zhimei Sun | group leader
The administrator of ICME
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Name: Dr. Linggang Zhu | supervisor
Master's thesis supervisor in ICME
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