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

1. 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. In this work, ***crossover*** and a variety of ***mutation*** operators are used to improve the sampling efficiency of the algorithm. The energy above hull is used as **Fitness function** for population iteration. After iterations, the candidates then further validated with a carefully considered screening criteria.
2. Given the extensive crystal material database, we can search for new materials through **element substitution** based on **structural prototypes**. I adopted this strategy for the impressive **GeTe-Sb2Te3 pseudo-binary line** of the Ge-Sb-Te system, due to the large number of phase-change storage materials found along it. The overall process is similar to the above work, with a more stringent energy screening criterion due to the prevalence of metastable cubic phases in structures along pseudo-binary line.

The works above is expected 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 DPA-2, CHGNet, MACE, 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 / Pymatgen

MD

LAMMPS / ASE / VMD / OVITO

CSP

USPEX / CALYPSO

Others

ATAT / VESTA / Atomate2 / Phonopy / 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
Email: lgzhu7@buaa.edu.cn