Zixun Wang

wangzx1120@mails.jlu.edu.cn mix142@usask.ca · GPA:3.9/4.0 TOEFL: 108 (R30/L28/S23/R27)

Education

Institute of Physics Chinese Academy of Sciences, Beijing, China 2021 – Present

Undergraduate Student in Yanjici Honor Program, expected 2024

Jilin University (JLU), Changchun, China 2020 – Present

Undergraduate Student in Tangaoqing Honor Program Physics, expected 2024

Research Experience

Metadynamics and Machine Learning University of Saskatchewan, Canada July. 2023 – Present

Summer Intern Professor: Yansun Yao

I have attempted to use machine learning molecular dynamics potentials for Metadynamics simulations to study phase transitions. In comparison to traditional molecular dynamics, this method allows for simulations at a larger scale (around 500,000 atoms). I have already conducted benchmarks on Si and GaN. We hope that it can address the phase transition process of compressing onion carbon into diamond.

One-dimensional Ferroelectric Westlake University, China Dec. 2022 – Present

Research Assistant Professor: Shi Liu

I employed density functional theory (DFT) to obtain a family of stable 1D nanothreads from cutting III-V two-dimensional triatomic layers anti-ferroelectric materials. This is the first predicted one-dimensional anti-ferroelectric structure. These nanothreads exhibit anti-ferroelectric phases, along with radial polarization. The radial polarization can be reversed under the influence of an electric field. This discovery holds significant promise for memory applications, marking a breakthrough in the field of low-dimensional anti-ferroelectrics. The results will be submitted in the form of a research paper.

Ideal Strength Calculation Software Jilin University, China Jan. 2022 – May. 2023

Research Assistant Professor : Hanyu Liu

I have developed software for calculating the ideal strength of materials based on first-principles calculations, building upon the previous work of our research group. This software can compute the ideal strength of materials under arbitrary stress directions and supports simulations with different indenter shapes, such as simulating Vickers hardness. The source code has been uploaded to: https://github.com/Zixun-Wang/MatElastPy . The results are being submitted as a research paper, and a preprint version is available at: https://arxiv.org/abs/2309.01137

Skills

- Programming Languages: Python, shell scripts, C/C++, LaTeX
- Software: VASP, LAMMPS, Quatumn Espresso, Deepmd-kit

Honors and Awards

National Scholarship 2022
University-level outstanding students 2022
University-level outstanding student cadres 2022/2023

Research interests

- Computational Physics/Chemistry : MD and DFT method development, ab-initio calculation, AI for Science