**Cu-Sn Machine Learning Interatomic Potential**

This repository contains a machine learning interatomic potential (MLIP) model for the Cu-Sn alloy system, developed using the **Deep Potential Generator (DP-GEN)** and **DeepMD-kit** frameworks. The trained model is provided as frozen\_model.pb.

Using this DP model, we performed molecular dynamics (MD) simulations to compute the **energy–volume (E–V) curve**, **elastic moduli**, and **phonon spectra** of Cu-Sn compounds. The simulation results show excellent agreement with density functional theory (DFT) calculations, demonstrating that the developed model achieves DFT-level accuracy while maintaining significantly higher computational efficiency.

**Software Used**

* **DP-GEN**: Automated active learning workflow for training interatomic potentials
* **DeepMD-kit**: Neural network potential training package
* **LAMMPS**: Molecular dynamics engine for simulation

**Repository Structure**

├── result/ # MD results: energy–volume curves, phonon spectra

├── Dataset/

│ ├── init\_data/ # Initial dataset used to bootstrap DP-GEN

│ └── training\_data/ # New data added during iterative training

├── frozen\_model.pb # Final trained Deep Potential model

└── report/ # Experimental report and summary