Benchmarking Foundation Machine-Learned Interatomic Potentials for the Elastic Properties of $LiCoO_2$ Battery Cathodes

Nasser Zibaei [1, †], Mohammad Shams [1], Reza Ebrahimi [1]

[1] Department of Chemistry, Faculty of Science, Semnan University, Semnan, Iran
[†] Corresponding author's email: nas.zib334@gmail.com

Abstract

Mechanical stability is a critical factor in the performance and durability of lithium-ion battery electrodes, particularly layered $LiCoO_2$ cathodes, where elastic anisotropy influences their response to mechanical stresses (Cheng2017; Sailuam2023). Recent advances in foundation machine-learned interatomic potentials (MLIPs) offer computationally efficient alternatives to density functional theory (DFT) (Deng2023; Batatia2025).

In this work, we propose a systematic assessment of two pretrained MLIPs, CHGNet and MACE-MP, for predicting the mechanical properties of $LiCoO_2$. The elastic constants, bulk modulus, shear modulus, Young's modulus, and elastic anisotropy will be evaluated using stress–strain calculations and compared with reference DFT results (deJong2015). Particular attention will be given to the accuracy of the predicted elastic tensor and the mechanical response along different crystallographic directions.

To provide a comprehensive comparison, the equilibrium crystal structures will first be optimized using DFT and both machine-learned potentials. Small tensile, compressive, and shear strains will then be applied to calculate the corresponding stress responses. The deviations in elastic constants and derived mechanical properties will be quantified using statistical error metrics. Furthermore, the computational efficiency of each approach will be evaluated to examine the trade-off between prediction accuracy and computational cost.

An additional focus will be placed on the ability of pretrained potentials to capture the intrinsic mechanical anisotropy of layered $LiCoO_2$. Due to its distinctive crystal structure, the mechanical response along the crystallographic c-axis can differ significantly from that within the basal plane (Sailuam2023). Direction-dependent elastic moduli will therefore be analyzed to determine whether CHGNet and MACE-MP can reproduce the anisotropic behavior predicted by DFT. By comparing predictions obtained from identical reference geometries and independently relaxed structures, the contributions of structural optimization errors and elastic response inaccuracies will be distinguished. This analysis will provide further insight into the transferability of foundation MLIPs to mechanically anisotropic battery materials.

This study aims to identify the strengths and limitations of foundation MLIPs in predicting the mechanical behavior of layered battery materials and assess their potential for accelerating computational materials characterization.

References

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