Contribution ID: **68** Type: **Poster**

Exploring the Efficacy of Machine Learning in Interatomic Potentials and Neutron Scattering Spectra Predictions

Tuesday 9 April 2024 18:30 (20 minutes)

Machine learning-based atomic potentials have become instrumental in forecasting the structure and dynamics of diverse materials. These potentials, claiming "ab initio accuracy with the efficiency of classical force field," raise questions about their true generalizability across a broad spectrum of materials. This generalizability, a key factor in extrapolating learned information to new systems, minimizes the need for extensive training data for each material, enhancing efficiency and applicability. To assess these claims, we decided to rigorously test various machine learning-based atomic potentials, calculating structure and lattice dynamics properties for a dozen intriguing systems and comparing results to our own neutron spectra data. In the first part of the talk, we will discuss our findings. In the second part of the presentation, we explore an alternative approach using the Atomistic Line Graph Neural Network (ALIGNN) method to directly predict inelastic neutron spectra without phonon calculations. By training on extensive datasets from the **JARVIS** database, ALIGNN learns intricate patterns and correlations, providing a swift and efficient alternative to traditional simulation methods to predict INS spectra for a large number of systems.

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Session Classification: Posters

Track Classification: MLC