Systematic assessment of various universal machine-learning interatomic potentials

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Abstract
Machine learning-based interatomic potentials have revolutionized materials modeling at the atomic scale, enabling simulations of ab initio quality over significantly larger time and length scales. Recently, several universal machine-learning models have been proposed as "out-of-the-box" solutions, eliminating the need to train and validate specific potentials for each material of interest. In this poster, we review and evaluate four different universal machine learning interatomic potentials (uMLIPs), all based on graph neural network architectures that have demonstrated transferability across different chemical systems. The present evaluation leverages data from both a recent verification study of density-functional theory (DFT) implementations and the Materials Project. This comprehensive assessment aims to guide materials scientists in selecting appropriate models for their specific research challenges, provide recommendations for model selection and optimization, and stimulate discussion on potential areas for improvement in current machine-learning methodologies within materials science.

References

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Figures

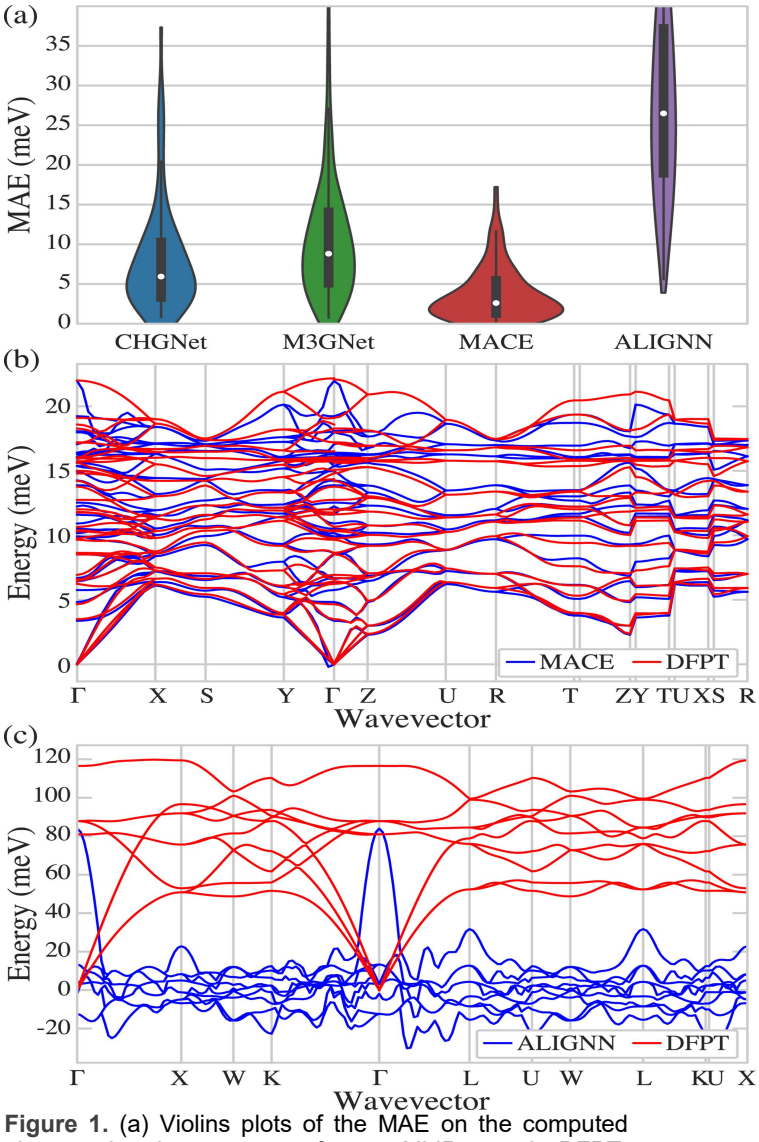

Figure 1. (a) Violins plots of the MAE on the computed phonon band structures from uMLIPs and DFPT. (b) Comparison of the phonon band structures computed with DFPT and MACE for the compound (mp-567744: SrBr2) with the smallest MAE (0.3 meV). (c) Comparison of the phonon band structures computed with DFPT and ALIGNN for the compound (mp-1569: Be2C) with the largest MAE (75.4 meV).