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Potential transferability and the Knowledgebase of Interatomic Models

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ABSTRACT

Empirical (fitted) interatomic potentials are widely used to predict the response of materials and structures in atomistic simulations. The ability of a potential to predict behavior that it was not fitted to reproduce is referred to as its "transferability." Despite the importance of the notion of transferability in selecting an empirical potential for a specific application, it has not yet been rigorously addressed by the materials simulation community. This is now possible due to the forthcoming Knowledgebase of Interatomic Models (https://openkim.org) which promises to serve as an abundant source of predictions of potentials and the corresponding first principles and experimental data for various material properties. Making use of this novel data resource in a cumulative manner, we compare representations of atomic environments as well as nonparametric supervised learning algorithms which can be used to systematically define and predict the transferability of empirical potentials.