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Invited Paper

An Efficient Ensemble Learning Framework for Crystal Structure Classification in Atomistic Simulations

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ABSTRACT

Nowadays, atomistic simulations act as an important means to guide the design of functional materials, while Identifying atoms' structures from simulation trajectories is one crucial first step. In general, traditional methods are only available to certain types of structures, where human knowledge has been well built. To achieve successful classification for new crystal structures, machine learning methods, especially deep-learning based model, appear to be a sound solution, but they typically require large amounts of training data and often have efficiency problems in their retraining for incorporating new information. To address this challenge, here we propose a Lightweight and Extendable Stacked Structure (LESS) classifier, which adopts bond orientational order parameters as input features. Via this ensemble learning approach, our model recognizes a variety of crystal structures, including amorphous, mono, and binary structures, with an over 97% accuracy on our validation data-set, outperforming many current methods even including some deep-learning methods. The model can also conduct probabilistic classification, that aids in the interpretation of atomic structures in complicated environments such as heterogeneous interfaces. Furthermore, when exposed to a completely unknown crystal structure, our framework can incorporate this new knowledge efficiently with generative sampled data from the current model. Overall, the LESS classifier exhibits great potential as an accurate and flexible atomic structure identification tool, featuring high efficiency in both learning and retraining.