On-Lattice Machine Learning Model for Lattice Monte Carlo Simulations of Complex Oxides with First-Principles Accuracy

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First-principles calculation based on the laws of quantum physics has established itself as a powerful tool for predicting materials properties from atomistic structures. However, its high computational cost means that it is rather limited in the ability to cover the combinatorially exploding compositional, structural, and configurational space required for materials design. This has started to change in recent years with the development of machine-learning surrogate models that closely mimic first-principles calculations at a small fraction of the computational cost. Especially, machine learning potentials that reproduce interatomic forces and total energies from given atomic coordinates has been instrumental in enabling large-scale long-time molecular dynamics (MD) simulations with first principles accuracy [1]. Here, we discuss the application of such potential models to lattice Monte Carlo (MC) simulation, which, unlike MD, enables fast equilibration and sampling of atomistic configurations at finite temperature even for slowly relaxing systems. This is especially advantageous for computational prediction of the configurations and physical properties of many-component crystalline systems such as metal alloys and complex oxides. To maximize the efficiency for lattice MC simulation, we propose to train machine learning potentials to predict the total relaxed energy from ideal on-lattice coordinates. This on-lattice model is trained in an iterative manner: an initial (possibly inaccurate) model is used to generate "thermodynamically balanced" MC samples, which are added to the training set if the error is larger than a given threshold. The model training and data set generation using the model is performed iteratively until sufficient accuracy is reached. A python framework for facilitating this process has been implemented in our open-source abICS code [2,3]. In the talk, I will discuss the application of this approach to ion conducting oxides and their interfaces [3,4].

References

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