Development of efficient and accurate machine-learning potentials for the simulation of complex materials

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Many complex materials for energy applications such as heterogeneous catalysts and battery cathode materials have compositions with multiple chemical species and properties that are determined by complex structural features. This complexity makes them challenging to model directly with first principles methods. As an alternative, machine-learning techniques can be used to interpolate first principles calculations. Such machine-learning potentials (MLPs) enable linear-scaling atomistic simulations with an accuracy that is close to the reference method at a fraction of the computational cost. Here, I will give an overview of recent applications of MLPs based on artificial neural networks (ANNs) [1] to the modeling of challenging materials classes, e.g., nanoalloys in solution [2], oxide nanoparticles [3], and amorphous materials [4, 5, 6].

The original multi-species ANN potential formalism [7] scales quadratically with the number of chemical species. This has previously prevented the modeling of compositions with more than a few elements. To overcome this limitation, we have recently developed an alternative mathematically simple and computationally efficient descriptor with a complexity that is independent of the number of chemical species [8,9]. The new methodology has been implemented in our free and open source atomic energy network (aenet) package (http://ann.atomistic.net) [9]. This development creates new opportunities for the modeling of complex materials for example in the field of catalysis and materials for energy applications.

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