**A hybrid approach combining artificial neural network potentials with first-principles calculations**

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Constructing accurate potential-energy surfaces (PES) as a function of atomic position is an important subject in both condensed matter physics and materials science to perform reliable atomic simulations. Recently, artificial neural networks (ANN) have been suggested to be a promising technique for constructing the PES of complicated systems. Reliable ANN potentials have several advantages in terms of efficiency and accuracy compared with other interatomic potentials and can replace first-principles calculations for crystal structure search in which a vast number of configurations should be optimized to find the global minimum. However, for successful application of ANN potentials to crystal structure search, improving its accuracy and choosing proper training sets remain a challenging issue to overcome.

In this work, we propose a hybrid approach combining ANN atomic potentials with first-principles calculations, which improves the efficiency of crystal structure search. We generate high-dimensional ANN potentials for Si using the Behler-Parrinello approach. The weight parameters for the ANN potentials are optimized by using the machine learning technique. For applications to crystal structure search, these ANN potentials are combined with the conformational space annealing algorithm for global optimization. In each generation, we employ the so-called self-learning training in which configurations generated by the conformational space annealing algorithm are used as training sets. Although the self-learning ANN potentials cover a variety of structures, the accuracy of these potentials is still not sufficient to perform the local energy minimization. To remove the residual forces and stresses, first-principles calculations are additionally performed for low-energy configurations prior to sorting configurations for the next generation. Our results show that ANN potentials can be used as an efficient local minimizer with the help of first-principles calculations, greatly improving the crystal structure search for the stable as well as diverse metastable phases with reduced computational costs.