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High-dimensional artificial neural network potentials for boron and its application to searching for new structures WOOHYUN HAN, Department of Physics, Korea Advanced Institute of Science and Technology, IN-HO LEE, 2Korea Research Institute of Standards and Science, KEEJOO CHANG, Department of Physics, Korea Advanced Institute of Science and Technology — The construction of accurate potential-energy surfaces (PES) with respect to lattice parameters and atomic coordinates is an important step for the atomistic simulations of structural phases. Recently, artificial neural networks (ANN) have been suggested to be a promising technique for constructing the PES of complex systems due to advantages in efficiency and accuracy, as compared to interatomic potentials and first-principles calculations. Elemental boron exhibits a variety of allotropes consisting of icosahedra as structural units, which are attributed to the electron deficiency, compared with carbon. Thus, it is a challenging task to generate accurate potentials for boron. In this work, we report high-dimensional ANN potentials for elemental boron, which are generated by the Behler-Parrinello approach. The weight parameters for the ANN potentials are optimized by using the machine learning technique, and training sets are obtained from first-principle calculations. The generated ANN potentials well reproduce the energy vs volume curves, phonon spectrum, and molecular dynamics simulations for several known boron allotropes. We combine the ANN potentials with the conformational space annealing algorithm for global optimization and discuss its applications.

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