Accurate deep neural network potential for predicting properties of solids

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Density Functional Theory is a very versatile tool which allows to compute multiple properties of materials. Nowadays, it is routinely applied for predicting, e.g., binding and cohesive energies of molecules and solid, electronic band structures, vibrational properties at 0K. Nevertheless, as the computational complexity of the DFT calculations scales non-linearly with the system size, the applications are often limited to the systems containing at maximum a few hundreds of atoms. It is therefore difficult to apply DFT for studying, e.g., solids with defects, properties of the materials at finite temperature, dynamical effects. To overcome these issues, the "classical" interatomic potentials are applied. Usually, these potentials approximate the energy of interaction between atoms by some kind of analytical function with the parameters which are adjusted to match experimentally known properties. The main disadvantage of these potentials is the lack of accuracy and transferability. The machine-learning technics provide the way to produce the interatomic potentials which are addressing deficiencies of the "classical" interatomic potentials while staying computationally efficient.

We present an interatomic machine-learning potential trained on DFT calculations using artificial neural networks (ANN). Our algorithm simultaneously trains on the DFT data for energies and atomic forces. This leads to the more efficient utilization of the DFT data as well as an increased accuracy of the potential. Our machine-learning potential is also universal in terms of the size of the system and its chemical composition. We demonstrate its versatility and accuracy via computing various properties of solids and compare the results with direct DFT calculations.