A Fourth-Generation High-Dimensional Neural Network Potential with Accurate Electrostatics Including Non-local Charge Transfer

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Machine learning potentials have become an important tool for atomistic simulations in many fields, from chemistry via molecular biology to materials science. Most of the established methods, however, rely on local properties and are thus unable to take global changes in the electronic structure into account, which result from long-range charge transfer or different charge states. In this work we overcome this limitation by introducing a fourth-generation high-dimensional neural network potential that combines a charge equilibration scheme employing environment-dependent atomic electronegativities with accurate atomic energies. The method, which is able to correctly describe global charge distributions in arbitrary systems, yields much improved energies and substantially extends the applicability of modern machine learning potentials. This is demonstrated for a series of systems representing typical scenarios in chemistry and materials science that are incorrectly described by current methods, while the fourth-generation neural network potential is in excellent agreement with electronic structure calculations.
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