Universität Basel

Research Project

Development of a Neural Network Potential with Accurate Electrostatic Interactions

Third-party funded project

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In recent years, a new generation of interatomic potentials based on machine learning techniques has been introduced. These potentials, which provide a direct functional relation between the atomic positions and the potential-energy, combine the accuracy of electronic structure methods with the efficiency of simple empirical potentials. Because of the absence of system-specific terms they allow to perform extended simulations of a large variety of systems. Most of these potentials rely on atomic properties like energies and charges depending only on the local chemical environments of the atoms. Such local charges are, however, unable to capture long-range charge transfer. This prevents the accurate description of systems in which distant structural features have global effects on the charge distribution in the system. Examples for such systems are semiconductors including defects, polar surfaces of oxides and metal-organic molecules with different possible metal oxidation states. In order to overcome these intrinsic limitations of current machine learning potentials, we propose to combine high-dimensional neural networks with the charge equilibration neural network technique. The resulting new method will be generally applicable to all types of systems, which we will demonstrate by analyzing the potential-energy surfaces of different model systems covering all types of bonding using the minima hopping method.

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