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Four Generations of Neural Network Potentials

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Abstract

A lot of progress has been made in recent years in the development of machine learning potentials (MLP) for atomistic simulations [1]. Neural network potentials (NNPs), which have been introduced more than two decades ago [2], are an important class of MLPs. While the first generation of NNPs has been restricted to small molecules with only a few degrees of freedom, the second generation extended the applicability of MLPs to high-dimensional systems containing thousands of atoms by constructing the total energy as a sum of environment-dependent atomic energies [3]. Long-range electrostatic interactions can be included in third-generation NNPs employing environment-dependent charges [4], but only recently limitations of this locality approximation could be overcome by the introduction of fourth-generation NNPs [5,6], which are able to describe non-local charge transfer using a global charge equilibration step. In this talk an overview about the evolution of high-dimensional neural network potentials will be given along with typical applications in large-scale atomistic simulations.

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