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Lecture ”Four Generations of Neural Network Potentials”

Monday, 13 September 2021 14:15 (1 hour)

A lot of progress has been made in recent years in the development of machine learning (ML) potentials for atomistic simulations [1]. Neural network potentials (NNPs), which have been introduced more than two decades ago [2], are an important class of ML potentials. 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 ML potentials 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 ML potentials [5], which are able to describe non-local charge transfer using a global charge equilibration step. In this talk an overview about the evolution of NNPs will be given along with typical applications in large-scale atomistic simulations.

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[5] T. W. Ko, J. A. Finkler, S. Goedecker, J. Behler, Nature Comm. 12 (2021) 398.

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