Neural Network Potentials for Catalysis

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Interatomic potentials relying on machine learning have become a promising tool for atomistic simulations of complex systems. Neural network potentials (NNP) are an important class of machine learning potentials, and to date four generations of NNPs have been proposed [1]. While the first generation of NNPs has been restricted to small molecules, the second generation extended the applicability of NNPs to high-dimensional systems containing thousands of atoms by constructing the total energy as a sum of environment-dependent atomic energies. Long-range electrostatic interactions can be included in third-generation NNPs employing environment-dependent charges, while the limitations of this locality approximation could be overcome by the introduction of fourth-generation NNPs, 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 a discussion of applications relevant for heterogeneous catalysis.

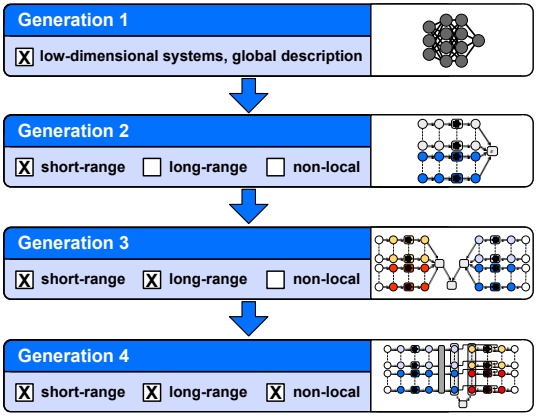

Figure 1: Four generations of neural network potentials.

[1] J. Behler, Chem. Rev., 2021, **121**, 10037, DOI: 10.1021/acs.chemrev.0c00868.