Four Generations of Neural Network Potentials

Jörg Behler
Theoretische Chemie, Institut für Physikalische Chemie,
Georg-August-Universität Göttingen, Germany

A lot of progress has been made in recent years in the development of atomistic potentials employing machine learning (ML). In contrast to most conventional potentials, which are based on physical approximations to derive an analytic functional relation between the atomic configuration and the potential-energy, ML potentials rely on simple but very flexible mathematical terms without a direct physical meaning. Instead, in case of ML potentials the topology of the potential-energy surface is "learned" by adjusting a number of parameters with the aim to reproduce a set of reference electronic structure data as accurately as possible. Due to this bias-free construction they are applicable to a wide range of systems without changes in their functional form, and a very high accuracy close to the underlying first-principles data can be obtained.

Neural network potentials (NNPs), which have first been proposed about two decades ago, are an important class of ML potentials. While first generation NNPs have been restricted to small molecules with only a few degrees of freedom, second generation NNPs [1] relying on local atomic environments are applicable to high-dimensional systems containing thousands of atoms. Long-range electrostatic interactions beyond the local environments can be included based on environment-dependent charges in third generation NNPs [2]. Recently, several limitations of these local approaches have been recognized resulting in the development of the fourth generation of NNPs, which is now able to describe long-range charge transfer and is applicable to systems in multiple charge states [3]. In this talk the basic ideas of NNPs are presented with a special focus on constructing NNPs for high-dimensional condensed systems. Applications for different types of systems, from bulk materials via liquid water to processes at interfaces are presented.

[1] J. Behler and M. Parrinello, Phys. Rev. Lett. 98 (2007) 146401.
[2] N. Artrith, T. Morawietz, and J. Behler, Phys. Rev. B 83 (2011) 153101.
[3] T.W. Ko, J.A. Finkler, S. Goedecker, J. Behler, arXiv:2009.06484.