INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

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High-Dimensional Neural Network Potentials for Atomistic Simulations

The reliability of the results obtained in computer simulations in chemistry, physics and materials science depends on the quality of the underlying potential-energy surface (PES) providing the systems' energy and forces. While the most accurate approach is to use electronic structure calculations like density-functional theory on-the-fly, the resulting ab initio molecular dynamics simulations are restricted to small systems and short simulation times. Consequently, a lot of effort has been invested for several decades in constructing more efficient atomistic potentials of varying form and complexity, which provide a direct functional relation between the atomic positions and the potential energy. Often these potentials are based on physical approximations, which necessarily reduce the accuracy of the PES.

In recent years a paradigm change has taken place by the introduction of machine learning potentials [1], which employ very flexible mathematical functions without a direct physical meaning to represent a reference set of electronic structure data as accurately as possible. While the first ML potentials based on artificial neural networks have been proposed already in 1995 [2], early neural network potentials (NNPs) were only applicable to small systems containing a few degrees of freedom. Nowadays, machine learning potentials have become a practical tool for large-scale simulations based on three central concepts: the introduction of environment-dependent atomic energy contributions [3], the development of rotationally, translationally and permutation invariant descriptors [3], and a systematic way to build reference data sets for training NNPs [4]. In this talk I will provide an overview about the general methodology of high-dimensional NNPs. Remaining challenges and limitations will be discussed, and some typical applications covering interfaces and bulk materials will be presented.

[1] J. Behler, J. Chem. Phys. 145 (2016) 170901.
[2] T. B. Blank, S. D. Brown, A. W. Calhoun, D. J. Doren, J. Chem. Phys. 103 (1995) 4129.
[3] J. Behler, M. Parrinello, Phys. Rev. Lett. 98 (2007) 146401.
[4] N. Artrith, J. Behler, Phys. Rev. B 85 (2012) 04543.