# Understanding Complex Systems
# Using High-Dimensional Neural Network Potentials

*Jörg Behler*
*Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum,*
*D-44780 Bochum, Germany*

The reliability of the results obtained in computer simulations critically depends on the quality of the employed interatomic potentials. While electronic structure methods like density-functional theory provide an accurate description of many systems, the high computational costs severely limit the number of atoms that can be included in these studies. The construction of more efficient but equally reliable interatomic potentials applicable to molecules, solids and surfaces is a frustrating challenge because of the very different types of bonding present for instance in molecules, ionic solids and metals. Many functional forms have been suggested for a variety of systems, but a general-purpose potential suitable for all types of materials is still lacking. In recent years artificial neural networks (NNs) have become a promising new approach to fill this gap and to construct potential-energy surfaces with nearly ab initio quality. NN potentials are numerically very accurate, can be combined with any electronic structure method and, once constructed, allow to perform large-scale molecular dynamics simulations. In this talk the basic concepts of neural network potentials will be outlined, and several examples including solids, nanostructures at surfaces, liquid water and solid-liquid interfaces will be presented to illustrate the applicability of this method to many different types of problems.