O 59: Invited Talk (Jörg Behler)

Time: Thursday 9:30–10:15 Location: H36

Invited Talk O 59.1 Thu 9:30 H36

Interatomic Potentials for Molecules, Solids, and Surfaces Based on Artificial Neural Networks — •Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

The reliability of the results obtained in molecular dynamics simulations strongly 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 limit the system size that can be studied. The construction of more efficient but equally reliable and unbiased interatomic potentials applicable to molecules, solids and surfaces is a frustrating challenge because of the very different types of bonding present for instance in organic molecules, ionic solids and metals. A wide range of functional forms has been suggested for a variety of systems, but a general-purpose potential suitable for all types of applications 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 for many systems. 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. Recent methodical developments aiming at applications to chemical processes at surfaces will be presented. The scope and current limitations of NN potentials will be discussed employing a number of realistic benchmark systems.