I15

Molecular Dynamics Simulations of Solid-Liquid Interfaces with First-Principles Accuracy Using High-Dimensional Neural Network Potentials

Jörg Behler

Theoretische Chemie, Georg-August-Universität Göttingen, Tammannstr. 6, D-37077 Göttingen, Germany

E-mail: joerg.behler@uni-goettingen.de

Understanding the structural and dynamical properties of water at solid-liquid interfaces is essential for unravelling the atomistic details of key steps in electrochemistry, heterogeneous catalysis and corrosion. In recent years, in particular ab initio molecular dynamics simulations (MD) based on density-functional theory (DFT) have contributed significantly to the understanding of these processes. Still, due to their high computational costs, ab initio MD simulations of water interacting with solid surfaces are restricted to comparably small systems and short simulation times. This limitation can be overcome by employing high-dimensional neural network potentials (NNPs), which are constructed from a set of electronic structure data and enable carrying out large-scale simulations with close to first-principles accuracy for a variety of systems.

In this talk first the methodology of high-dimensional NNPs is discussed. Using this method, NNPs for liquid water interacting with metal and oxide surfaces using copper and zinc oxide as benchmark systems are presented. First, the convergence of various properties as a function of the supercell size and the thickness of the water layer in typical slab approaches will be investigated allowing to assess the reliability of conventional ab initio MD simulations. Then, the influence of copper and zinc oxide surfaces on various properties of water will be discussed addressing in particular the local water structure, its density fluctuations, changes in the molecular mobility and the mechanisms of proton transfer events.