**Neural network simulations for aqueous systems**

Matti Hellström* and Jörg Behler

Universität Göttingen, Inst. für Physikalische Chemie, Theoretische Chemie

The potential energy surface (PES) of a system lies at the heart of many problems in materials modeling and computational chemistry. Neural networks, one of the most widely used machine learning techniques, can be parameterized to provide a computationally inexpensive way of predicting the PES, by training to reference data obtained from quantum mechanical calculations. In this way, neural networks can be used together with molecular simulation techniques to model materials in a realistic environment. Here, the strategies for parameterizing the neural networks, as well as some results from simulations for electrolyte solutions and solid/liquid interfaces, are presented.