O 54: Poster New Methods: Theory

Time: Tuesday 18:00–20:00 Location: P2

O 54.1 Tue 18:00 P2

Increasing the Transferability of Machine Learning Potentials by Learning Atomic Properties — •Johann Richard Springborn[1,2], Gunnar Schmitz[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

In the last decade, Machine Learning Potentials (MLPs) have become an established tool for describing potential energy surfaces (PESs) of complex systems. While they significantly speed up the evaluation of the energy and forces in comparison to *ab-initio* methods, they require high-quality reference data for training. Depending on the systems to be studied, generating this training data can become the computational bottleneck and it is of high interest to reduce the number of structures to be computed as well as their complexity. We propose to achieve this goal by training MLPs on atomic properties instead of global quantities such as the system's total energy. This approach aims to increase the transferability of the resulting MLPs to more complicated systems while still utilizing easily accessible reference data.