Molecular Dynamics Simulations of Water Based on High-Dimensional Neural Network Potentials

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Despite the simple geometry of the H_2O molecule, the description of liquid water by atomistic simulations has remained a challenge for many years. High-accuracy *ab initio* methods are computationally demanding; therefore, their applicability is limited to rather small systems and short simulation times. On the other hand, computationally efficient potentials such as simple classical forces fields are not able to capture many interesting phenomena, in particular if they have not been included in the parameterization explicitly. The introduction of Machine Learning Potentials like High-Dimensional Neural Network Potentials (HDNNP) allows to overcome those limitations by combining the accuracy of electronic structure calculations with the efficiency of empirical force fields [Behler2007] and several applications to large-scale simulations of liquid water have been reported to date [Morawietz2016, Daru2022].
The aim of this hands-on workshop is an introduction to High-Dimensional Neural Network Potentials and their application in Molecular Dynamics Simulations. The first part of the tutorial will consist of an analysis of the reference data set, the training and validation of a HDNNP for bulk water. The second part will focus on utilization of obtained potential by running HDNNP-driven Molecular Dynamics Simulations and an analysis of the resulting trajectories. The knowledge of any specific software is not required. However, familiarity with Bash and Python is recommended.

Places: 6
Location of the workshop: Theoretische Chemie II, Gesundheitscampus Süd 25

[Behler2007] J. Behler, M. Parrinello, Phys. Rev. Lett. 98 (2007) 146401.
[Morawietz2016] T. Morawietz, A. Singraber, C. Dellago, J. Behler, PNAS 113 (2016) 8368.
[Daru2022] J. Daru, H. Forbert, J. Behler, D. Marx, Phys. Rev. Lett. 129 (2022) 226001.