Welcome to the Group of Prof. Dr. Jörg Behler

On 1. February 2017 the group has moved to the University of Göttingen

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(previous group photos)

The main focus of the Independent Junior Research Group is the investigation of chemical reactions at solid surfaces. We are particularly interested in the individual reaction steps in heterogeneous catalysis. This work is partially carried out in the framework of the collaborative research center "Metal-Substrate Interactions in Heterogeneous Catalysis" (SFB558). Here we are studying the structural and dynamical properties of metal clusters at oxide surfaces and their role in the catalytic process. Further, we are trying to understand the formation principles of complex adsorbate structures of organic molecules at metal surfaces and the possible influence of organic superstructures in directing heterogeneous catalysis.
We are also interested in the properties of materials under extreme conditions like high-pressures and temperatures. An example is the investigation of pressure-induces phase transitions in crystalline solids. For this purpose, we have recently developed an efficient method for crystal structure predicition by combining the metadynamics approach (A. Laio, and M. Parrinello, Proc. Nat. Acad. Sci. 99, 12562 (2002); R. Martonak, A. Laio, and M. Parrinello, Phys. Rev. Lett. 90, 75503 (2003)) with a high-dimensional Neural Network potential (J. Behler, and M. Parrinello, Phys. Rev. Lett. 98, 146401 (2007)).
We employ a variety of methods like molecular dynamics and metadynamics simulations to study these processes. The reliability of the results obtained in atomistic simulations strongly depends on the accuracy of the underlying potentials. Due to the large system size required to address many interesting questions, density-functional theory is the most important electronic structure methods in our studies. Still, long simulations of large systems can be very time-consuming, if they are based directly on density-functional theory. A central topic of our group is therefore the development of new methods to represent potential-energy surfaces using artificial Neural Networks.
These methods are also employed for the study of solvation effects in the context of the research focus Solvation Science@RUB.

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