Universität Basel

Research Project

Structure and dynamics of materials based on advanced electronic structure calculations

Third-party funded project

Project title Structure and dynamics of materials based on advanced electronic structure calculations
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In atomistic simulations the positions of all the involved atoms are individually known. In this way the structure as well as the dynamics of molecular systems can be studied and understood in depth. A prerequisite for such atomistic simulations is the availability of a high quality potential energy surface and methods to explore it efficiently. Potential energy surfaces calculated on the density functional level are usually considered to be state of the art, even though their accuracy is not sufficient in numerous cases. In this project several key aspects of atomistic simulations will be addressed. Based on our recently developed methods to navigate in the configurational space, the efficiency of our structure prediction schemes will be further improved and its applicability enlarged. In addition we will deduce from our exploration of the potential energy surface not only structural but also dynamic properties. Improved density functional methods will be implemented to give higher accuracy potential energy surfaces and consequently improved predictability for atomistic simulations. We will work both on the validation of methods within mainstream density functional schemes as well as on some non-standard approaches inspired by quantum chemistry methods. For some specific systems, machine learning based force fields will be constructed that are not only highly accurate but also orders of magnitude faster to evaluate than potential energy surfaces resulting from density functional calculations. All these developments will allow to find new materials with useful properties faster and to predict their properties with higher reliability. In particular we will apply these methods to study molecular crystals and cluster assembled materials.

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Add documents

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