Universität Basel

Research Project

Towards Quantifying the Synthesizability of Materials

Third-party funded project

Project title Towards Quantifying the Synthesizability of Materials
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The discovery of new materials is an essential ingredient for technological progress. It is generally agreed upon that simulation methods can make important contributions to this field and extensive research activities are under way worldwide. In this context unbiased structure prediction methods have revealed a large number of possible structures for numerous materials. However only a relatively small fraction of these structures can be found in nature or can be synthesized in the laboratory. This observation poses fundamental and technological challenges. One would like to understand whether the unobserved structures can for some hitherto unknown fundamental reason not exist or whether simply the correct synthesis recipe has not yet been found. If they can not exist, synthesis should not be tried for these materials. If they may exist, simulation could give guidance to synthesis efforts. Since a time resolved atomistic simulation of the actual nucleation and growth processes occurring during synthesis is not feasible in connection with a high-accuracy description of the potential energy surface, we will use concepts from thermodynamics to predict the final structure without following the relevant processes in time. In this context, it will be necessary to develop much more efficient methods to calculate free energies. To understand the behavior of the free energy at formation conditions requires developing improved methods to calculate this quantity at high temperatures, where the harmonic approximation breaks down. To obtain the correct energetic ordering at room temperature, it is frequently necessary to include nuclear quantum effects into the free energy calculations. Applying some of the latest mathematical tools, we will develop novel algorithms that are considerably more powerful than the existing ones. Finally we will also search for new quantities that can be obtained from the potential energy surface at affordable numerical cost and that contain relevant information about the synthesizability of a material. All these new methods should then finally allow to directly assess the synthesizability of a material. The new methods will be used for several materials that have potential applications in energy production and storage. Preferentially materials will be used that have already been studied in the group and for which fast machine learning force fields will be available when the project starts.

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