Hydrogen Storage in High Entropy Alloys

Genetic Algorithm and ML-NEB

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Hydrogen related technologies are getting more attention again in the past months. Just recently, Germany and the European Union decided to follow their new “hydrogen strategies” for a clean and environmental friendly future. [1,2] Hydrogen has a strong potential as an alternative fuel with zero CO_2 emission. Still, an open question to most of hydrogen related technologies is how to store the hydrogen efficiently and safe. In this context, metal hydrides have been widely studied and especially so-called high entropy alloys (HEAs) were used for hydrogen storage and showed a superior storage capacity compared to other metal hydrates. [3-6] Many studies for different metal compositions have been experimentally performed, but still the question about the reason for this high storage capability could not been answered. Since the materials are called high entropy alloys, most studies dedicate the properties of the HEAs to entropic effects. We on the other hand assume, that electronic effects might be responsible for favorable hydride phase formation. In a previous study, we found that due to micro strain and due to differences in electronegativity the ligand effect might play a critical role for binding and reaction barriers in alloy materials.[7] Similar effects could play an important role in HEAs and lead to local hydrate formation at electronically favorable sites. This raises the question, whether a HEA is needed to create an alloy with high hydrogen storage capacity, or whether additionally alloys with less than five different element types (one of the definitions of HEAs) will be able to show similar hydrogen storage capacity.

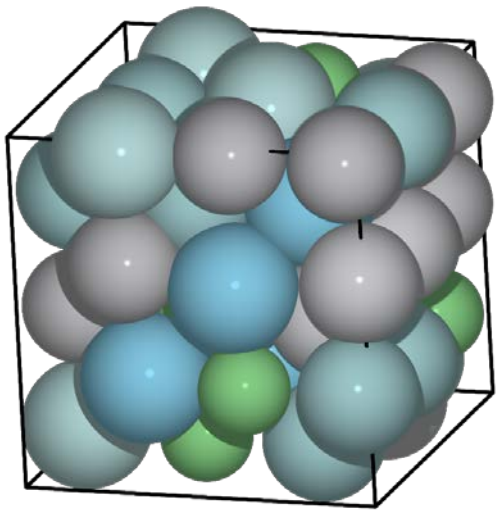

Figure 1: BCC cell of a high entropy alloy containing 54 atoms of six different elements

In this project we will determine the reason for the special stability of the hydride phases in the HEA. Therefore, we will use a genetic algorithm to determine most stable phases in the material. In addition, we will use nudged elastic band calculations based on an on-the-fly created machine learning potential to investigate migration pathways through the material. A deeper look into the electronic structure of the most stable phases of the HEA hydrides will help us to understand the extraordinary properties of this class of materials. In addition, we will be able to formulate new design principles for alloy based hydrogen storage materials.

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