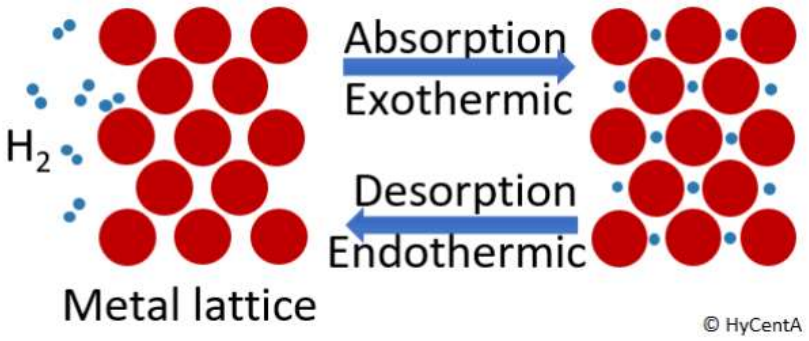
Machine learning methods for predicting storage properties of material-based hydrogen storage

Description

Due to hydrogen's low density at ambient conditions, efficient storage remains an open issue. Currently hydrogen is typically stored compressed to high pressures (CGH2) or in its liquid form (LH2). While CGH2 requires compression power, has a relatively low volumetric energy density and poses an increased safety risk due to elevated pressures, LH2 requires significant energy for liquefaction at low temperatures of 20 K.

An alternative method for hydrogen storage is material-based storage, offering high potential volumetric storage densities at near-ambient conditions. Different material group such as metal hydrides, metal-organic frameworks and carbon-based materials are studied. Due to the high number of possible material permutations, investigating the storage properties solely by experimental methods is not feasible. The use of machine learning (ML) methods can thus aid the pre-selection of promising material candidates.

The thesis aims to (1) research and select suitable ML methods, (2) train the model based on existing material data, and (3) demonstrate the model accuracy via comparison with the validation data set.



Work Packages

- Literature research on existing ML methods for predicting material properties (1 month)
- Definition of data features and generation of training data for ML based on existing material databases (1,5 month)
- Implementation of ML model and demonstration of model accuracy with validation set (2,5 months)
- Written thesis (1 months)

- **Start**: immediately
- **Duration**: approx. 6 months
- **Paid Master Thesis**
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