Designing New Materials for Ammonia Storage Using Density Functional Theory and Genetic Algorithms

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ABSTRACT:

Metal halide ammines, e.g. Mg(NH3)6Cl2 [1] and Sr(NH3)8Cl2 [2], can reversibly store ammonia, with high volumetric hydrogen storage capacities. The storage in the halide ammines is very safe, and the salts are therefore highly relevant as a carbon-free energy carrier in future transportation infrastructure. The so far known compounds, are not optimal because they release the ammonia in several steps and generally at too high temperatures. In this project we are searching for improved mixed materials with optimal desorption temperatures and kinetics, optimally releasing all ammonia below 100 °C in as few steps as possible.
The stored energy can be released by using fuel cells, which can either be run directly on ammonia in a high temperature SOFC, in a direct ammonia fuel cell (DAFM) operating at intermediate temperatures, or be decomposed, and the hydrogen can be used in a low temperature PEMFC, which is a much more mature technology [3].
We apply Density Functional Theory, DFT, calculations on mixed compounds selected by a Genetic Algorithm (GA) [4], relying on biological principles of natural selection. The GA is evolving from an initial (random) population and selecting those with highest fitness, a function based on e.g. stability, release temperature, storage capacity and the price of the elements. The search space includes all alkaline earth, 3d and 4d metals in combination with chloride, bromide or iodide, and mixtures thereof. In total the search space consists of millions of combinations, which makes a GA ideal, to reduce the number of necessary calculations. We are screening for release from either a hexa or octa ammine, and we have found promising candidates, which will be further investigated – both computationally and experimentally.

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KEYWORDS: Indirect Hydrogen Storage - Ammonia Storage - Metal Halide Ammines
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