Computational Search for Improved Ammonia Storage Materials

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Metal halide ammines, e.g. Mg(NH3)6Cl2 and Sr(NH3)8Cl2, 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. In this project we are searching for improved mixed materials with optimal desorption temperatures and kinetics, optimally releasing all ammonia in one step.

We apply Density Functional Theory, DFT, calculations on mixed compounds selected by a Genetic Algorithm (GA), 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 thousands of combinations, which makes a GA ideal, to reduce the number of necessary calculations. We are screening for a one step release from either a hexa or octa ammine, and we have found promising candidates, which will be further investigated – both computationally and experimentally.