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Peter Bjerre Jensen[1]*, pbjen@dtu.dk, Steen Lysgaard*[1]*, Ulrich Quaade*[2]*, Tejs Vegge*[1]*. (1) DTU Energy Conversion, Technical University of Denmark, Kgs Lyngby, Denmark, (2) Amminex A/S, Søborg, Denmark*

Metal halide ammines, e.g. $Mg(NH_3)_6Cl_2$ and $Sr(NH_3)_8Cl_2$, 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. In this project we are searching for improved mixed materials with optimal desorption temperature 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, e.g. stability, release temperature and storage capacity. The search space includes all alkaline, alkaline earth, 3d and 4d metals and the four lightest halides. In total the search space consists of almost two million combinations, which makes a GA ideal, to reduce the number of necessary calculations.

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