Metal halide ammines, e.g. Mg(NH3)6Cl2 and Sr(NH3)8Cl2, can reversibly store ammonia, with high volumetric hydrogen storage capacities. In this project we are searching for improved mixed materials with optimal desorption temperature and kinetics. We apply 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, giving in total almost two million combinations.