Accelerated DFT-Based Design of Materials for Ammonia Storage

Future energy carriers are needed in order to lower the CO2 emissions resulting from the burning of fossil fuels. One possible energy carrier is ammonia, which can be stored safely and reversibly in metal halide ammines; however, the release often occurs in multiple steps at too high temperatures. Therefore, there is a need for new materials, releasing the ammonia in a narrow temperature interval. To search for new mixed metal halide chlorides, we use DFT calculations guided by a genetic algorithm (GA) to expedite the search, as the defined search space allowing up to three different metals contains more than 100,000 different structures. Here, we search for materials releasing the ammonia between 0 and 100 °C, a temperature range suitable for system integration with low-temperature polymer electrolyte membrane fuel cells (PEMFC). The efficiency of the implemented algorithm is verified by three trial runs capable of finding the same optimal mixtures starting from different random populations, testing <5% of the candidates. Some of the best candidates are already confirmed experimentally, and others offer a record high, accessible hydrogen capacity exceeding 9 wt %. Among the identified materials is the first known high-capacity ternary metal halide ammine, which we have subsequently synthesized and confirmed the ammonia storage properties using temperature-programmed desorption (TPD).

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