

Technical University of Denmark



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

Jensen, Peter Bjerre; Lysgaard, Steen; Quaade, Ulrich J.; Vegge, Tejs

*Publication date:*  
2014

[Link back to DTU Orbit](#)

### *Citation (APA):*

Jensen, P. B., Lysgaard, S., Quaade, U. J., & Vegge, T. (2014). Designing New Materials for Ammonia Storage Using Density Functional Theory and Genetic Algorithms. Abstract from International Discussion on Hydrogen Energy and Applications, Nantes, France.

**DTU Library**  
Technical Information Center of Denmark

---

### **General rights**

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

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

P.B. Jensen <sup>1</sup>, S. Lysgaard <sup>1</sup>, U. Quaade <sup>2</sup>, T. Vegge <sup>1</sup>

<sup>1</sup>DTU Energy Conversion - Kgs. Lyngby (Denmark)

<sup>2</sup>Amminex Emmissions Technology - Søborg (Denmark)

---

### ABSTRACT:

Metal halide ammines, e.g. Mg(NH<sub>3</sub>)<sub>6</sub>Cl<sub>2</sub> [1] and Sr(NH<sub>3</sub>)<sub>8</sub>Cl<sub>2</sub> [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.

### References :

- [1] Sørensen RZ, Hummelshøj JS, Klerke A, Reves JB, Vegge T, Nørskov JK, et al. Indirect, reversible high-density hydrogen storage in compact metal ammine salts. *J Am Chem Soc* 2008;130:8660–8.
- [2] Lysgaard S, Ammitzbøll AL, Johnsen RE, Norby P, Quaade UJ, Vegge T. Resolving the stability and structure of strontium chloride amines from equilibrium pressures, XRD and DFT. *Int J Hydrogen Energy* 2012;37:18927–36.
- [3] Klerke A, Christensen CH, Nørskov JK, Vegge T. Ammonia for hydrogen storage: challenges and opportunities. *J Mater Chem* 2008;18:2304–10.
- [4] Lysgaard S, Landis DD, Bligaard T, Vegge T. Genetic Algorithm Procreation Operators for Alloy Nanoparticle Catalysts. *Top Catal* 2013. DOI:10.1007/s11244-013-0160-9

**KEYWORDS:** Indirect Hydrogen Storage - Ammonia Storage - Metal Halide Ammines  
Density Functional Theory - Genetic Algorithms.

---