Designing mixed metal halide ammines for ammonia storage using density functional theory and genetic algorithms - DTU Orbit (04/11/2019)

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Metal halide ammines have great potential as a future, high-density energy carrier in vehicles. So far known materials, e.g. Mg(NH₃)₆Cl₂ and Sr(NH₃)₈Cl₂, are not suitable for automotive, fuel cell applications, because the release of ammonia is a multi-step reaction, requiring too much heat to be supplied, making the total efficiency lower. Here, we apply density functional theory (DFT) calculations to predict new mixed metal halide ammines with improved storage capacities and the ability to release the stored ammonia in one step, at temperatures suitable for system integration with polymer electrolyte membrane fuel cells (PEMFC). We use genetic algorithms (GAs) to search for materials containing up to three different metals (alkaline-earth, 3d and 4d) and two different halides (Cl, Br and I) – almost 27000 combinations, and have identified novel mixtures, with significantly improved storage capacities. The size of the search space and the chosen fitness function make it possible to verify that the found candidates are the best possible candidates in the search space, proving that the GA implementation is ideal for this kind of computational materials design, requiring calculations on less than two percent of the candidates to identify the global optimum.

General information
Publication status: Published
Organisations: Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic Scale Materials Modelling, Department of Physics, Amminex Emissions Technology A/S
Contributors: Jensen, P. B., Lysgaard, S., Quaade, U. J., Vegge, T.
Pages: 19732-19740
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 16
ISSN (Print): 1463-9076
Ratings:
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.29 SJR 1.771 SNIP 1.231
Web of Science (2014): Impact factor 4.493
Web of Science (2014): Indexed yes
Original language: English
Electronic versions:
Jensen_2014_PCCP_DesigningMixedMetalHalides_DFT_GA.pdf
DOIs:
10.1039/C4CP03133D

Bibliographical note
© the Owner Societies 2014. Open Access article
Source: FindIt
Source ID: 269736514
Research output: Contribution to journal › Journal article – Annual report year: 2014 › Research › peer-review