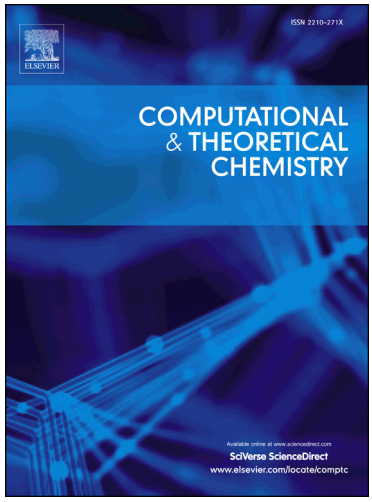

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Cation/anion dependence of metal ammine borohydrides/chlorides studied by *ab initio* calculations

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Abstract

Ammonia (NH_3), which contains about 18 mass% of hydrogen, is regarded not only as one of the most promising hydrogen storage materials but also as an efficient carbon-free energy carrier which can be directly used by *e.g.* high-temperature solid oxide fuel cells. For the development of the NH_3-based sustainable society, it is important to improve NH_3 storage technologies. In this paper, we have studied the microscopic properties of NH_3 absorption in metal borohydrides and metal chlorides by *ab initio* calculations. We have revealed that there is a systematic cation dependence in the NH_3 absorption properties of such materials, and the properties of NH_3 absorption are mainly governed by NH_3-cation interactions and NH_3-anion repulsions.

Keywords: ammonia storage, hydrogen storage, ab initio, microscopic property

1. Introduction

The development of a carbon-free sustainable society is one of the most important tasks for the human beings, and the society in which energies are generated from renewable energy sources and are stored and transferred in hydrogen (H_2) is regarded the most promising answer for this task.

Ammonia (NH_3) can be regarded as one of the most promising hydrogen storage materials since it contains about 18 mass% of hydrogen atoms and can be liquefied at about 1 MPa. We can obtain H_2 molecules from NH_3 by thermal decompositions or chemical reactions. For the latter, H_2 molecules are easily obtained from MH-NH_3 system (MH: alkali metal hydride) [1, 2], and the hydrogen desorption property of this system depends on the ionicity of alkali

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