

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Effect of Mg Doping in NaAlH₄ RAJEEV AHUJA, University of Uppsala, SA LI, Virginia Commonwealth University, C. MOYSES ARAUJO, University of Uppsala, PURU JENA, Virginia Commonwealth University — First principles calculations based on density functional theory have been carried out to search for suitable catalysts that can lower the hydrogen desorption temperature from sodium alanate (NaAlH₄). We focus here on the possibilities of doping Mg in bulk sodium alanate. The result shows that Mg prefers to occupy the Na site and weakens the covalent bond between Al and H. The energy needed to remove a hydrogen atom from (Mg,Na)AlH₄ is found to be significantly lower than that from NaAlH₄. The effect is similar to Ti doping which is supposedly the best catalyst found to date for hydrogen desorption from sodium alanate. Furthermore, the Mg doping is shown to promote the formation of Na vacancy which in turn plays an important role in the hydrogen desorption process.

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Date submitted: 23 Nov 2004

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