A cluster density functional theory study of the interaction of the hydrogen storage system NaAlH$_4$ with transition metal catalysts

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I

A Ti atom added to the surface of NaAlH$_4$ preferably substitutes a lattice Na near the surface, when using the NaAlH$_4$ cluster with Ti adsorbed as the reference system and keeping the substituted atoms within the model (Chapter 3 of this thesis).

II

Ti$_2$ prefers to adsorb as atomic Ti rather than as a Ti$_2$ above Na sites, with the Na atoms being displaced towards the subsurface region. Ti is more stable in the subsurface region of the NaAlH$_4$ than on the surface, and its exchange with Na is preferred. Almost equally stable is the exchange with one Na and one Al, as long as the resulting structure contains a direct Ti-Ti bond (Chapter 4 of this thesis).

III

TiH$_2$ adsorbs on the surface above a Na site, pushing the Na atom subsurface. However, exchanging the whole TiH$_2$ unit with the subsurface displaced Na atom is more favorable (Chapter 5 of this thesis).

IV

A key difference between Ti, Zr, and Sc on the one hand, and Pd and Pt on the other hand is that exchange of the Ti, Zr and Sc atoms with a surface Na ion, whereby Na is pushed on to the surface, is energetically preferred over surface absorption in an interstitial site, as found for Pd and Pt. This explains why Ti, Zr and Sc are good catalysts for release of hydrogen, and Pd and Pt are not good catalysts (Chapter 6 of this thesis).
The release and re-uptake of H\textsubscript{2} from NaAlH\textsubscript{4} can be made reversible by adding a catalyst like Ti.


Experiments show that partial decomposition of undoped NaAlH\textsubscript{4} particles is possible if the particles are very small (nano-sized), the decomposition starting at low temperature.


Traditional hydrogenation catalysts like Pd and Pt are poor catalysts for hydrogen release from NaAlH\textsubscript{4}.


There are experiments that suggest Ti to be present in NaAlH\textsubscript{4} itself.


Our universe is a book. At each era of human life, a new discovery appears that adds a new paragraph to this book.

Helping poor people should not only consist of giving them food to eat. Giving them the opportunity to perform research and to learn about science is also important.