Hydrogen Storage For Fuel Cells - A Density Functional Theory Study of Hydrogen Adsorption on Aluminum Clusters

Researchers from Accelrys have carried out a study of hydrogen adsorption by Aluminum clusters, a promising candidate for fuel cell hydrogen storage devices.

The simulations revealed that a lot of H atoms can be adsorbed easily on the surface of the Al clusters.

These findings are important because light metals such as Aluminum are inexpensive and can store large amounts of hydrogen - factors that are crucial in fuel cell design.

Hydrogen storage is a crucial issue in fuel cell design and application - a safe, compact, and inexpensive system that is capable of storing a relatively large amount of hydrogen is highly desirable. Many light metals, e.g. magnesium and Aluminum, show promise for hydrogen storage devices owing to their potential high storage densities and safe endothermic hydrogen release.

However, the experimental study of the structure of metal clusters is problematic due to high reactivity. It is important to understand cluster size and hydrogen-site specific effects in order to provide a contribution to a unified description of the bridging between the properties of clusters, nanowires, and cluster crystals.

In this study, researchers from Accelrys,[1] using MS Modeling's $DMol^3$, simulated the interaction of both hydrogen atoms and hydrogen molecules with the surface of an Al_{13} cluster. Optimized and and transition state (TS) structures were obtained for $Al_{13}H_n$ (n = 1-12) clusters.

According to jellium model, the Al_{13}^- anion, having a complete outer shell of electrons, should be more stable than its neutral counterpart, Al_{13}. The simulations revealed this to be the case - the anion being 2.75eV lower in energy than the neutral ground sate. It was also found that the Al_{13}^{2-} anion is also more stable than the neutral one. This finding shows that the Al_{13} cluster can favor, from an electronic point of view, the surface adsorption of more than one hydrogen atom.

The optimized structures of three different isomers of the $Al_{13}H$ cluster with the hydrogen atom being adsorbed in different positions on the cluster surface were obtained and studied. The transition states were also obtained.

Structures with two or more hydrogen atoms adsorped on the cluster surface were also investigated.

It was found that:

- Hydrogen can be adsorped on the Al_{13} cluster surface without crossing a potential barrier. However, the binding energy was not high enough to dissociate the hydrogen molecule (the hydrogen molecule being repelled by the cluster surface)
- The $Al_{13}H$ cluster has three different stable minima with the hydrogen atom being attached to one Al atom, being displaced between two Al atoms and being displaced between three Al atoms. The most stable isomer is with hydrogen atom attached to one Al atom. The most stable isomer leads to significant distortions of the cluster.
- With the increase of the number of hydrogen atoms adsorped on the Al_{13} cluster surface the distortion is reduced and the binding energy with small fluctuations does not change.

Al clusters of different sizes, Al nanowires, and Al cluster crystals can be considered as potential materials for hydrogen storage devices.[2,3]

References

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