Storage Of Hdrogen In Transition Metal Decorated Carbon Nanostructures

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One key issue for the advancement of fuel-cell technologies is the development of safe and inexpensive ways of storing hydrogen aboard vehicles. Currently, a lot of effort is being devoted to engineering nanomaterials that are required to dissociate H_2 molecules into H atoms and reversibly absorb hydrogen molecules at ambient conditions. Much work has focused on carbon-based materials such as nanotubes, and metal hydrides such as alanates. It is found that, while the hydrogen-carbon interaction is too weak for hydrogen storage at ambient conditions, the metal-hydrogen interaction is too strong for fast hydrogen release at moderate temperatures.

Guided by our own work on Ti-doped sodium alanates [1], we have found a way to overcome this difficulty by forming artificial metal-carbide-like structures on single-wall carbon nanotubes (SWNT) [2] and fullerenes [3], which we have used as model systems to prove the new concept. From accurate first-principles calculations, we have shown that a single Ti atom adsorbed on a SWNT or C_{60} molecule can strongly bind up to four hydrogen molecules. At large Ti coverage, these idealized systems can store H_2 molecules up to 8wt.%, exceeding the commonly accepted minimum requirement of 6wt.% for practical applications. Further, these systems are not expected to suffer from the low H_2 absorption and desorption kinetics that hampers the use of other storage media (e.g. complex hydrides) in applications. We are currently extending our investigations to more realistic nanostructured carbons in order to determine whether this concept for hydrogen storage remains valid and identify metals that overcome some of the experimental difficulties found when Ti is used (i.e., oxidation and segregation).

References:

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