Nanotubes: A Confinement Space to Store and Activate Molecules

B. Tangour*

Preparatory Institute for Engineers Study, Université de Tunis El Manar, Tunisia

*Author for correspondence e-mail: baha.tangour@gmail.com

Efficient use of hydrogen as a clean energy source requires two challenges, *a priori* connected by a paradox. Indeed, it is not sufficient to confine the hydrogen within a container or a material, but it is necessary to release it easily in order to facilitate its reactivity. On the other hand, we cannot separate the hydrogen storage from the catalysis process needed to operate a fuel cell.

To meet these objectives, we have undertaken some studies on the confinement of dihydrogen molecule in various carbon nanotubes. They differ in their chirality and diameter. Our study involved low diameters single-wall nanotubes. We were able to mark different rings for each tube. The first, established from the outer wall, is a space under control of carbon atoms chemical reactivity. The second concerns the stabilizing influence of van der Waals forces. Between those two regions, there is a space under the control of the repulsive part of the van der Waals interactions. The existence of the latter space allows interpreting the diffusion acceleration of liquids or ions for a particular diameter of the nanotube. The hydrogen stored under certain conditions, is activated and would be better prepared for chemical reactivity.

On the other hand, hydrogen fuel cells often use platinum as a catalyst for dissociating the dihydrogen molecule. In order to replace this catalyst, we studied the ability of titanium dioxide nanotubes to catalyze the formation of H_2 from water and store it for use in a continuous flow.

The hydrogen can be also stored as hydrides but the problem lies in its subsequent release. We studied then the possibility of storing the hydrogen in the channels formed by some nanostructured hydrides as IrH_3.

All studied methods allow manufacturing, store and releasing large quantities of dihydrogen promoter making their industrial use.

All calculations have been performed by Gaussian 09 using the B3LYP and CAM-B3LYP functionals.