ON MOLECULAR HYDROGEN ADSORPTION ON THE EXTERNAL SURFACE OF CARBON NANOTUBES

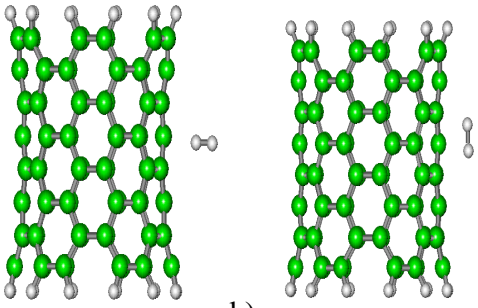
Zaporotskova I.V., Lebedev N.G., Zaporotskov P.A.
Volgograd State University, University Avenue, 100, Volgograg, 400062, Russia
* *E-mail: irinaz@rbcmail.ru*

Introduction

It is known that some substances, including carbon nanotubes [1 - 3], have being absorbing significant amount of hydrogen on mass or volume unit. Such materials are perspective as fuel elements for vehicles. And the use of nanotubes in quality hydrogen sorption materials will allow to lower considerably gross weight of system by weight reduction of a sorbent (in this case carbon).

Results and discussion

Semi-empirical researches of molecular hydrogen adsorption on an external surface of carbon nanotube (6, 6) and at the presence of the catalyst-hydrogen atom, have been carried out. The hydrogen molecule has been placed in the central part of nanotube molecular cluster to reduce the influence of boundary effects (Fig. 1).



a) b)

Fig. 1. The (6, 6) nanotube cluster with molecule H_2:
a) The case of the arrangement of molecule H_2 perpendicularly to nanotube surfaces;
b) The case of the arrangement of molecule H_2 in parallel nanotube surface.

As a whole 12 most probable ways of H_2 adsorption on the external surface of the tube have been investigated: 4 variants for case of the arrangement of molecule perpendicularly to nanotube surfaces and 8 variants for case of the arrangement of molecule in parallel nanotube surface. It has been found that during the attack of nanotube surface the molecule H_2 breaks up to two atoms, each of which is adsorbed on the nanotube surface.

As a rule in hydrogen gas except for molecules some amount of atomic hydrogen is present. Therefore it has been investigated the hydrogen molecule adsorptions at the presence of sorbed atomic hydrogen. The cases of the arrangement of molecule H_2 perpendicularly and parallel to nanotube surfaces have been investigated. In all variants H_2 settled down above the same atom of carbon of the central part of the cluster. The hydrogen atom settled down consistently over each carbon atom on nanotube perimeter (fig. 2). It has been found that at the presence of atom H the hydrogen molecule did not lose the integrity. Curves of potential energy of adsorption complexes «nanotube - molecule H_2 - atom H» have been constructed and adsorption energies of molecule H_2 have been calculated (fig. 3).

Conclusions

It has been found that during the attack of nanotube surface the molecule H_2 breaks up to two atoms H, each of which is adsorbed on the nanotube surface, on the bonding carbon atoms C-C. That is the molecular hydrogen adsorption on a surface single wall carbon nanotube without additional influence on the system is impossible.

The research of the simultaneous adsorption of hydrogen molecule on tube surface at the presence of the catalyst (hydrogen atom) - has allowed to make a conclusion that H_2 adsorption on carbon nanotube surface without the dessociation of the molecule is possible only under condition of simultaneous presence of atomic hydrogen acting in a role of the catalyst of the process.

Acknowledgements

The work has been supported by Russian Foundation for Basic Researches (project 04-03-96501).

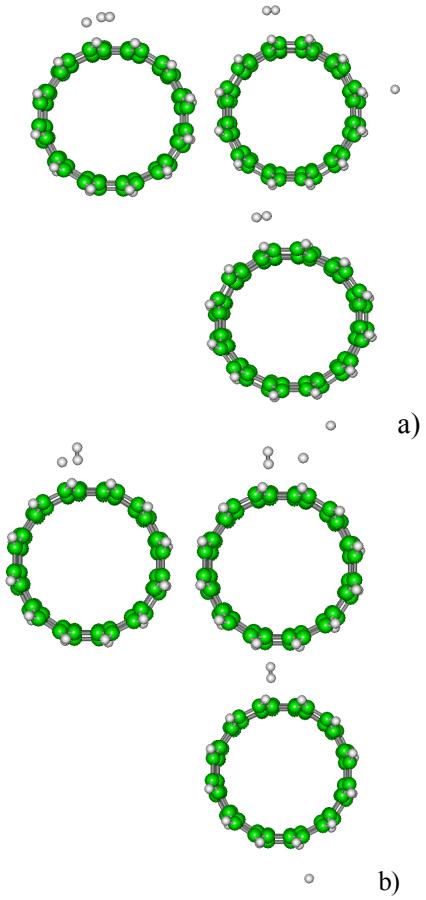


Fig. 2. Nanotube (6, 6) fragment with adsorbing hydrogen molecule and atom of the catalyst H:
а) H_2 is placed in parallel tube surface;
б) H_2 – orthogonal to tube surface.

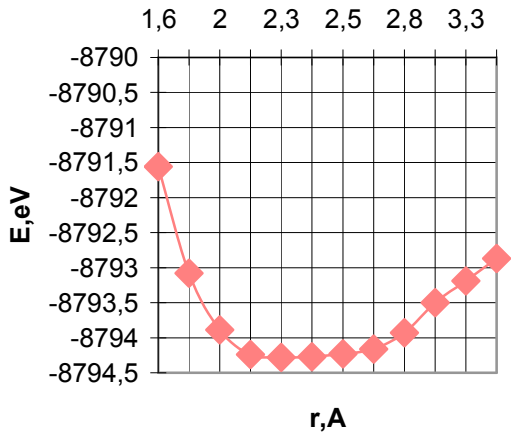


Fig. 3. A character curve of the potential energy of adsorption complex «nanotube - molecule H_2 - atom H».

References

1. Dresselhaus M.S., Dresselhaus G., Eklund P.C. Science of Fullerenes and Carbon Nanatubes, Academic Press, 1996, 965 P.
2. Eletskii A.V. Sorbcionnie svoistva uglerodnih nanostructur (Sorption properties of carbon nanostructures). Uspehi Fiz. Nauk, 2004, **174**(11), 1191 - 1230.
3. Zaporotskova I.V., Lebedev N.G., Chernozatonskii L.A. Quantum-chemical investigations of single wall carbon nanotube hydrogenation processes. Hydrogen materials science and chemistry of carbon nanomaterials. NATO Science Ser., II Mathematics, Physics and Chemistry, 2004, **172**, 243 - 258.