RESEARCH OF THE MECHANISMS OF THE INTERNAL SATURATION OF SINGLE WALL CARBON NANOTUBES OF A SMALL DIAMETER BY ATOMIC HYDROGEN

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Introduction

It is known that some substances can absorb the significant amount of hydrogen on unit of weight or volume. Such materials are intensively investigated, as their use as fuel elements is extremely perspective. As hydrogen adsorbing materials can be used carbon nanotubes [1-5] being the good hydrogen accumulator. The theoretical quantum chemical researches executed to the present time have proved an opportunity of an effective multiple atomic hydrogen adsorption on an internal and external carbon nanotube surface [2, 4, 5]. However the mechanism of carbon nanotube internal filling by hydrogen atoms is not found out finally yet.

Results and discussion

Two ways of adsorbing hydrogen atom introduction inside tube have been offered: 1) capillary - when the taking root atom will penetrate inside tube through a face aperture of nanotube (Fig. 1); 2) introduction by "wetting" - when the taking root atom will penetrate inside трубки through nanotube lateral surface (Fig. 2).

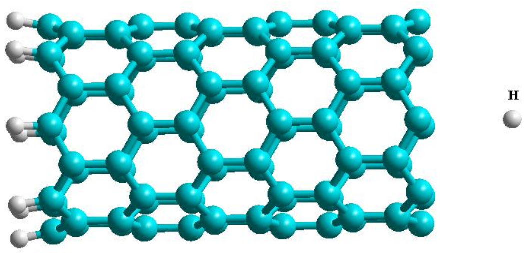

Fig. 1. Model of (8, 0) nanotube internal saturation process by "capillary" way.

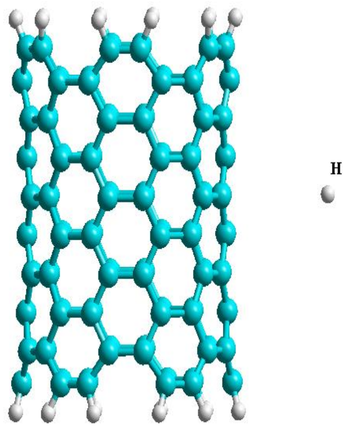

Fig. 2. Model of (6,6) nanotube saturation process by surface “wetting” method.

Quantum chemical semi-empirical investigations of the offered mechanisms of single wall carbon nanotube saturations by atomic hydrogen have been carried out. The molecular clusters types (n, n) and (n, 0) nanotubes containing 6 and 8 hexagons on perimeter have been considered. The atom H took root inside tubes and in case 1 it passed through the centre of tube face aperture, and in case 2 - through middle of surface hexagon.

The potential energy curves have been constructed and the potential barriers, which atom is overcome for introduction process (fig. 2, 3), have been calculated. The ways of overcoming of a barrier by atom H: classical and quantum (tunneling), have been investigated. The basic characteristics of these processes have been found. The opportunity of carbon nanotube saturations by atomic hydrogen and realization of both offered mechanisms have been proved. The energetically most favourable ways of atom H penetrations inside nanotubes have been determined.

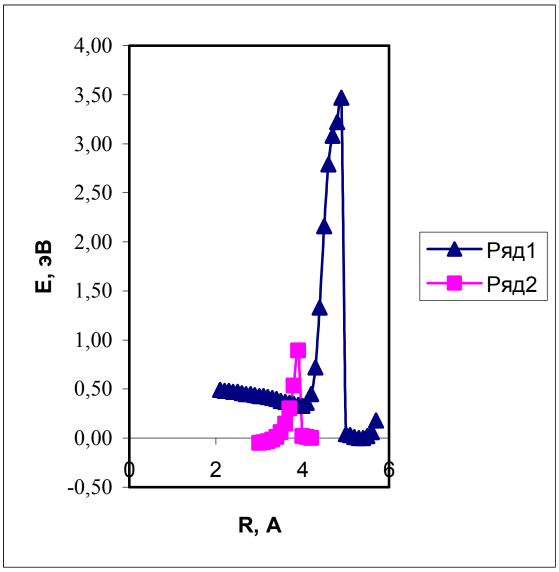

Fig. 3. Curve of potential energy of carbon nanotube internal saturation process by "capillary" method for 1) (6, 6) and 2) for (8, 0).

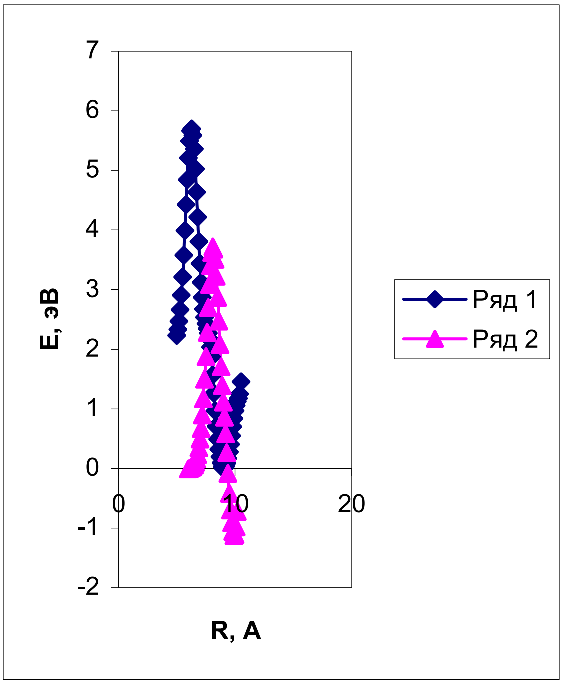

Fig. 4. Curve of potential energy of carbon nanotube internal saturation process by surface "wetting" method for 1) (8, 0) and 2) (6, 6).

Conclusions

1. It has been obtained that the most effective way of (n, 0) nanotube saturation is the capillary way. The (n, n) nanotube saturation is energetically more effective by surface "wetting".

2. The quantum chemical calculations have predicted that for a capillary way of nanotube filling the classical overcoming of a potential barrier by hydrogen atoms to be appeared the most probable process. One should to note that the influence of the functional groups which could are on tube border due to the unsaturated boundary chemical bonds on the process characteristics has been not investigate in the paper. It is a subject of the further research.

3. It has been established that the most stable state of hydrogen atom penetrating in tube is the center on investigated nanotybe on a longitudinal axis.

Acknowledgements

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