The adsorption of a hydrogen atom on the two types of boron sheets surface

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Abstract. The possible connection between the atom of hydrogen and the surface of two-dimensional boron sheets have been investigated. The calculations were carried out within the model of molecular cluster with the use of quantum chemical MNDO scheme. Two types of BS were studied: triangular BS (TBS) and α-sheet of boron atoms (αBS). The hydrogen atoms attacking BS have been simulated by a step-by-step approach for all atom locations. The surface patterns of potential energy for these processes were built. The analysis of curves showed that the active atom of hydrogen is adsorbed on the surface of BS. The adsorption distances (R_{ad}) and the adsorption energy (E_{ad}) were calculated. We have proved that αBS has a greater sorption capacity than hydrogen TBS.

1. Introduction

The search for suitable materials for hydrogen storage has driven attention to different light-weight nanostructures. Among them there are carbon nanostructures including carbon nanotubes (CNTs) which were intensively investigated during the last years. Many layered materials demonstrate their ability to form nanotubular structures. These nanotubes could be potential candidates to store molecular hydrogen because of their large surface area. Among the light-weight elements, besides C, boron would be a good candidate. Nowadays, many research teams and laboratories are engaged in the researches connected with boron and its compounds [1].

In 2004, the single-walled boron nanotubes have been synthesized [2]. Recently, scientists are interested in two-dimensional boron sheets (BS) [3]. Synthesis of this novel two-dimensional material attracts considerable interest because of its unique properties. The two-dimensional boron is expected to be used in many fields of science and technology including hydrogen energetic.

2. The adsorption mechanism of hydrogen atoms on the surface of a boron sheets

The first step of our research was the investigation of the binding opportunity between the atom of hydrogen and the surface of two-dimensional BS and the mechanism of this process. The calculations were carried out within the model of molecular cluster with the use of quantum chemical MNDO scheme [4]. We have studied two types of BS: triangular BS (TBS) and α-sheet of boron atoms (αBS). The examples of an αBS and a triangular BS are shown in figure1.

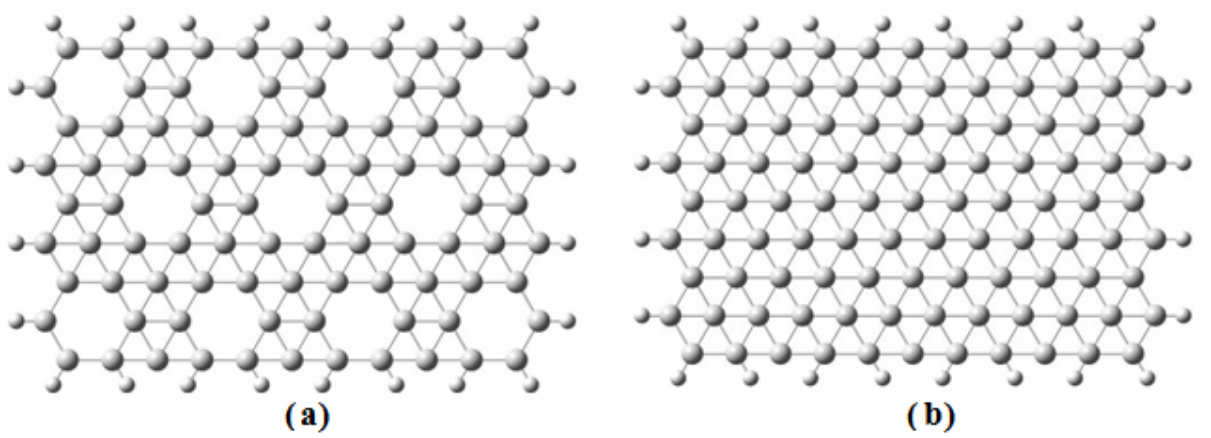

Figure 1. The cluster of pure boron sheets (BS): (a) an α-sheet of boron atoms (αBS); (b) a triangular boron sheet (TBS).

We studied three positions of the adsorbed H atom relative to the αBS surface: (I) over a boron atom in the hexagon node, (II) over a boron atom in the hexagon centre, (III) over the hexagon centre (figure 2) and one position of the adsorbed atom H relative to the TBS surface: (I) over a boron atom (figure 3).

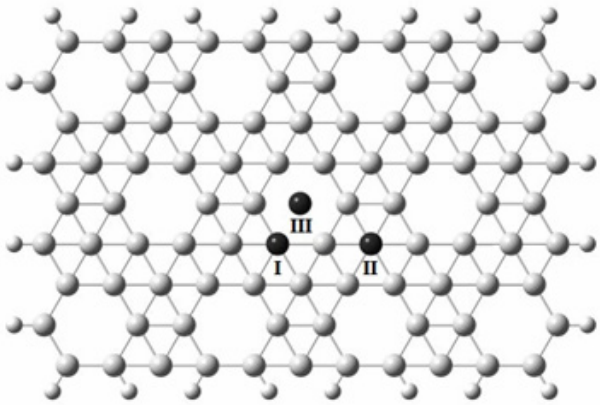

Figure 2. Three positions of adsorbed atoms over the surface of αBS: (I) over a boron atom in the hexagon node, (II) over a boron atom in the hexagon centre, (III) over the hexagon centre.

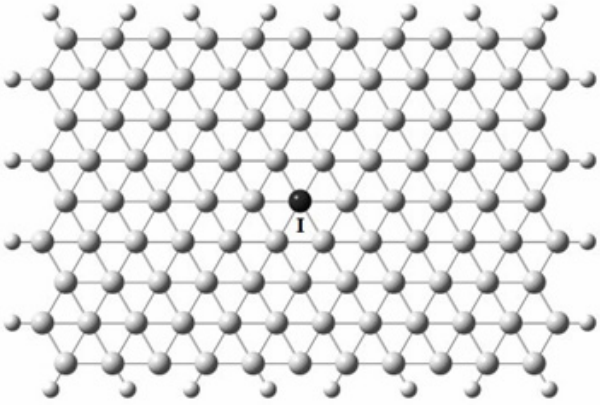

Figure 3. Position of adsorbed atoms over the surface of TBS: (I) over a boron atom.

The process of adsorption for all positions was simulated by step-by-step approach (with a step of 0.1 Å) of the adsorbed atom to a B atom (or a dummy atom) perpendicular to the surface of BS. The calculations have allowed to model profiles of potential energy surface of the given processes (figures 4, 5). The energy curves of these processes show a minimum (excepting the case where an H atom was placed in the position III) which illustrates the fact of a chemical bond formation between H atoms and a B atom on the surface of BS. An H atom is not adsorbed over the centre of a boron hexagon of αBS surface. The basic characteristics of the adsorption process for the hydrogen atom are shown in table 1 and table 2. The analysis of adsorption energy values showed that αBS has a greater sorption capacity with respect to hydrogen than TBS.

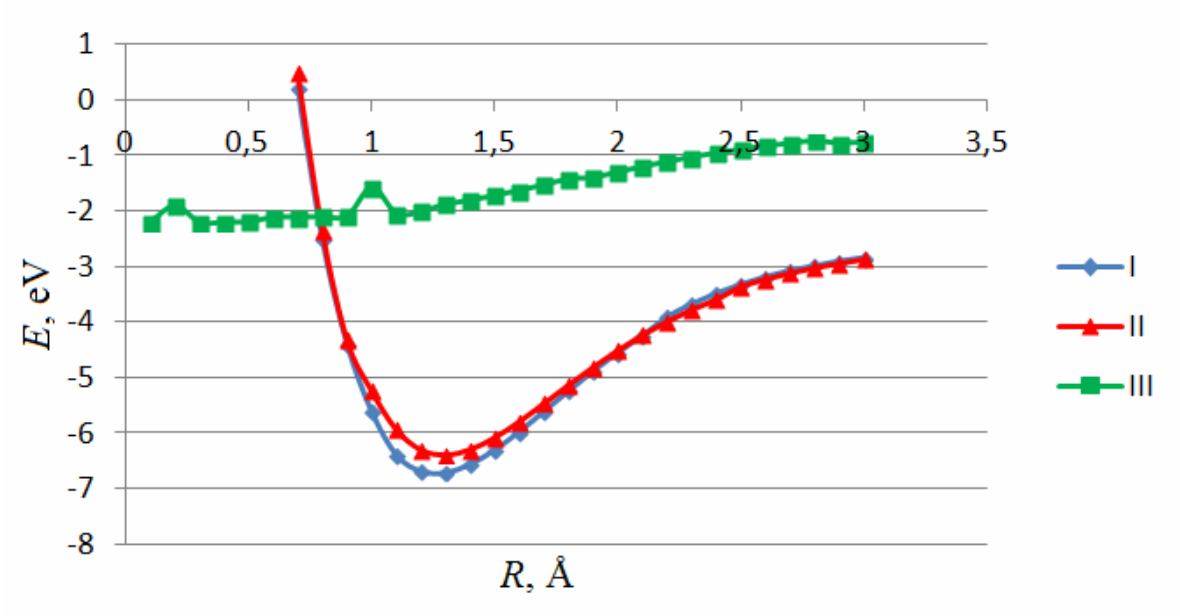

Figure 4. Profiles of surface potential energy of the H atom interaction with the surface of αBS: (I) position I – over a boron atom in the hexagon node, (II) position II – over a boron atom in the hexagon centre, (III) over the centre of a boron hexagon.

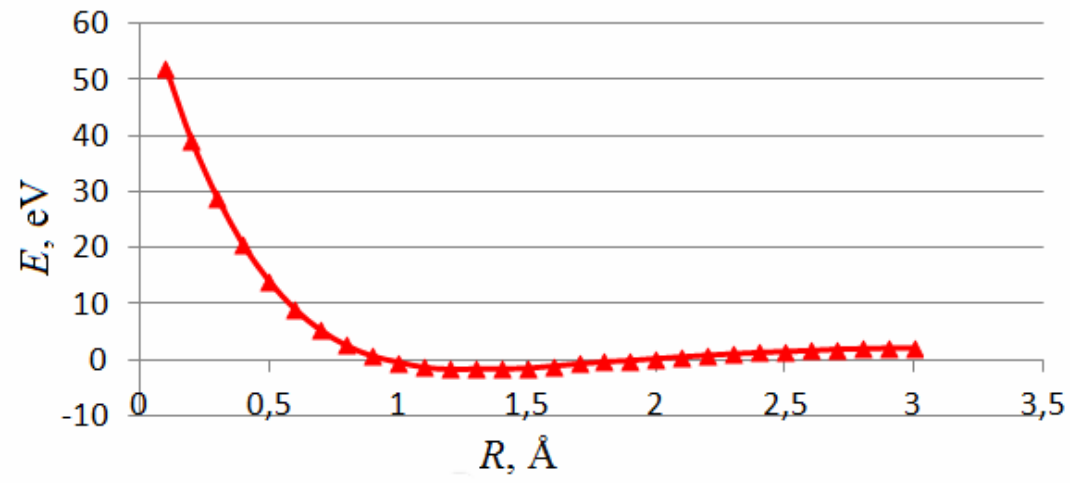

Figure 5. Profile of surface potential energy of the H atom interaction with the surface of TBS: position I – over a boron atom in the hexagon centre.

Table 1 The basic characteristics of the adsorbed H atom over the surface of αBS: (I) over a boron atom in the hexagon node, (II) over a boron atom in the hexagon centre; E_{ad} – the energy of adsorption, eV; R_{ad} – the distance of adsorption, Å; ΔE_g – the width of band gap zone, eV; q_B and q_H – the charges on B and H atoms respectively.

Positions of Hydrogen Atom	E_{ad}, **eV**	R_{ad}, **Å**	ΔE_g, **eV**	q_B	q_H
I	-6,68	1,2	1,98	-0,18	0,03
II	-6,4	1,3	1,91	-0,14	-0,003
αBS			0,09		

Table 2 The basic characteristics of the adsorbed H atom over the surface of TBS: (I) over a boron atom; E_{ad} – the energy of adsorption, eV; R_{ad} – the distance of adsorption, Å; ΔE_g– the width of band gap zone, eV; q_B and q_H – the charges on B and H atoms respectively.

Positions of Hydrogen Atom	E_{ad}, **eV**	R_{ad}, **Å**	ΔE_g, **eV**	q_B	q_H
I	-1,64	1,2	1,53	-0,09	0,01
TBS			1,51		

Also, we investigated the qualitative change of the band-gap of the considered hydrogen composites on the base of BS (figures 6, 7). The width of the energy gap increases in all cases considered. For αBS the band-gap is equal to about 1,9 eV and for TBS the band-gap is equal to about 1,5 eV. However, we should note that calculations were carried out using the molecular model. In this case the value of the band-gap is a little bit higher because the infinity boron sheets are modeled by limited-size clusters. Therefore, we can assume that hydrogen composites based on BS will exhibit semi-conductive properties.

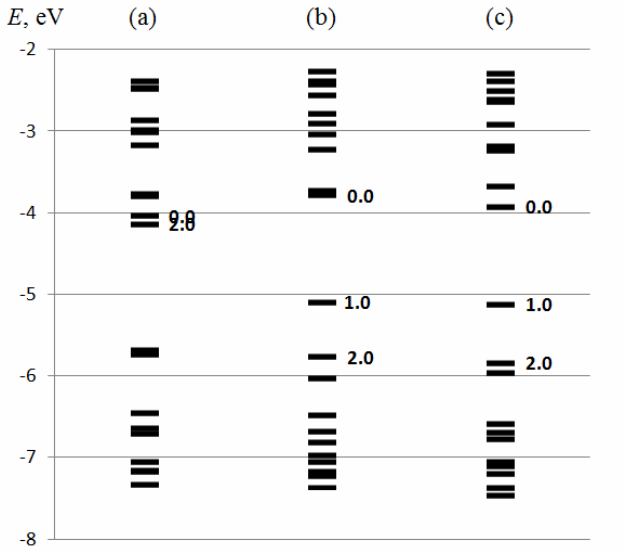

Figure 6. Single electron energy spectra of: (a) pure αBS, (b) αBS with an H atom in the position I, (c) αBC with an H atom in the position II.

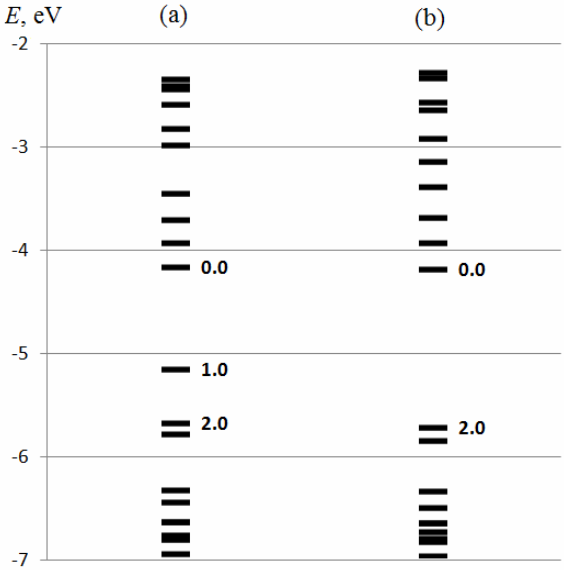

Figure 7. Single electron energy spectra of : (a) pure TBS, (b) TBS with an H atom.

3. The study of regular hydrogenation of boron sheets

The issue of major importance is the question of hydrogenation of surface structures. For graphene this question has been studied in [5, 6]. We consider it necessary to study this phenomenon in boron sheets. We calculated hydrides of two types of BS and studied regular hydrogenation of BS.

To define the most probable hydride structures the calculations for the following two positions of hydrogen atoms relative to a BS surface were carried out: (1) H atoms are located over B atoms, wherein hydrogen atoms are not displaced from each other; (2) the hydrogen atoms are displaced relative to each other for the length of B-B bond (figures 8, 9). The distance of adsorption was taken from the tables 1, 2. The difference of total energies of these positions for both BS is very small and equal to zero within the error limits. So, the analysis of the total energy and charge distribution has showed that the both options of regular hydrogenation for each kind of boron sheets (α and triangular) are available and the new structures are stable. Thus, we can assert that formation of gas-phase hydrogen composites on the basis of boron sheets is possible.

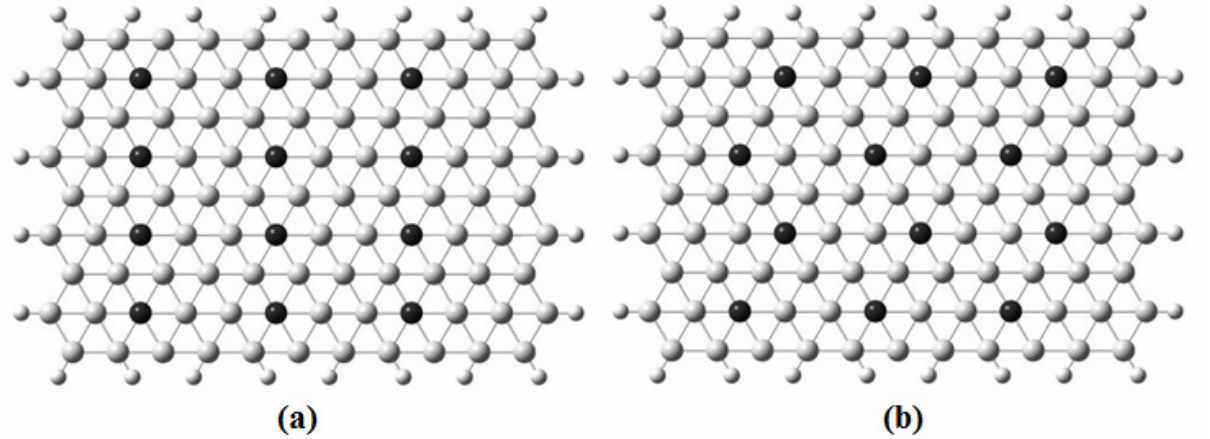

Figure 8. The cluster of TBS with indications of H atom positions on the surface: (a) position 1; (b) position 2.

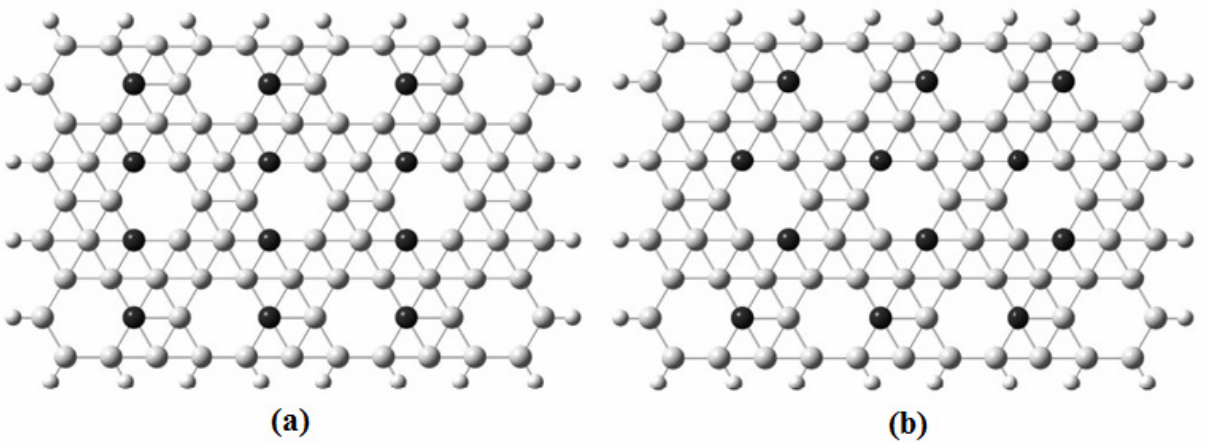

Figure 9. The cluster of αBS with indications of H atom positions on the surface: (a) position 1; (b) position 2.

4. Conclusion

The research of adsorption mechanism for the hydrogen atom on the surface of two-dimensional boron sheets has been investigated. There were three positions of hydrogen adsorption for αBS and one position for TBS. The possibility of adsorption in the position over a B atom has been proofed for both BS. The adsorption energy and the optimal distance of adsorption have been determined.

The process of regular adsorption of hydrogen atoms on the surface of αBS and TBS has been studied. Formation of gas-phase hydrogen composites on the basis of boron sheets is proofed.

References

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