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Molecular Simulation of Hydrogen Adsorption onto Single-Walled Carbon and Boron-Nitride Nano-Cones

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Abstract

In this paper, we have studied the hydrogen adsorption onto CNCs and BNNCs nano-cones using GCMC simulations. The effects of length and cone apex angle on adsorption property have been investigated. Our results show that with increasing the pressure and decreasing the cone length and cone apex angle except for CNC-300°, the hydrogen adsorption onto the BNNCs and CNCs was increased. It was also found that BNNCs can uptake more hydrogen in comparison with CNCs at the same thermodynamically conditions. Further, more hydrogen adsorption can be achieved in both CNCs and BNNCs with 240°apex angle. This finding attributed to high surface area as well as strong interactions between hydrogen molecules and respected nano-cones. Also, results of hydrogen adsorption with unit of mol/m3 are corresponded of the energy of hydrogen adsorption.

Keywords: GCMC; adsorption; nano-cones; CNC; BNNC; hydrogen.

1.Introduction

Hydrogen is an attractive energy carrier for clean energy uses, which can be produced from all renewable sources; therefore, it is introduced as one of the most promising candidates for the replacement of current energy systems [1]. In order to provide safe and practical hydrogen storage, a number of techniques have been employed [2, 3, 4]. Possible current techniques for hydrogen storage include physical storage via compaction of the liquid, chemical storage in irreversible hydrogen carriers, reversible metal and chemical hydrides and gas-on-solid adsorption [5, 6].

Although each of above mentioned approaches for hydrogen storage possesses favourable advantageous, none of them improves the performance of transportation vehicles on their efficiencies, safety requirements and even their sizes, weights and costs [5]. Therefore, hydrogen adsorption with a safe, effective and stable storage medium remains a main challenge. Among various materials, carbon nanostructured materials have been attracted considerable interest as suitable candidate for hydrogen storage due to their high hydrogen storage capacity at ambient conditions [7-17].

Dillon et al. were the first people who investigated the hydrogen adsorption on carbon nanotubes (CNTs) by using new Raman spectroscopy-based technique [8]. Since their study, numerous theoretical and experimental attempts have been devoted to hydrogen adsorption capacity of these novel nanostructered materials [9-17].

Nano-cone is one of the well-known allotropes of nanotubes. Carbon nano-cones (CNCs) are the first nano-

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cone synthesized by industrial process (Kvaerner Carbon Black & Hydrogen Process) [18]. Boron-nitride nano-cones (BNNCs), on the other hand, are another type of nano-cones which have been prepared chemically [19].

Indeed, a nano-cone is a nanotube with an open-ended side while another side is capped with a cone which this cone can be a part of a fullerene. Then this cone can be created with a small or large angle. Consequently; a large-open angle cone would be similar to graphite or graphene. For instance, a CNC can be easily constructed if a graphene sheet is divided in to m×60◦ sector (m varying from 1 to 5) and then, removed m sectors from a flat graphite sheet so that, new bonds that have been existed from removing m sectors, being fused together while for each removing sector, one additional pentagon is introduced at the conic tip. Therefore, a series of five single-walled nano-cones (SWNCs) is obtained (because of varying m), with a linear angle at the cone apex equal to 112.9˚, 83.6˚, 60.0˚, 38.9˚ and 19.2˚ which are named according to the part removed 60˚, 120˚, 180˚, 240˚, 300˚, respectively [18-22]. Figure 1 illustrates the single-wall carbon nano-cone (SWCNC) and boron-nitride (SWBNNC) nano-cone for 60˚ and 300˚ apex angles.

In this work, Grand canonical Monte Carlo (GCMC) simulations were carried out to evaluate the hydrogen adsorption capacity of the SWCNC and SWBNNC. This paper is organized as follows. In section 2, we explain briefly the simulation technique implemented in this work. In section 3, hydrogen adsorption isotherms and energy of adsorption for both SWCNC and SWBNNC systems are calculated and compared.

2. Molecular simulation section

2.1 GCMC simulation procedure

For systems under consideration we have employed GCMC technique which is recognized to be a powerful tool for realistic simulation of energy storage materials at ambient conditions. In each GCMC simulation, using grand canonical ensemble, the probability of a configuration is given by $\rho_i = C \times f(\{N\}_i) \times exp[-\beta E_i]$ (where C is an arbitrary normalization constant, β is the reciprocal temperature and E_i is the total energy of configuration i). Moreover, temperature, volume and chemical potential are kept constant during the simulation. The total energy of interacting systems was expressed by the following term:

$$E_i = E_{i,SS} + E_{i,SF} + U_{i,S} \qquad (1)$$

where $E_{i,SS}$ relates to the intermolecular energy between the sorbate molecules (here H_2), $E_{i,SF}$ signifies to the interaction energy between the sorbate molecules and framework (here are CNC or BNNC), and $U_{i,S}$ denotes total intermolecular energy of the sorbate molecules. Furthermore; three types of moving; displacement, creation and deletion with equal probabilities are used in each GCMC simulation. In addition, the operations are repeated until the number of H_2 molecules in the simulation cell comes to equilibrium. Further details with respect to the GCMC simulation technique as well as computational manner have been given elsewhere [23]. In this study, C-C and B-N bonds length were set to 1.42 and 1.44 Å, respectively [X6]. Each point of computation was carried out at 298.25 K and the number of trial moves in a typical GCMC simulation was 2×10^7 iterations, that half of first iterations are considered as equilibration which has been discarded. Then, remained iterations have been applied to calculate ensemble averages of thermodynamics parameters. Also, interactions between H_2 molecules with each other and with nano-cones were simulated through the Lennard–Jones (LJ) (12-6) potentials [11], which have derived from the Lorentz-Berthelot mixing rules [24, 25].

Table1: LJ (12-6) parameters of H2 and nano-cone's atoms [11] [24]

LJ parameter	σ (nm)	ε/kB (K)
H_2	0.2958	**36.7**
C (CNC)	0.34	**28.2**
B (BNNC)	0.3453	**47.8**
N (BNNC)	0.3365	**72.9**

Table 2. The structural details of SWCNC and SWBNNC

CNC, apex angle (°)	CNC heights (nm)	BNNC, apex angle (°)	BNNC heights (nm)
60	3	60	4
	4		
120	3	120	4
	4		
	5		
180	4	180	4
	5		
	6		
240	4	240	4
	5		
	6		
	7		
300	4	300	4
	5		
	6		
	7		

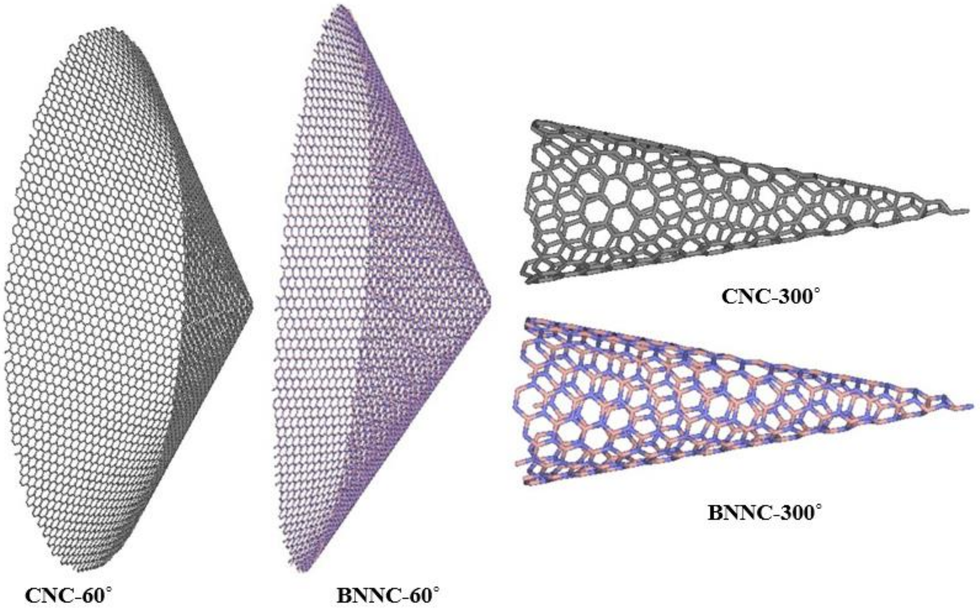

Figure 1. The structure of SWCNC and SWBNNC with apex angle of 60° and 300°.

2.2 Simulation details

Table 1 represents the LJ parameters considered for the interacting species. It should be noted that in the present work, the nano-cones were assumed to be a rigid body and all atoms carry out any charge in the systems under consideration. These investigations have performed in the pressure range from zero to 16 MPa, and tube lengths of 3-7 nm for CNCs while for BNNCs the tube length is fixed at 4 nm. Furthermore, for both nano-cones, five different apex angles: 60°, 120°, 180°, 240° and 300° are considered (see Table 2). Periodic boundary conditions (PBC) are set at SWCNCs and SWBNNCs systems during the GCMC displacements. However, it should be considered that in actual calculation, the spherical cut-off distance is set a little smaller than the half of simulation cell. Moreover, for comparison the isotherms of H_2 in both SWCNC and SWBNNC are illustrated at 298 K.

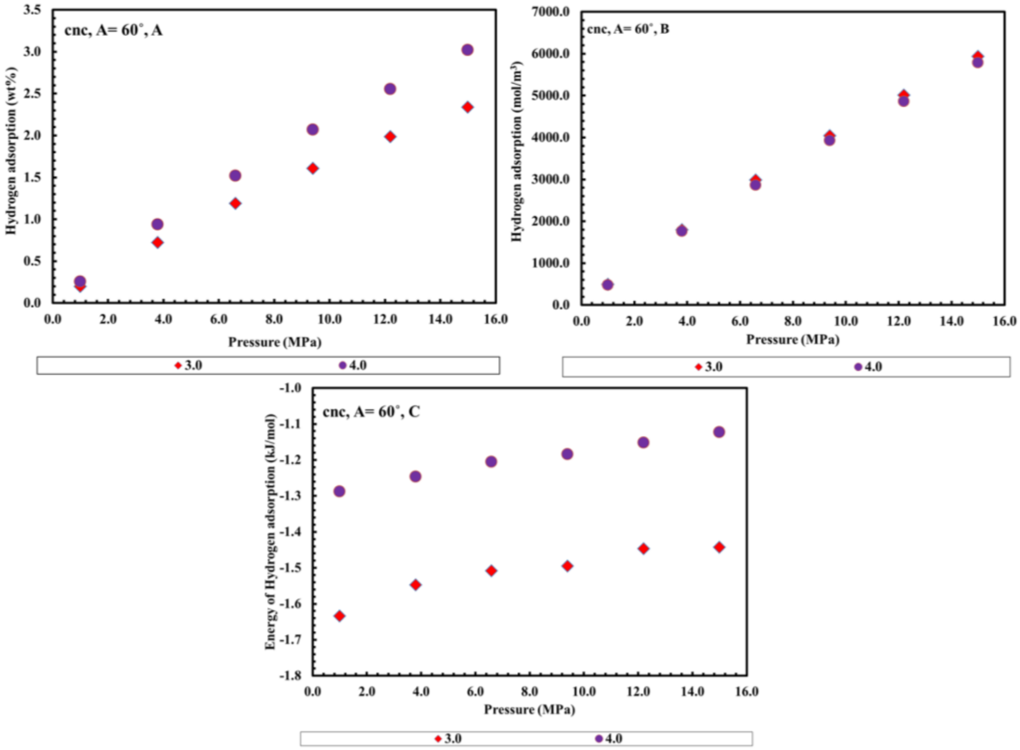

Figure 2. Adsorption isotherm of hydrogen in SWCNC 60˚ (A) The hydrogen adsorption in unit of wt% (B) The hydrogen adsorption in unit of mol/m³ (C) energy of hydrogen adsorption.

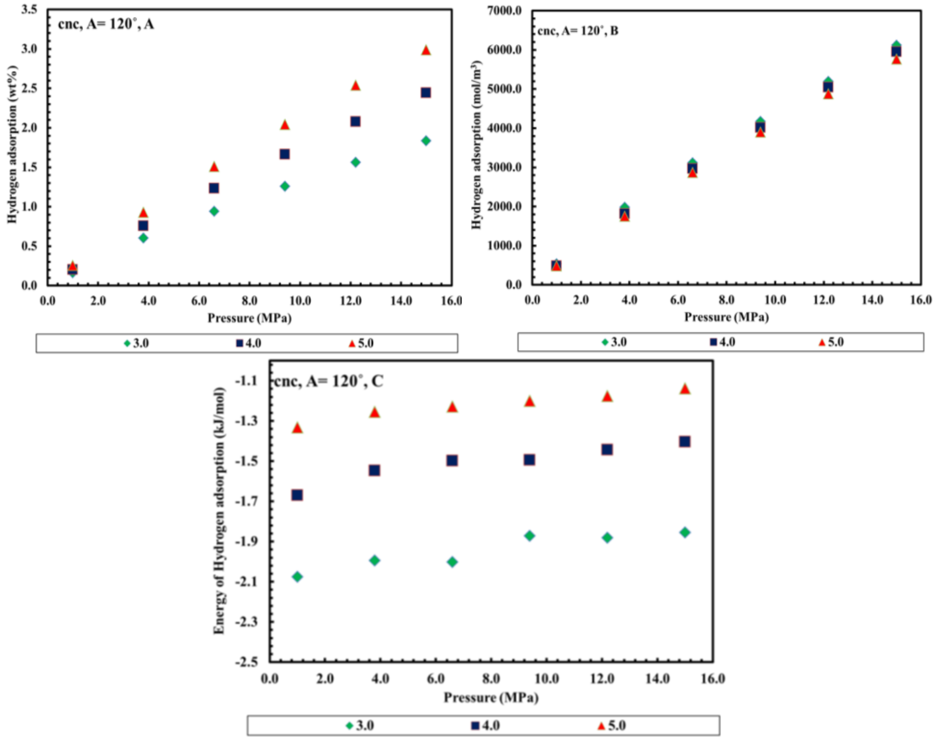

Figure 3. Adsorption isotherm of hydrogen in SWCNC 120˚ (A) The hydrogen adsorption in unit of wt% (B) The hydrogen adsorption in unit of mol/m³ (C) energy of hydrogen adsorption.

3. Result and discussion

In this paper, first of all, we have plotted the isotherm of hydrogen adsorption (with H_2/system wt% and mol/m^3 units. mol/m^3 means "mol" of hydrogen that are adsorbed in "m^3" of nano-cones) against pressure in SWCNCs. Then, we have investigated the effect of length and apex angle of both SWCNC and SWBNNC on hydrogen adsorption. In the first step, two parameters; the tube length and the pressures were varied at fixed apex angle. Figure 2 shows the hydrogen adsorption isotherms for SWCNC with 60° and 3 and 4 nm lengths in H_2/system wt% and mol/m^3 units, respectively. As it can be seen from the figure, the hydrogen adsorption was increased with increasing of the pressure. Furthermore, according to the figure units, shorter SWCNC with unit of mol/m^3 has more adsorption capacity. Besides, it is proved by Figure 2 (c) that shorter SWCNC can adsorb more hydrogen molecules in comparison with other counterparts. It's well known that the correct unit of hydrogen adsorption is "mol/m^3".

In fact, it seems that increasing of the SWCNC length causes increasing the amount of available space for the hydrogen adsorption. Also, with increasing nanotube length, the volume of simulation cell will be increased. Therefore, increasing the tube length and the volume of simulation cell are two reverse factors that can impact on hydrogen adsorption.

In order to investigate the influence of the length and angle of cone apex on hydrogen adsorption, we have calculated the hydrogen adsorption on SWCNCs with 120°, 240° and 300° of apex angle which are presented in following.

The results of the simulation of CNC-120° (carbon nano-cone with 120° apex angel) are displayed in Figure 3-A, B and C with length of 3, 4, 5 nm, respectively. It is clear from this figures that more hydrogen adsorption with the wt% of unit, takes place in larger length nano-cone (Figure 3-A) and with mol/m^3 of unit of adsorption, as a result, more hydrogen adsorption was observed in shorter length NCN (3 nm) (see Figure 3-B). Also, the energy of hydrogen adsorption (Figure 3-C) for CNC-120° with the less length (3 nm) tends forward more negative (more absolute energy of adsorption).

Furthermore, Figure 3-A shows that by increasing the pressure, the weight percentage (wt%) of hydrogen adsorption is increased with increasing the nano-cone lengths. In the moderate pressure (4-10 MPa) and at high pressure (>10 MPa) the hydrogen adsorption with considering wt% of unit, is increased more clearly in longer CNC-120°. Also, Figure 3-B shows that with increasing the pressure, the hydrogen adsorption in the different lengths will be increased, but it seems there are little differences between nano-cones on hydrogen adsorption. According to, Figure 3-B and C, we can find that in CNC-120°, at low pressure with increasing the pressure, less space is available to adsorb and the energy of repulsion increases compared with CNC-60°. However, at high pressure (>10MPa) available space to hydrogen adsorption is very low, because of filling in CNC by the hydrogen molecules. In fact, at moderate pressure (from 4-10 MPa), the hydrogen adsorptions on CNC with various lengths, have similar behavior and increasing of the length of CNC almost does not change the amount of adsorbed hydrogen. This observation, has already reported [26] which confirms our present result. Also, Figure 3-B and C show that the unit of mol/m^3 is correct unit of the hydrogen adsorption, because at high absorptivity, the energy of hydrogen adsorption will be more and the CNC-120° with 3 nm tube length has more hydrogen and more energy adsorptions.

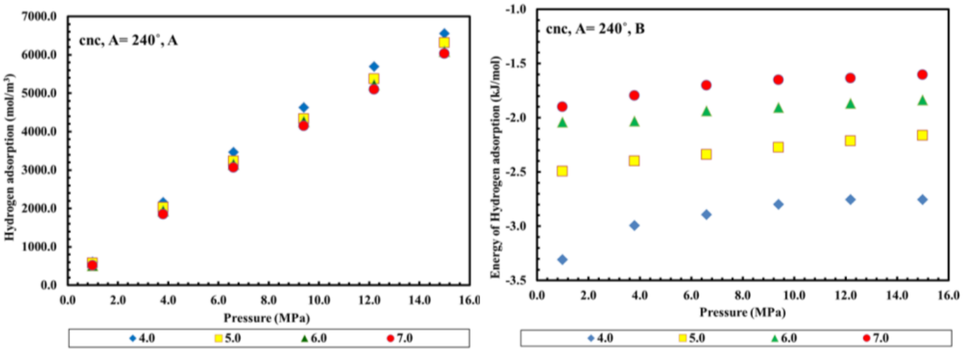

Figure 4. Adsorption isotherm of hydrogen in SWCNC 240° (A) The hydrogen adsorption in unit of wt% (B) The hydrogen adsorption in unit of mol/m^3 (C) energy of hydrogen adsorption.

So, we select the hydrogen adsorption unit of mol/m^3 in our continuation report. Also, in order to briefly description of our results we do not present the CNC-180° of results because, the results of hydrogen adsorption behaviors on CNC-180° are very close to results of hydrogen adsorption behaviors of CNC-120°.

In following, the hydrogen adsorption and the energy of adsorption onto the CNC-240° with length of 4, 5, 6 and, 7 nm have evaluated and the results shown in Figure 4. As shown in Figure 4-B, the hydrogen adsorption has more absolute adsorption energy in smaller CNC (see energy of adsorption in Figures 2-C, 3-C and 4-B). The comparison between the adsorption energy in the CNC-240° and smaller angle shows that the absolute adsorption energy for small angles is more than larger angles in the same thermodynamic conditions. Thus, it can be concluded that the decreasing the apex angle increases the absolute adsorption energy. Also, Figure 4-A, shows that the hydrogen adsorption is increased with increasing the pressure, and will be increased slowly with increasing the length in moderate pressure (4-10 MPa). Two reasons usable support our results: Firstly, when the CNC length increases, the available space and the probability of interaction of hydrogen-hydrogen will be increased. Hence, the interaction of hydrogen with nano-cone's wall is reduced and then the influence of nano-cone's wall interaction energy is reduced, which causes the hydrogen adsorption to decrease. Secondly, another reason is related to reducing the interactions between hydrogen and the tip of nano-cone. Because the maximum of adsorption potential is occurring on the cone tip and the adsorption potential will be decreased while hydrogen cannot close to the cone tip. So, the interaction between hydrogen and nano-cone will be decreased. Our observation has been concluded by using first principle study [26]. Therefore, as depicted in Figures 2, 3 and 4, the hydrogen adsorption in shorter nano-cones is most probable with considering the absolute energy of adsorption and inner space of nano-cones.

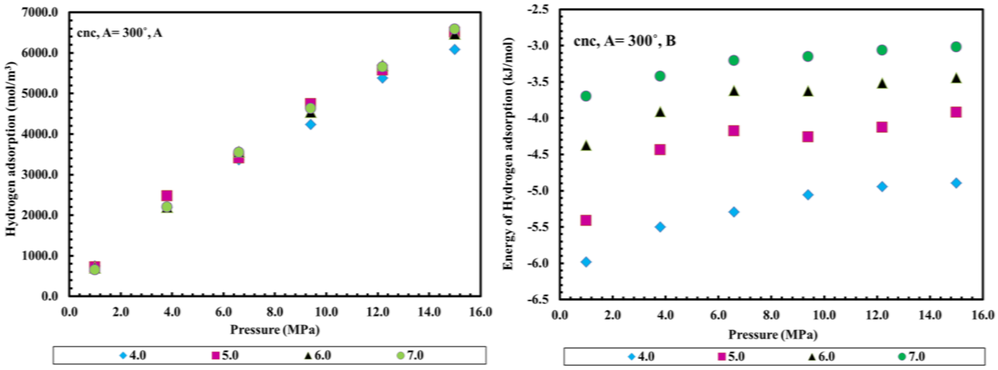

Figure 5. Adsorption isotherm of hydrogen in SWCNC 300° (A) The hydrogen adsorption in unit of wt% (B) energy of hydrogen adsorption.

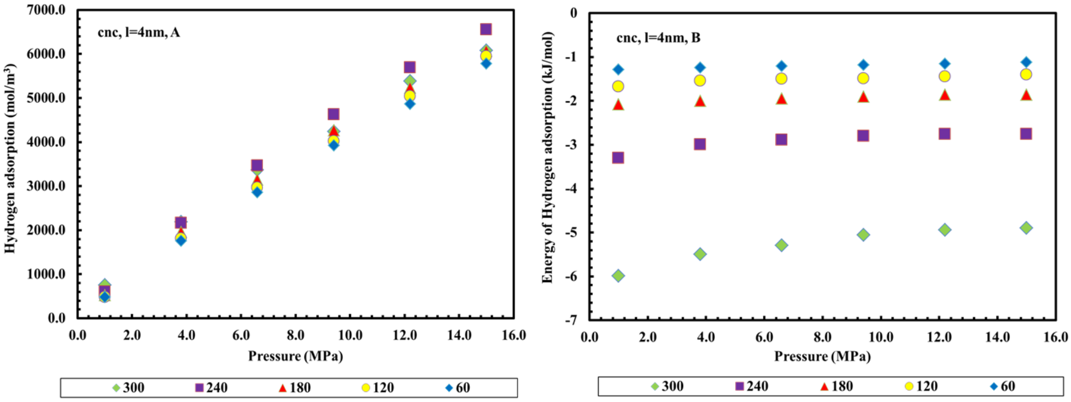

Figure 6. Adsorption isotherm of hydrogen in SWCNC at different apex angle. (A) The hydrogen absorbed energy. (B) The hydrogen adsorption unit in mol/m^3 (C) hydrogen adsorption unit in percentage by weight.

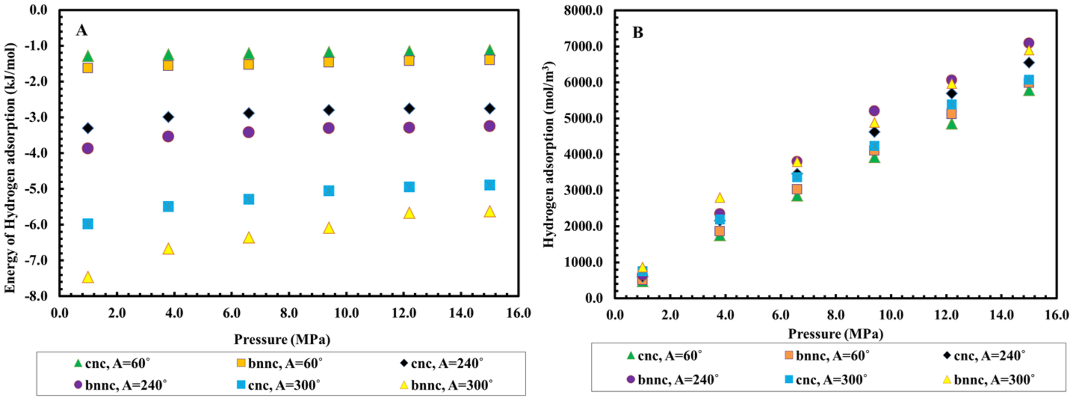

Figure 7. Adsorption isotherm of hydrogen in SWCNC and SWBNNC with 4 nm length. (A) The hydrogen absorbed energy. (B) The hydrogen adsorption unit in mol/m^3.

On the other hand, the results of hydrogen adsorption behaviors onto CNC-300° is different from the other counterpart. The hydrogen adsorption in the CNC-300º with 4, 5, 6 and, 7 nm of length is shown in Figure 5-A. Also, Figure 5-B shows that the smallest angle nano-cone (CNC-300°) has more absolute adsorption energy. In fact, the adsorption energy in the CNC-300° emphasizes that the hydrogen adsorption must be more than other nano-cones. Furthermore, Figure 5-A shows that in the CNC-300°, longer nano-cone (7 nm) adsorbs more hydrogen while in other nano-cones, shorter nano-cone adsorb more hydrogen. Also, the maximum of absolute energy of hydrogen adsorption onto CNC-300° is related to shorter nano-cone (3 nm) that is inconsistent with logical principles of adsorption. It is clear that, the reason for this behavior is related to decreasing the apex angle from 60° to 300°. In fact, the available space inside the nano-cone greatly reduces when the apex angle is decreased, and this space limitation does not allow the hydrogen molecules to be closed to the tip of the cone. Thus; a considerable proportion pore volume (especially near the tip) will actually be empty and this causes that with increasing the pressure, the hydrogen adsorption in nano-cones with very small apex angle and with longer length would be more than short ones. Consequently, important factor onto hydrogen adsorption in nano-cones is the apex angle following the length of nano-cones.

For finding complete investigation, we have considered the effect of apex angles on hydrogen adsorption. The hydrogen adsorption comparison between CNC in fixed length and various apex angles (60°, 120°, 180°, 240° and 300°) were studied. Figure 6-A, B present the hydrogen adsorption and the energy of adsorption onto CNCs respectively. So, Figure 6-A shows that CNC-240° at fixed length has more hydrogen adsorption. The reason of its, is described before. Also, Figure 6-B shows that the absolute adsorption energy by the CNC-300° is significantly more than the other angles and with decreasing the apex angles, the adsorption energy will be decreased too. It is related to various angles on cone-tip that led to different slopes would be made on the cone-wall, which these slopes can be caused stronger/weaker confined hydrogen molecules. For instance, in the angle of 60° and 120°, the walls of the cone are opened and the interaction between nano-cone's wall and hydrogen occurs rarely. It means that the hydrogen molecules in these cases just are sensitive the wall as graphite plane. So, the interactions between hydrogen molecules and cone's atom are decreased. But, with increasing the cone apex angle (>120°), configuration of the wall become closer together. Hence, confined hydrogen can interact more effectively between together and between walls-hydrogen than before. Figure 6-A shows that with increasing the pressure, the adsorption will increase on all angles and hydrogen adsorptivity onto CNCs are slightly different together and the maximum adsorption will be related to CNC with angle Thus: 60°< 120°< 180° < 300° <240°. This is due to the decrease of the interaction potentials on very low volume. In these cases, with increasing the pressure, the repulsive potential will increase and the adsorption will decrease. Also, these results observed in Ref. [27]. As a result, the adsorption decreases with increasing the cone apex angle that this is due to the decreasing interactions between hydrogen molecules and atoms of cones.

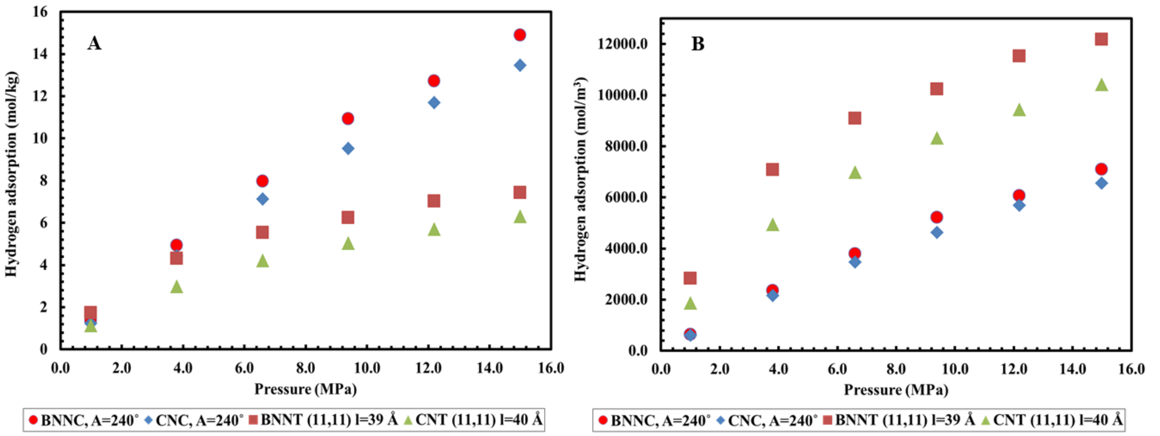

Figure 8. Adsorption isotherm of hydrogen in SWCNC and SWBNNC with 4 nm length and apex angle of 240° with comparison by SWCNT (11, 11) and SWBNNT (11, 11). (A) unit of adsorption is mol/kg (B) unit of adsorption is mol/m^3.

To sum up discussion, it can be concluded, that with increasing the apex angle of the cone and by reducing the pore width on the cone, the hydrogen adsorption will decrease. Of course, according to Figure 6-A, this conclusion has an exception. In fact, with sharp decreasing of pore width (in apex angle of 300°), the hydrogen adsorption will decrease because of low space available to interacting.

In the following, we describe the hydrogen adsorption at different pressures on boron-nitride nano-cones (BNNC) with equal length (4nm) and different angles then we will compare with obtained results of CNCs. The purpose of comparison is to investigate the effect of pressure and apex angle of the cone on the hydrogen adsorption onto CNC and BNNC. Figure 7-A and B are displayed the hydrogen adsorption and energy of adsorption onto CNCs and BNNCs respectively. From Figure 7-A we can find that the hydrogen adsorption onto CNCs and BNNCs at different pressure and the apex angle 60°, 240° and 300° show that the adsorption energy on the BNNCs are more than on the CNCs and this difference on the adsorption energy, decreases with increasing the cone apex angle (see Figure 7-B). So, the values of the adsorption energy for CNCs and BNNCs on the 300°, are very close together. But at the hydrogen adsorption isotherm in Figure 7-A, we can be observed that on these three angles, the hydrogen adsorption for BNNC is more than CNC. Also, according to the previous conclusion, the adsorption at the pressures under 6 MPa for CNC-300° has the most value but with increasing the pressure, the CNC-240° has the most adsorption (See Figure 7. A). However; the difference between the hydrogen adsorption onto CNC and BNNC is related to ε for C, B and N. Because of that the ε values for B and N are more than C. Thus; the interaction between hydrogen and BNNC is stronger than CNC and the hydrogen adsorption onto the BNNC is more. So, BNNC-240° has more hydrogen adsorption than CNC-240° and CNC-60° has less hydrogen adsorption. However; the first important factor onto hydrogen adsorption in nano-cones is ε, it means that the intermolecular interactions between all atoms of guest and adsorbent, secondly factor, is the apex angle and third factor is length of nanotube.

Finally, to the best understand of the hydrogen adsorption onto nano-cones, we have been simulated the hydrogen adsorption onto (11, 11) single walled carbon nanotube (SWCNT) and (11, 11) boron-nitride nanotube (SWBNNT) with 4 and 3.9 nm respectively. The SWCNC and SWBNNC have 4 nm lengths with 240° of apex angle. In this comparison, we select that cones have more hydrogen adsorption than others (See Figure 7-B). Also, the weight of CNC, BNNC, SWCNT and SWBNNT were considered the same. Here, the hydrogen adsorptions have presented in Figure 8. Figure 8-A and B show the hydrogen adsorption with unit of mol/kg and mol/m^3 respectively. According to Figure 8-B, nanotubes have more hydrogen adsorption rather than nano-cones. But, Figure 8-A shows that the hydrogen adsorption onto nano-cones are better than nanotubes. This latter result is against of results of Figure 8-B. It seems that the selection of “unit” in practical experience is very important. In fact, with weigh scale, the unit of “mol/kg” is appropriate units, while unit volume scale is appropriate “mol/m^3.

4. Conclusions

In this paper, we have investigated the effect of length and cone apex angle on the hydrogen adsorption of SWCNCs and SWBNNCs. In summary, the simulation results obtained in this work shows that with increasing of pressure and cone apex angle and decreasing of the cone length, the hydrogen adsorption will be increased onto the SWBNNCs and SWCNCs. But, the results of hydrogen adsorption behaviors onto CNC-300° due to space limitations is different from the other angles. Also, we compare the hydrogen adsorption onto the SWCNCs and SWBNNCs. Our simulation results show that the SWBNNCs have more hydrogen adsorption than SWCNCs on the same thermodynamics conditions. The most importance result is that, SWCNCs and SWBNNCs with apex angle of 240° adsorbed more hydrogen than other one because of both the most space availability and the most interactions between hydrogen molecules and atoms of cones. Finally, the percentage by weight unit is NOT a suitable unit for physical adsorption and is not compatible with the result of the conclusion of the adsorbed energy. Also, in experimental view, we must be considered the weight or volume scales to use nano-cones or nanotubes.

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