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Structure induced Hydrogen storage in Carbon and Boron Nanostructures

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Abstract: Enhancing hydrogen storage through Nanostructures is one of the thrust area of research today. Among several materials studied, this allotropic form of carbon, namely Carbon Nanotubes (CNTs) proves to be one of the promising system owing to its unique properties like high surface area, porous and high stability to a list few important one. The possibility of hydrogen storage both in the inner and outer surfaces are well investigated by lot of theoretical as well as experimental works. The role of defects, doping and Structural variations of the different Nanomaterial are also analysed and found that some of these strongly affects the storage capacity. But still the DOE target could not be achieved that makes this issue an interesting topic of study.

Here, the dependence of the hydrogen binding energy on the bond length and angles of the Nanotubes are analysed. Different types of Nanotubes like metallic and semiconductor with varying structures are considered for this study (1.57 Å length of the C – C bond gives the binding energy value of 0.061eV). Apart from CNTs other contending materials such as Boron nitride are also considered. The adsorption binding energy values (as a function of different orientations of molecule and at different sites of Nanostructures) are compared and the results will be discussed in detail for hydrogen storage applications.

Keywords: Hydrogen storage, Deformed SWCNT, Adsorption.

Introduction and Computational details:

It has excellent mechanical strength and elasticity characteristics, electronic properties ranging from metals to semiconductor, high electronic sensitivity to chemical adsorbents and mechanical strains, and very large aspect and surface to volume ratios respectively [1]. A lot of theoretical and experimental works (like inner and outer surfaces, defects, doping and structural variations) were done to enhance the storage capacity [2-6]. But still the DOE target (6.5 wt%) could not be achieved that makes this issue an interesting topic of study. The mechanical strain / stress were strongly influenced the bond length and angle of the CNT by various theoretical investigation [7-9]. In this paper, the dependence of the hydrogen binding energy on the bond length and angles of the nanotube are analysed.

Molecular Dynamics simulation have been performed on the (5,5) SWCNT comprising 100 atoms and 5 unit cells respectively. For stretching, one end of the tube is kept fixed while other end of the tube is moved. Due to the stretch, the bond length has been changed from 1.42Å to 1.57Å respectively. Density Functional Theory (DFT) calculation is performed for evaluating the adsorption binding energy of hydrogen atom on the outer surface of opened SWCNT and deformed SWCNT. In our present calculation involves Generalized Gradient Approximation (GGA) for the electron exchange and correlation effects, Perdew Burke Enzerhof (PBE) as potential and Double Numerical Polarization (DNP) as basis set. The binding energy values are estimated from the well-known following equation

$$E_b = E_{\text{CNT}} + E_{\text{H}} - E_{(\text{CNT} + \text{H})}$$

Where, E_{CNT} , E_{H} and $E_{(\text{CNT} + \text{H})}$ are total energy of the corresponding free CNT, single hydrogen atom and CNT with hydrogen atom respectively. The energy values are minimized by adjusting the separation between the hydrogen atom and adsorption site from the wall of the CNT.

Results and Discussion:

In this section, the binding energy of the system was calculated for single hydrogen atom and for which the hydrogen atom axis positioned perpendicular and above carbon ring. This is the more stable configuration among the other two configurations such as parallel to the carbon ring and parallel to the C-C bond [4]. Since the atom is able to fit better into the electron density valley that exists on the centre of the hexagons. As a first case, (5,5) SWCNT the binding site requires the nanotube wall & hydrogen atom separation of 2.75Å and the binding energy value is 0.091eV. The corresponding binding energy changes as a function of separation for (5,5) shown in fig.1. As in the second case, structural deformation could be performed in two different directions. One is along the axis of the nanotube (Z) and another one is perpendicular to the axis of the nanotube (Y). In this case, the bond length could be elongated from the CNT default bond length (1.42Å) to 1.57Å. We have observed that the adsorption binding energies of hydrogen atom on the deformed nanotubes were 0.061eV (Z) & 0.067eV (Y) with the hydrogen atom separation (D_{Eq}) as 1.75Å & 2.0Å from wall of the nanotube. The corresponding binding energy changes as a function of separation for (5,5) deformed CNT shown in fig. 2 & 3. The binding energy (E_b) and separation distance (D_{eq}) for the hydrogen atom adsorption on the SWCNT and deformed SWCNT is presented in Table-1.

It is observed from the present study the bond length and angle of the single walled carbon nanotube of armchair configuration had strongly affected the hydrogen storage capacity. Further it will be extended to various nanostructures and different configurations under investigation.

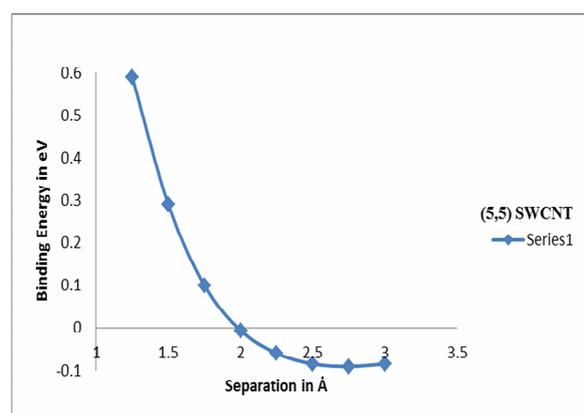


Fig: 1: binding energy variation of hydrogen atom as a function of separation for (5,5) SWCNT.

Table: 1: The binding energy (E_b) and separation distance (D_{eq}) for the hydrogen atom adsorption on the SWCNT and deformed SWCNT

TUBE	SWCNT		DEFORMED SWCNT			
			Y		Z	
	E_b (eV)	D_{Eq} (Å)	E_b (eV)	D_{Eq} (Å)	E_b (eV)	D_{Eq} (Å)
(5,5)	0.091	2.75	0.067	2.00	0.061	1.75

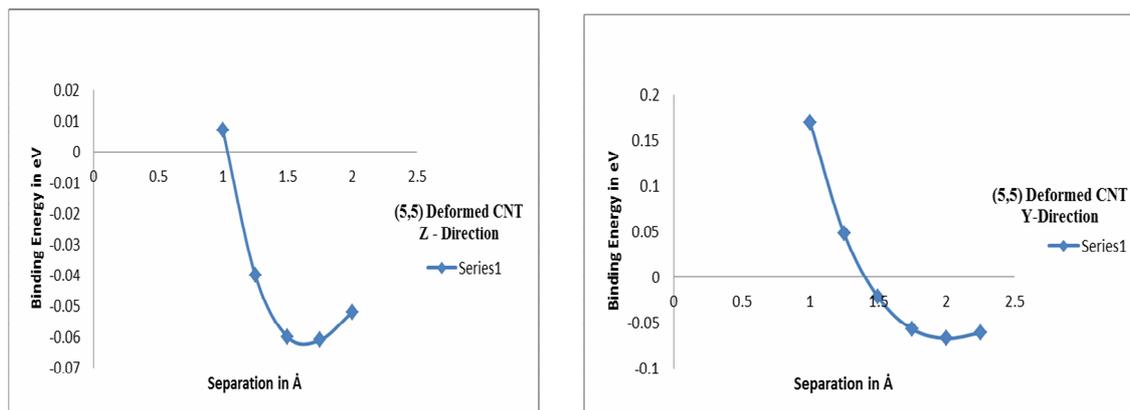


Fig: 2 & 3: Binding energy variation of hydrogen atom as a function of separation for (5,5) deformed SWCNT.

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