

## Structural aspect on carbon dioxide capture in nanotubes

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**Abstract:** In this work we reported the carbon dioxide adsorption ( $\text{CO}_2$ ) in six different nanostructures in order to investigate the capturing capacity of the materials at nanoscale. Here we have considered the three different nanotubes including zinc oxide nanotube (ZnONT), silicon carbide nanotube (SiCNT) and single walled carbon nanotube (SWCNT). Three different chiralities such as zigzag (9,0), armchair (5,5) and chiral (6,4) having approximately same diameter are analyzed. The adsorption binding energy values under various cases are estimated with density functional theory (DFT). We observed  $\text{CO}_2$  molecule chemisorbed on ZnONT and SiCNT's whereas the physisorption is predominant in CNT. To investigate the structural aspect, the tubes with defects are studied and compared with defect free tubes. We have also analyzed the electrical properties of tubes from HOMO, LUMO energies. Our results reveal the defected structure enhance the  $\text{CO}_2$  capture and is predicted to be a potential candidate for environmental applications.

**Keywords:** Carbon nanotube; Silicon carbide nanotube; Zinc oxide nanotube;  $\text{CO}_2$  adsorption; Density functional theory.

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### I. Introduction

Carbon dioxide is the one of the major green house gases (GHGs) that may have direct linkage to global climate changes. It exists in gaseous state, due to their large concentration in the atmosphere, it affect the greenhouse effect [1]. The emission of carbon dioxide from industry and burning of fossil fuel has directly pumped to the atmosphere and it leads to undesirable climate changes. In recent years its concentration increases rapidly and efforts already have been taken to control the emission of  $\text{CO}_2$  and the process is going on. Human life in the earth is in need of perfect membrane for carbon dioxide capture so as to live peaceful and healthy life. There are several methods employed to adsorb and confine the  $\text{CO}_2$  in order to produce the clean environment. Hectic research was carried out on to control the emission of  $\text{CO}_2$  using bulk metal oxide surface, metal organic framework, zeolites and nanostructures. Recently, it is one of the thrust areas of work for scientist and researchers all over the world. There is lot of research papers devoted both theoretically and experimentally on this issue.

Because of their unique properties and applications in emerging filed, CNTs are being tried as a membrane for  $\text{CO}_2$  capture. The gas molecule adsorption in carbon nanotubes and nanotube bundles was carried out by Zhao et al. [2]. Cinke et al. [3] have carried out the work on  $\text{CO}_2$  adsorption in SWNT and concluded the  $\text{CO}_2$  is physisorbed on to the nanotubes. The vibrational behavior of adsorbed  $\text{CO}_2$  on SWNTs was investigated by Yim et al. [4]. A DFT study of  $\text{CO}_2$  adsorption on SWNTs was reported by Quinonero et al. [5]. They analyzed that the SWNTs are good potential candidate for  $\text{CO}_2$  capture and storage in reducing the gas emissions. A comparative study on MWCNTS and activated carbon charcoal was reported by Khalili et al. [6]. They observed the high amount of  $\text{CO}_2$  capture in these materials.  $\text{CO}_2$  adsorption in single walled bamboo-like carbon nanotubes (SWBCNT) are analyzed by Husain [7]. They reported the  $\text{CO}_2$  molecule was adsorbed more strongly with larger adsorption energy on SWBCNTs. Thermodynamics and regeneration studies of  $\text{CO}_2$  adsorption on MWNTs was studied by Hsu et al. [8]. The effect of Fe doping on adsorption of  $\text{CO}_2/\text{N}_2$  within carbon nanotubes with dispersion corrections was carried out by Du et al. [9]. Sonawane et al. [10] have performed the work on interaction of  $\text{O}_2$ ,  $\text{CO}_2$ ,  $\text{NO}_2$  and  $\text{SO}_2$  adsorptions on Si-doped carbon nanotubes. MgO decorated carbon nanotubes for  $\text{CO}_2$  adsorption was studied by Feng et al. [11]. Fatemi et al. [12] worked in improving  $\text{CO}_2/\text{CH}_4$  adsorptive selectivity of carbon nanotubes by functionalization with nitrogen-containing groups and investigated the multi walled nanotubes containing nitrogen groups shows much higher adsorption capacity of  $\text{CO}_2$ .

Apart from CNTs other nanostructures such as aluminium nitride nanotubes (AlNNT), boron nitride nanotubes (BNNT), and boron carbide (BCNT) are also considered for  $\text{CO}_2$  adsorption as the phenomena is largely structural dependent one. Effective capture by BNNT in ambient condition was reported in literature [13, 14]. Jiao et al. [15] was carried out the work on DFT study of  $\text{CO}_2$  and  $\text{N}_2$  adsorption on AlNNTs. The  $\text{CO}$  adsorption in Al doped BNNT was carried out by Shao et al. [16]. Mahdavi et al. [17] have performed the theoretical studies on AlN, BN and SiC nanotubes for  $\text{CO}_2$  adsorption and predicted AlNNTs could be promising candidate for this purpose. Bagherinia et al. [18] carried out the work on adsorption of GHGs in

silicon carbide nanotubes. They observed SiCNTs has got best gas adsorptive ability at ambient pressure and low/high pressure. Theoretical investigation of CO<sub>2</sub> adsorption on graphene was carried out by Lee et al. [19]. A DFT study on CO<sub>2</sub> capture in BN sheet with boron vacancy was investigated by Jiao et al. [20]. Several authors performed the study on the oxide surfaces for gas adsorption [21, 22]. It is observed from the above literatures, there are only few studies on CO<sub>2</sub> adsorption in ZnO and SiC nanotubes. Silicon carbide nanotubes have high thermal stability and mechanical strength and find applications in optical and optoelectronic devices [23, 24]. Similar to SiCNTs, zinc oxide nanotubes shows interesting properties and has already proven applications in gas sensors [25]. Not much work exist on SiCNT and ZnO nanotube for CO<sub>2</sub> capture and this motivates us to take the present investigation on CO<sub>2</sub> adsorption on these nanotubes along with CNT. Though many aspects of on CO<sub>2</sub> capture are reported, to the best of our knowledge, the effect of structural defect on CO<sub>2</sub> capture is yet to be probed.

Here we have performed the CO<sub>2</sub> adsorption in different novel structures with hexagonal network. In our work we have selected the three different types of nanotubes such as ZnONT, SiCNT and CNT. In each case we have considered the three different chirality of nanotubes, such as, (5,5) armchair, (9,0) zigzag and (6,4) chiral, which has approximately the same diameter. The adsorption of CO<sub>2</sub> through nanotube sidewall has been done for which the molecular axis positioned perpendicular and above the corresponding hexagonal ring. In order to study the role of structural defect, the pentagon and heptagon are introduced deliberately in the hexagonal structures. The HOMO-LUMO energy gap ( $E_g$ ), electronic chemical potential ( $\mu$ ), electrophilicity ( $\omega$ ) and hardness ( $\eta$ ) of the tubes are also calculated from the HOMO, LUMO energies. The computational details are given in the next section.

## II. Computational details

The ab initio density functional theory based calculation is performed for estimating the adsorption binding energy ( $E_{ads}$ ) of CO<sub>2</sub> on outer surface of opened single-walled ZnONT, SiCNT and CNT. The total energy of the system was calculated using Kohn-Sham equation. In this work, we have included the Generalized Gradient Approximation (GGA) for the electron exchange and correlation effects. We have used Perdew, Burke and Enzerhof (PBE) potential and the Double Numerical Polarization (DNP) atomic orbital basis set [26]. The binding energy values are estimated from the well-known equation,

$$E_b = E(\text{nanotube}) + E(\text{CO}_2) - E(\text{nanotube}+\text{CO}_2) \quad (1)$$

where,  $E(\text{nanotube}+\text{CO}_2)$ ,  $E(\text{nanotube})$  and  $E(\text{CO}_2)$  are the total energy of the corresponding nanotube with CO<sub>2</sub> molecule, free nanotube, and the energy of CO<sub>2</sub> molecule respectively. The energy values are minimized by adjusting the separation between the molecule and adsorption site from the wall of the nanotubes.

We are interested in calculating the binding energies in six different structures namely as defect free CNT (DFCNT), DFSiCNT, DFZnONT, defected CNT (DCNT), DSiCNT and DZnONT. Our motivation is to study the trend in the binding energy variation in above nanostructures. All calculations are performed in finite systems at zero K.

## III. Results and Discussion

We present the results of CO<sub>2</sub> adsorption in different types of nanotubes for the defect free and defected cases. As mentioned earlier tube chiralities are also taken into account. The ZnONT and SiCNT have hexagonal structure as like in CNTs and are constructed by replacing an alternative carbon atom in CNT by Zn and O in the case of ZnONT and Si and C in the case of SiCNT. We have considered the 40, 36 and 50 number of atoms corresponding to (5,5) (9,0) and (6,4) nanotubes.

### 3.1 Defect free case

For the present study we have considered the hexagon (CO<sub>2</sub> molecule adsorbed perpendicular to nanotube wall with respect to hexagon) site for CO<sub>2</sub> adsorption for all kinds of nanotubes. The molecule adsorbed on the outer surface of (5,5) DFZnO nanotubes gives the stable nanotubewall-CO<sub>2</sub> distance of 1.97 Å with the binding energy of 1.136 eV. We could observe there is an increment of binding energy of 0.853 eV in zigzag ZnONT compared to armchair. The chiral (6,4) DFZnONT gives still higher binding energy of about 2.578 eV than these two types. This large value of binding energy indicates that the CO<sub>2</sub> molecule is chemisorbed on the outer surface of ZnONT which implies that there is strong hybridization takes place between the ZnONT and CO<sub>2</sub> molecule. The interaction of CO<sub>2</sub> with the one of the oxygen in ZnONT gives the stable carbonate structure leads to very high adsorption as expected. Fig. 1 gives the schematic diagram of CO<sub>2</sub> adsorption in (5,5) ZnONT. Our results are in coincidence with the existing literature [21].

In the case of SiCNT the indirect band gap semiconductor armchair (5,5) gives the large value of binding energy 1.859 eV with the nanotube wall-molecule separation of 1.45 Å. The direct band gap semiconductor of (9,0) SiCNT gives the binding energy value of 1.446 eV. We obtain 0.319 eV decrement in binding energy in chiral (6,4) SiCNT. Similar to ZnONT, We could observe a strong formation of chemical bond between the

surface of SiC nanotube and the CO<sub>2</sub> molecule. This may be due to sharing of electrons of oxygen in CO<sub>2</sub> with the SiCNT as reported earlier [10]. Fig. 2 shows a schematic diagram of CO<sub>2</sub> adsorption in (9,0) DFSiCNT.

Since single wall CNTs is one of the potential candidate for gas adsorption we have investigate all kinds of CNTs with respect to CO<sub>2</sub> molecule. Binding energy for armchair, zigzag and chiral works out to be 0.570 eV, 0.1573 eV and 0.254 eV. We obtain this lower value due to van-der-Waals interaction between the tube wall and the CO<sub>2</sub>. Our results are in good agreement with the reported one [3]. Fig. 3 represents the CO<sub>2</sub> adsorbed (6,4) DFCNT with respect to hexagon. Our present results are supported with the recent experiments reported by Khalili et al [6].

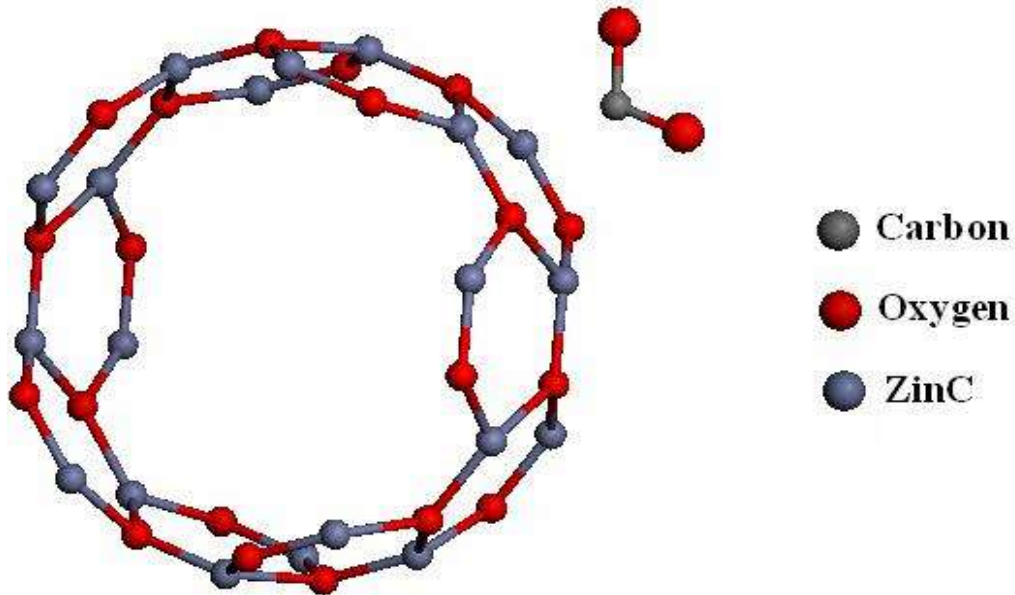


Fig. 1 CO<sub>2</sub> adsorption with respect to hexagon in (5,5) ZnONT

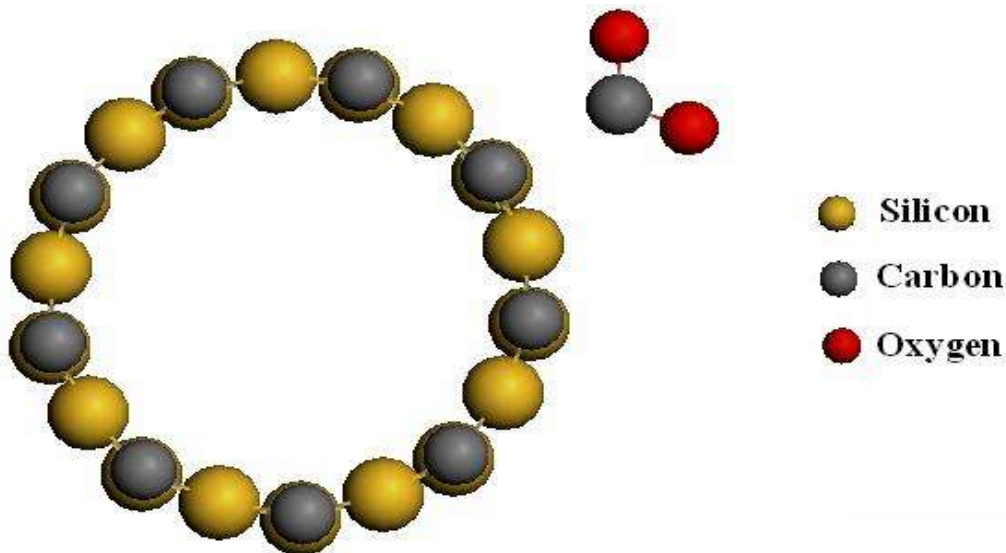


Fig. 2 CO<sub>2</sub> adsorption with respect to hexagon in (9,0) SiCNT

TABLE. 1 Increment in Binding Energy (%) between defected and defect free (5,5), (9,0) and (6,4) ZnONT, SiCNT and CNT.

Type of tube	Increment in BE (percentage)(defected and defect free)		
	CNT	SiCNT	ZnONT
(5,5)	14	43	43
(9,0)	78	17	31
(6,4)	24	11	6.6

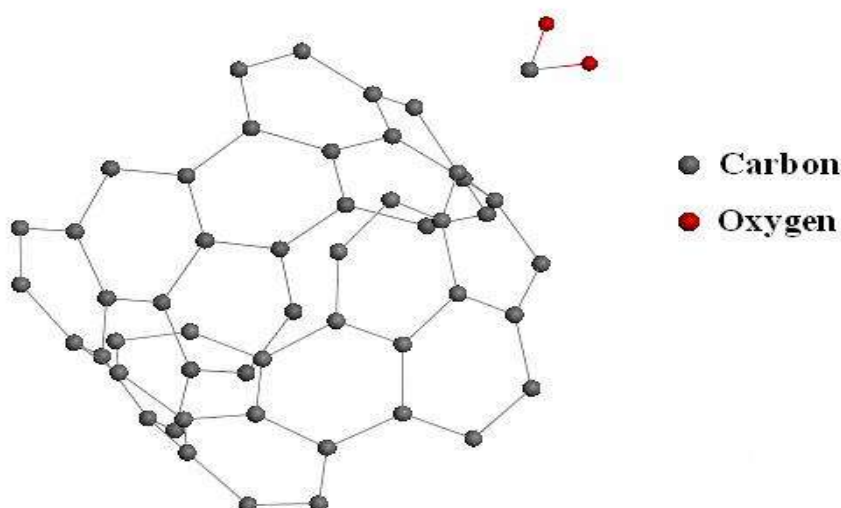


Fig. 3 CO<sub>2</sub> adsorption with respect to hexagon in (6,4) CNT

### 3.2 Defected case

Here we are interested to study the role of structural defects on CO<sub>2</sub> adsorption. The planar pentagon and the boat shaped heptagon is introduced oppositely leads to negative curvature at the inner side of the tube that gives small bend in the walls. The excess of electrons on the pentagon and a deficiency on the heptagon tend to form a six- $\pi$ -electron system [27]. Electronically it will modify the structure considerably it leads enhancement in molecule adsorption binding energy. The values are estimated to be 1.63 eV for the defected (5,5) DZnONT, which is about 43% higher than the defect free value. For the zigzag case we could observe an increment of 0.611 eV that is equal to 31% enhancement compared to defect free case. But there is only a small increment of about 6.6% for the chiral (6,4) tube. Fig. 4 gives the schematic diagram molecule adsorbed (9,0) DZnONT. Though the binding energy values are larger compared to zigzag and armchair type, it seems that the defects has lesser role in the chiral tubes. When we analyze the results of defected SiCNT armchair has 43% enhancement increment compared to defect free case. These values are 17% and 11% for the defected zigzag and chiral SiCNT. For both SiCNT and ZnONT effect of defect plays stronger role in armchair and zigzag than in chiral tube. From the results we could observe the very strong chemisorptions will take place in defected nanotubes than free tubes. The CO<sub>2</sub> adsorbed (6,4) DSiCNT is shown in Fig. 5. It is interesting to note the behavior of CNTs slightly different than the ZnONT and SiCNT. We got the highest value of increment of 78% binding in defected zigzag (9,0) CNT. The binding energy works out to be 0.280 eV corresponding to defected (9,0) zigzag CNT. It is also seen from the earlier literature reported by Mackie et al. [28], the binding energy of N-doped zigzag tube is 0.3023 eV. The amchair and chiral defected CNTs provides the very less improvement with respect to defects. TABLE 1 gives the increment in binding energy (percentage) between defected and free tubes for all kinds of nanotubes. Binding energy values with respect to chiral alge of nanotubes are plotted in Fig. 6-8.

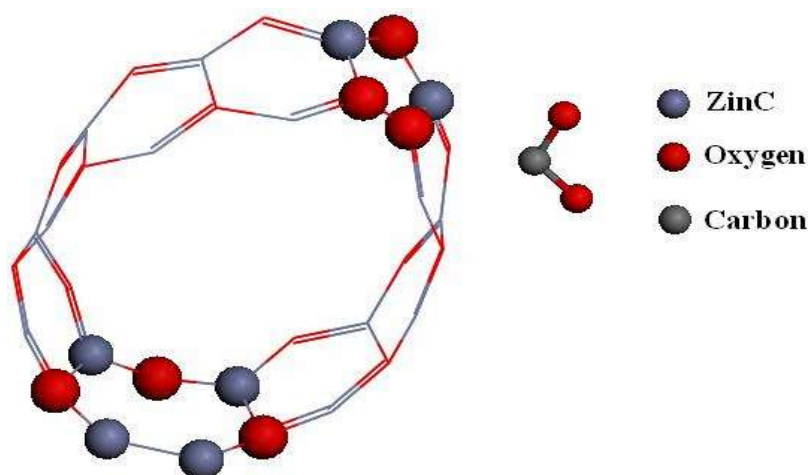


Fig. 4 CO<sub>2</sub> adsorption with respect to hexagon in defected (9,0) ZnONT

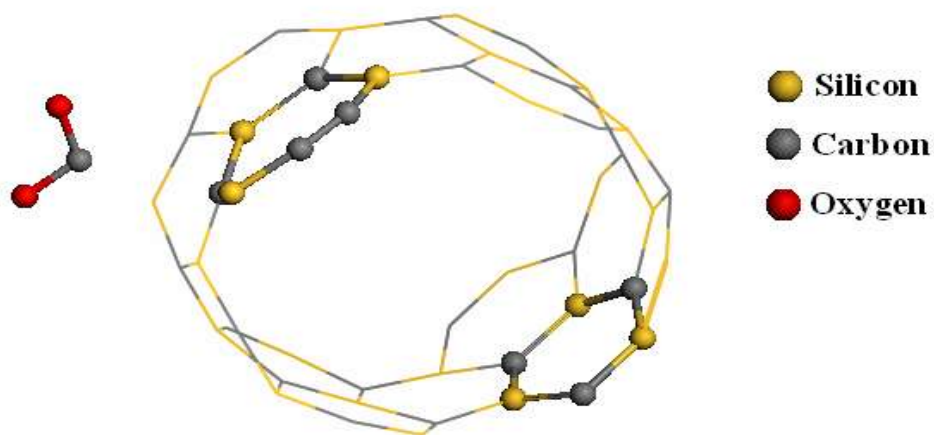


Fig. 5 CO<sub>2</sub> adsorption with respect to Hexagon in defected (6,4) SiCNT

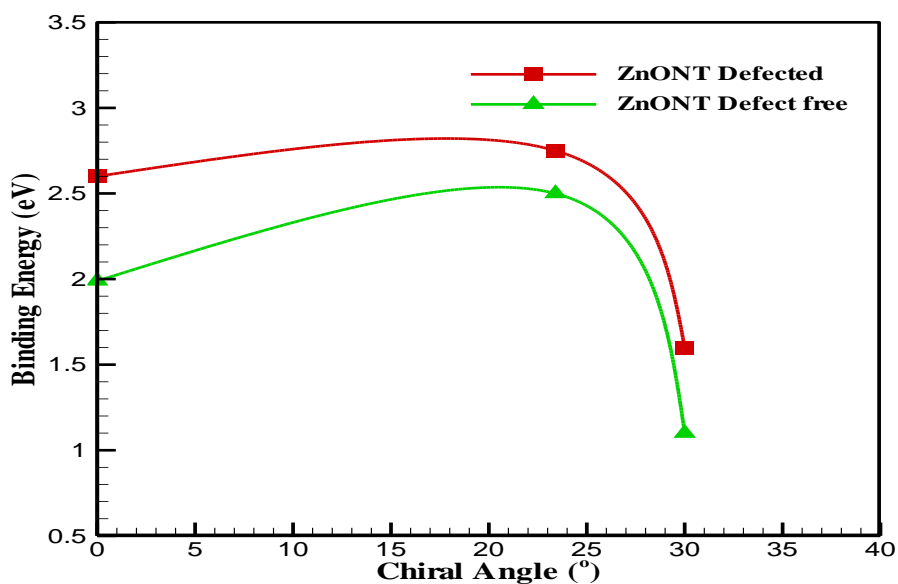


Fig. 6 Binding energy of CO<sub>2</sub> in (9,0), (6,4) and (5,5) ZnONT with respect to chiral angle

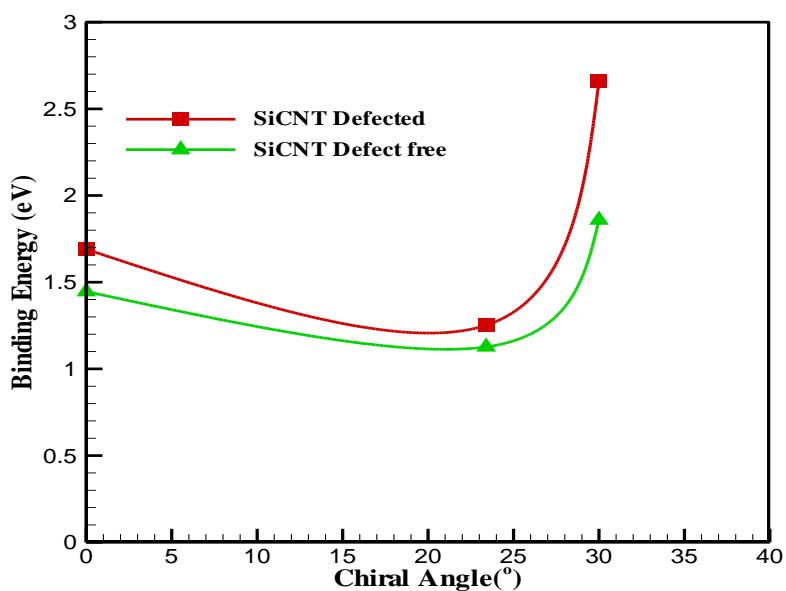


Fig. 7 Binding energy of CO<sub>2</sub> in (9,0), (6,4) and (5,5) SiCNT with respect to chiral angle



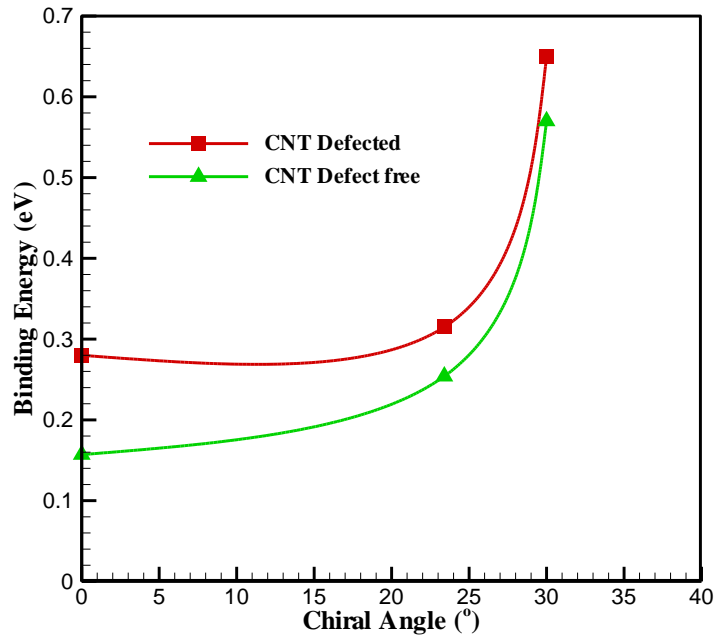


Fig. 8 Binding energy of CO<sub>2</sub> in (9,0), (6,4) and (5,5) CNT with respect to chiral angle

We have also analyzed the electrical properties of tubes through the estimation of various parameters such as HOMO-LUMO energy gap ( $E_g$ ), electronic chemical potential ( $\mu$ ), electrophilicity ( $\omega$ ) and hardness ( $\eta$ ). They are calculated from the HOMO, LUMO energies by the following Equations 2-4. The above parameters are listed in TABLE 2 to 4.

$$\mu = \frac{(E_{HOMO} + E_{LUMO})}{2} \quad (2)$$

$$\eta = \frac{(E_{LUMO} - E_{HOMO})}{2} \quad (3)$$

$$\omega = \frac{\mu^2}{2\eta} \quad (4)$$

where,

- $E_{HOMO}$  – Energy of highest occupied molecular orbital in eV
- $E_{LUMO}$  – Energy of lowest unoccupied molecular orbital in eV
- $\mu$  - Chemical potential in eV
- $\omega$  – Electrophilicity in eV
- $\eta$  – Hardness in eV

From the table, we could observe that there is a decrement in gap in all types of defected nanotubes than defect free tubes of ZnONTs. It is examined that the electronic chemical potential is decreased in all types of tubes. It is also noticed that the decrement in the hardness of the material after CO<sub>2</sub> adsorption in both defected and defect free ZnONT and it indicates the tubes become soft due to adsorption. In SiCNT, energy band gap value decreases in armchair and zigzag tubes due to CO<sub>2</sub> adsorption than the tubes are defect free. The trend is reversed in the presence of defects and CO<sub>2</sub> adsorption. Both these strongly modifies the molecular orbitals. It should be mentioned here that chiral tube is insensitive to CO<sub>2</sub> adsorption. Though chemical potential does not get changed, the tube becomes softer when CO<sub>2</sub> are adsorbed. There is overall increment in the hydrophilicity of the tubes and is more in defect free case than in defected case. Extensive analysis of the interior mechanism for this behavior is yet to be carried out for all types of tubes. In SiCNT the hardness of the material is decreased. We have observed that the hardness of the carbon nanotube remains same before and after adsorption in both cases of defected and defect free. We concluded from the results that the CO<sub>2</sub> adsorption changes the electrical properties of ZnONT, SiCNT and CNT and is more in metallic tubes. In all above nanostructures the electrophilicity index is increased before and after CO<sub>2</sub> adsorption that specifies the tube is chemically active.

**TABLE. 2 HOMO-LUMO band gap ( $E_g$  in eV), electronic chemical potential ( $\mu$  in eV), hardness ( $\eta$  in eV), softness ( $S$  in  $\text{eV}^{-1}$ ), and electrophilicity ( $\omega$  in eV) for the three different Bare and  $\text{CO}_2$  adsorbed ZnONT nanotube without and with defect.**

Without Defect							
ZnONT	HOMO	LUMO	$E_g$	$\mu$	$\eta$	S	$\Omega$
(5,5)+ $\text{CO}_2$	-5.333	-4.536	0.797	-4.9345	0.3985	2.509	30.551
(5,5) bare	-5.038	-2.998	2.04	-4.018	1.02	0.98	7.9138
(9,0)+ $\text{CO}_2$	-4.849	-4.058	0.791	-4.4535	0.3955	2.528	25.074
(9,0) bare	-4.546	-3.352	1.194	-3.949	0.597	1.675	13.060
(6,4)+ $\text{CO}_2$	-4.347	3.718	0.629	-4.0325	0.314	3.179	25.893
(6,4) bare	-4.052	-3.462	0.59	-3.757	0.59	1.694	11.9619
With Defect							
ZnONT	HOMO	LUMO	$E_g$	$\mu$	$\eta$	S	$\Omega$
(5,5)+ $\text{CO}_2$	-3.816	-3.541	0.275	-3.678	0.1375	7.272	49.191
(5,5) bare	-2.930	-2.645	0.285	-2.7875	0.1425	7.017	27.263
(9,0)+ $\text{CO}_2$	-4.871	-4.397	0.474	-4.634	0.237	4.279	45.303
(9,0) bare	-4.604	-3.996	0.608	-4.3	0.304	3.289	30.4111
(6,4)+ $\text{CO}_2$	-4.477	-4.103	0.374	-4.29	0.187	5.347	49.208
(6,4) bare	-4.158	-3.691	0.467	-3.92	0.233	4.282	32.975

**TABLE. 3 HOMO-LUMO band gap ( $E_g$  in eV), electronic chemical potential ( $\mu$  in eV), hardness ( $\eta$  in eV), softness ( $S$  in  $\text{eV}^{-1}$ ), and electrophilicity ( $\omega$  in eV) for the three different Bare and  $\text{CO}_2$  adsorbed SiCNT nanotube without and with defect.**

Without Defect							
SiCNT	HOMO	LUMO	$E_g$	$\mu$	$\eta$	S	$\Omega$
(5,5)+ $\text{CO}_2$	-5.420	-5.330	0.09	-5.375	0.045	22.22	321.006
(5,5) bare	-5.367	-5.097	0.27	-5.232	0.135	7.407	107.00
(9,0)+ $\text{CO}_2$	-5.394	-5.278	0.116	-5.336	0.058	17.241	245.45
(9,0) bare	-5.245	-5.001	0.244	-5.123	0.122	8.196	107.56
(6,4)+ $\text{CO}_2$	-5.336	-5.280	0.056	-5.308	0.028	35.714	503.122
(6,4) bare	-5.155	-5.099	0.056	-5.127	0.028	35.714	469.39
With Defect							
SiCNT	HOMO	LUMO	$E_g$	$\mu$	$\eta$	S	$\Omega$
(5,5)+ $\text{CO}_2$	-5.124	-4.960	0.164	-5.042	0.082	12.19	155.010
(5,5) bare	-4.881	-4.757	0.124	-4.819	0.062	16.12	187.280
(9,0)+ $\text{CO}_2$	-5.012	-4.920	0.092	-4.966	0.046	21.73	268.056
(9,0) bare	-4.682	-4.641	0.041	-4.6615	0.020	48.78	543.123
(6,4)+ $\text{CO}_2$	-5.055	-5.006	0.049	-5.030	0.0245	40.816	516.344
(6,4) bare	-4.826	-4.759	0.067	-4.792	0.033	29.85	347.928

**TABLE. 4 HOMO-LUMO band gap ( $E_g$  in eV), electronic chemical potential ( $\mu$  in eV), hardness ( $\eta$  in eV), softness ( $S$  in  $\text{eV}^{-1}$ ), and electrophilicity ( $\omega$  in eV) for the three different Bare and  $\text{CO}_2$  adsorbed CNT nanotube without and with defect.**

Without Defect							
CNT	HOMO	LUMO	$E_g$	$\mu$	$\eta$	S	$\Omega$
(5,5)+ $\text{CO}_2$	-6.280	-6.075	0.205	-6.177	0.102	9.756	187.03
(5,5) bare	-5.960	-5.778	0.182	-5.869	0.091	10.989	189.25
(9,0)+ $\text{CO}_2$	-6.566	-6.106	0.46	-6.336	0.23	4.347	87.271
(9,0) bare	-6.280	-5.750	0.53	-6.015	0.265	3.773	68.264
(6,4)+ $\text{CO}_2$	-6.211	-6.099	0.112	-6.155	0.056	17.857	338.250
(6,4) bare	-5.936	-5.826	0.11	-5.881	0.055	18.181	314.419
With Defect							
CNT	HOMO	LUMO	$E_g$	$\mu$	$\eta$	S	$\Omega$
(5,5)+ $\text{CO}_2$	-5.687	-5.262	0.425	-5.474	0.212	4.705	70.671
(5,5) bare	-5.301	-4.886	0.415	-5.093	0.207	4.809	62.65
(9,0)+ $\text{CO}_2$	-6.155	-5.917	0.238	-6.036	0.119	8.403	153.08
(9,0) bare	-5.821	-5.577	0.244	-5.699	0.122	8.196	133.109
(6,4)+ $\text{CO}_2$	-5.746	-5.524	0.222	-5.635	0.111	9.009	143.032
(6,4) bare	-5.465	-5.240	0.225	-5.352	0.112	8.888	127.87

#### IV. Conclusions

Doping in nanotubes, creating vacancies and functionalizing with N containing groups are sum of the techniques to improve the adsorption of CO<sub>2</sub> on the tube surfaces. We have compared our results corresponding to both defect free and defected cases and we concluded that the structural defect influences the CO<sub>2</sub> adsorption more than the above technique such as doping and functionalization which are experimentally complicated as it needs controlled growth of the nanostructures. We have also analyzed the band gap and hardness of material should be altered by adsorption and observed that the tube becomes softer due to CO<sub>2</sub> adsorption and becomes chemically active. This is an interesting result for the practical applications of nanostructures in controlling the environment pollution.

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