Journal of
Nanomedicine & Nanotechnology

Lone, J Nanomed Nanotechnol 2016, 7:1
http://dx.doi.org/10.4172/2157-7439.1000354

Research Article Open Access

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Abstract

The adsorption of cytosine on metallic pristine single walled carbon nanotubes (SWNT) surface is investigated using density functional theory with local density approximation. On the SWNT, cytosine is physis orbed by taking WKH Œ Œ LQWHUDFWLRQ %LQGLQJ HQHUJ\ UHSRUWHG LQ WKLV FDVH LV DURXQ F\WRVLQH 6:17 LQWHUDFWLRQ FDQ EH VWURQJO\ HQKDQFHG 7KH HQKDQFHG ELQ H9 LQ SUHVHQFH RI /L DQG &R DWRPV 8VLQJ SULVWLQH 6:17 HOHFWULF VHQVRU VHQVLWLYLW\ 5HSRUWHG ZRUN JLYHV LQVLJKW LQWR 6:17 EDVHG ELR VHQVRUV

Keywords SWNT; Cytosine; Adsorption; Biosensor

Introduction

A er the successful synthesis of experiment [1], carbon nanotubes have attracted much more interest to the research community. Carbon nanotubes have potentials applications in various elds such as architecture, eld-emission, molecular electronics, catalysis and bio-sensors [2-10].

e behavior of ds DNA molecule have been attached to SWCNT was investigated using molecular dynamics simulations [11], which reveals the –staking interaction between nucleo bases and side wall of the nanotubes. e selectivity of single nucleo bases towards adsorption chiral single-wall carbon nanotubes (SWCNTs) using DFT [12], suggested adsorption energies of the nucleo bases has in the order of G>A>T>C which validates experimental work.

To improve the sensitivity of graphene doped by Al shows signi cant interaction with CO molecule [13], it attributes metal doping could enhance sensitivity of graphene.

e biomolecules such as DNA nucleo bases, adsorbed on carbon nanotubes and graphene surface are extensively studied by di erent research groups across the globe.

eoretical Investigations reported in [14] shows that all nucleic acid bases (NABs) guanine, adenine, cytosine, thymine and uracil forms stable stacking with zigzag (7,0) single- walled carbon nanotubes. e interaction energy suggested that among the bases Guanine forms most stable stacking complex.

e interaction energy of nucleic acid bases with graphene and SWNT [15] using DFT-D and MP2 studied in terms of semiempirical molecular orbital method PM3 with dispersive corrections (PM3-D). ese results predicates semiempirical approach is more accurate and cost e ective. e binding energy of various nucleo bases Guanine, adenine, thymine and cytosine with (5, 5) SWNT [16] reported by applying the rst principal HF method.

e binding energy, physisorption, understanding of binding mechanism, interaction of nucleo bases phenomena with carbon nanotubes (SWNT) i.e. conducting, semiconducting have been investigated theoretically and experimentally respectively [17-39].

To exploit the potential of the applying single walled carbon nanotubes (SWNT-6,6) as sensing material, it is very important to understand an interaction between the SWNT(6,6) surface and adsorptive molecules. It is known that such types of interaction are dominated by chemical natures of the molecules and particularly preferential adsorption sites. Most of previous published investigations focused on interactions or adsorption of bimolecular (DNA) onto pristine single walled carbon nanotubes. To understand the e ects of adsorption/doping of the bimolecular-SWNT interaction is still very limited. In this work, we investigated the adsorption of cytosine on pristine single walled carbon nanotubes (SWNT-6,6) and metal-doped SWNT(6,6), applying rst-principles calculation.

Computational Methods

e calculations were performed in the framework of density functional theory with a plane wave basis set. To obtain stable atomic geometries and binding energies we used the Vienna Ab initio simulation package (VASP) [27] with ultra-so pseudo potentials [28]. is approach makes carrying out numerous computations feasible for system with a large number of atoms per unit cell. We expanded the cuto energy was increased up to 29.1 Ry (396 eV) to cheek the convergence of the result, further, we calculated exchange-correlation potential within the generalized gradient approximation (GGA) [29].

Each system consists of a 12.30 × 12.30 × 10 Å SWNT super cell (96 C atoms) with cytosine molecules adsorbed. We used a 1 × 1 × 3 Monkhorst–Packgrid [30] fork-point sampling of the Brillouinzone. e k-point is set to 3 × 3 × 1 for the Brillouin zone integration. e structural con gurations of the isolated SWNT (6, 6) are optimized through fully relaxing the atomic structures. With the same super cell and k-points sampling, the con gurations of the di erent molecule-SWNT systems were optimized through fully relaxing the atomic structures until the remaining forces are smaller than 0.01 eV/Å. e binding energy of cytosine on SWNT is calculated as

$$E_{ad} = E_{(molecule@SWNT)} - E_{(SWNT)} - E_{(molecule)} \quad (1)$$

e above calculation method was tested on a well-known system, e.g. the interaction of (6, 6) SWNTs with benzene, and reported binding energy of -0.12 eV, which is consistent with the previous reports [31].

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Received 'HFHPEHU Accepted)HEUXDU\ Published February

Citation: /RQH (% $GVRUSWLRQ RI &\WRVLQHRQ 6L Nanotubes. - 1DQRPHG 1DQRWHFKQRO GRL

e electron transport calculations were performed using the Atomistix Tool Kit (ATK) 2.0.4 package [32], which were implements DFT-based real-space, nonequilibrium Green's function (NEGF) formalism. e mesh cuto is chosen as 200 Ry to achieve a reasonable balance between calculation e ciency and accuracy.

Results and Discussion

To know nature of the cytosine and SWNT (6, 6) the chemical, simulated structures have been shown in (Figures 1a-1d) respectively.

To nd the most favorable adsorption con gurations, the molecule under investigation was initially placed at di erent positions above the graphene with di erent orientations. Figure 2 shows the possible adsorption con gurations of cytosine on pristine and metal doped graphenes. For convenience, the adsorption con gurations shown in Figures 2a-2e are referred as hollow, bridge and stack con gurations, respectively.

e corresponding binding energy for di erent con gures are tabulated in Table 1. In Table 1 adsorption energy (E_{ad}), Equilibrium SWNT-molecule distance (d) which is de ned as shortest atom to atom distance, and Mullikan charge (Q) of cytosine absorbed on metallic SWNT (6, 6) the stack con guration has a higher binding energy (-0.38 eV) than the hollow (-0.16 eV) or bridge (-0.26 eV), hence is the favorable adsorption con guration. Only small charge transfer occurs in all the three con gurations, which clearly shows that the interaction is physisorption. e mechanism of the interaction is attributed to - stacking. e calculated binding energies are close to that reported for the nucleoside/SWNT (-0.42 to -0.46 eV) [14] adenine/carbon nanotubes (-0.35 eV), [15] andinteraction energy of nucleic acid bases with graphene and carbon nanotubes [16] and Binding of nucleo bases with single-walled carbon nanotubes systems [17].

Two atoms were used to dope the metallic SWNT (6, 6). To study the e ect of metal doping in the optimize structure of SWNT-Li-Cytosine; practically there is no deformation in the geometry of SWNT and cytosine. In short, both remains near planer. Two hydrogen of the cytosine tilt slightly towards the SWNT (6, 6) between Li atom and cytosine is 2.26 Å, (Figure 3a) the distance i.e. shortest atom to atom distance is 2.26 Å, But in case of the geometry of the cytosine becomes deformed a er adsorbing onto the Co-doped SWNT (Figures 3b and 3c) shows strong interaction taking place. e distance between Co and cytosine is 1.95 Å. e reported binding energies are 0.56 and -0.20 eV for Li and Co doped single walled carbon nanotubes which con rms the Co doped SWNT's shows a stronger binding to bio molecule cytosine than Li doped SWNT's (6, 6). Figure 3 compares the electronic total charge density plot of the cytosine@Li-SWNT (6, 6) with that of the Co-SWNT (6, 6) the small gap of the electron orbital appears between Li atom and cytosine (Figure 3b). Whereas in case of the cytosine@Co-SWNT (6,6) the electronic charge strongly overlapped, which leading to more orbital mixing and a large charge transfer. e Mullikan population analysis reveals, the Co loaded on +1.92 were considered as positively charged ion in the adsorption adduct. e large charge (-0.61) is transformed from SWNT to cytosine in the presence of Co atom with high binding energy, depicts a strong chemical bond formed between the cytosine and Co-SWNT (6, 6) ,this re ects in the Table 1.

Figure 4 indicates the total electronic charge density of states (DOS) for the stack (Figure 2c) also metal doped con gurations (Figures 2d and 2e) respectively. Comparing with the metallic single wall carbon nanotubes (6, 6), the DOS of cytosine SWNT system indicates very minute change near the Fermi level (Figures 4a and 4b), on adsorption

Figure 2: 6FKHPDWLF YLHZ RI WKH F\WRVLQH DGVRUE GLIIHUHQW FRQ¿JXUDWLRQV D KROORZ E EULG 6:17 DQG H &R GRSHG ZLWK 6:17

System	E_{ad} (eV)	d (Å)	Q (e)
&\WRVLQH#KROORZ 6:17			
&\WRVLQH#EULGJH 6:17			
&\WRVLQH#VWDFN 6:17			
&\WRVLQH#/L 6:17			
&\WRVLQH#&R 6:17			

Table 1: $GVRUSWLRQ HQHUJLHV EULGJH 6:17 PROHFXOH GL DV WKH VKRUWHVW DWRP WR DWRP GLVWDQFH DQ DGVRUEHG RQ 6:17

Figure 3: 6FKHPDWLF YLHZ RI WKH F\WRVLQH DGVRUE GLIIHUHQW FRQ¿JXUDWLRQV D KROORZ E EULG 6:17 H &R GRSHG ZLWK 6:17

Figure 1: The schematic view of the cytosine: Chemical structure (a) ,simulated VWUXFWXUH DW E & 1 2 DQG + DWRPV DUH VKRZQ DV EDOOV DQG VWLFNV ZKLWH UHVSHFWLYHO\ E WRS YLHZ F\WRVLQH F 6:17 G

Figure 4: 7KH '26 RI D 7KH SULVWLQH 6:17 GDVKHG OLQH &\WRVLQH 6:17 VROLG OLQH E &R 6:17 GDVKHG OLQH &\WRVLQH &R 6:17 VROLG OLQH FDOFXODWHG IRU WKH FRUUHVSRQGLQJ FRQ¿JXUDWLRQV VKRZQ LQ)LJXUH F $ VFKHPDWLF LOOXVWUDWLRQ RI WKH 6:17 EDVHG FKHPLFDO VHQVRU IRU GHWHFWLQJ F\WRVLQH G $ FRPSDULVRQ SORW RI WKH , 9 FXUYHV IRU WKH GHYLFHV EDVHG RQ 6:17 &\WRVLQH#6:17 &R 6:17 F\WRVLQH#&R 6:17

there is no signi cant conductivity changes. e minute or little change in DOS near the Fermi level is consistent with relative to small binding energy. When the cytosine adsorbed on Co-doped SWNT a abrupt change occurs near the Fermi level which is agreement with the high binding energy values. erefore we conclude that metallic SWNT cannot suitable for cytosine as sensing material, whereas Co-doped SWNT shows high sensitivity.

To study the sensing properties of the metallic single wall carbon nanotubes (6,6), the electron transport properties and Co-doped SWNT were simulated using NEGF methods. e chemical sensing transducer is the resistance sensor which is the simplest one. In this type resistance change of the sensing materials upon the adsorption of chemicals is detected. SWNT-based resistance sensors are simulated using a model consisting of SWNT(6,6) contacted by two SWNT electrodes as depicted in Figure 4c, we determined series of current versus voltage (I-V) curves for SWNT junction with and without the adsorption of cytosine. e simulated I-V curves for the metallic SWNT and Co-doped SWNT before and a er cytosine adsorption are shown in Figure 4d.

e SWNT shows nonlinear behavior. e Co-SWNT is more conductive than the metallic SWNT (6,6) due to the possibility that the states of the SWNT are hybridized with 4s and 3d levels of the Coin the DOS near the Fermi level [40]. e I-V curves shows that the Co-SWNT has the highest response to cytosine. When the bias voltage is higher than 1.5 V, the Co-SWNT shows a sensitivity one magnitude higher than that of the metallic single wall carbon nanotubes.

Conclusion

Investigated calculations suggested that the cytosine have a very weak interaction with pristine single walled carbon nanotubeSWNT(6-6) surface. erefore, chemically or physically modify SWNT are required for more e ective adsorption to this molecule. We investigated that strong binding can be achieved by introducing metal atoms on the SWNT surface. Particularly, the Co-doped SWNT shows strong interaction with cytosine and consequently exhibits much higher sensitivity than the pristine SWNT. Reported result provides useful to develop novel SWNT -based for immobilization as well as detection of DNA molecules on SWNT surface.

Acknowledgements

7KH DXWKRUV DUH JUDWHIXO WR WKH ¿QDQFLDO VXSSRUW IURP GHSDUWPHQW RI VFLHQFH DQG WHFKQRORJ\ 1HZ 'HOKL ,QGLD XQGHU)$67 75$&. 6&+(0(IRU <281* 6&,(17,67 *5$17 1R 65)7 /6 2<6 7KH VLPXODWLRQ ZRUN ZDV FRQGXFWHG LQ WKH +LJK 3HUIRUPDQFH &RPSXWLQJ RI &HQWUDO 5HVHDUFK /DERUDWRU\ DW V. P. College, Vaijapur, Dist. Aurangabad, Maharashtra, India

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1. ,MLPD 6 KHOLFDO PLFURWXEXOHV RI JUDSKLW

Saito R, Dresselhaus G, Dresselhaus MS (1999) Physical Properties of carbon QDQRWXEHV ,PSHULDO &ROOHJH 3UHVV /RQGRQ

:LOOLDPV .$ 9HHQKXL]HQ 37 GH OD 7RUUH %* 1DQRWHFKQRORJ\ FDUERQ QDQRWXEHV ZLWK '1$ U

$OLGRUL 6 $VTLULGL . /RQGHUR 3 %HUJNYLVW 0 RNA and DNA with Functionalized Carbon Nanotubes. J Phys Chem C 1DQRPDWHU ,QWHUIDFHV

$EGXOD 1+7 &KHERWDUHY $3 KRLPDQL 07 5DKPDQL 0 6DHLGP DNA sensor model based on a carbon nanotube network in the degenerate FRQFHQWUDWLRQ 3HWUOHXP 3URF GHWHFWLQJ

&KHQ &/ <DQJ &) $JDUZDO 9 .LP 7 6RQNXVDOH GHFRUDWHG FDUERQ QDQRWXEH EDVHG FKHPLFDO oxide semiconductor circuitry. IOP Nanotechnology

7. &KHQJ 06 7RK &6 1RYHO ELRVHQVLQJ PHWKR GHWHFWLRQ RI YLUXVHV $QDO\VW

(UGHP $ 0XWL 0 .DUDGHQL] + &RQJXU * &DQDYD PRQLWRULQJ RI LQGLFDWRU IUHH '1$ K\EULGL]DWL PRGL¿HG GLVSRVDEOH JUDSKLWH VHQVRUV &ROO

9. *RQJ -/ 6DUND 7 %DGKXOLND 6 0XFKDQGDQL $ ELRVHQVRU IRU PHUFXU\ ,, EDVHG RQ VLQJOH VWUXFWXUH VZLWFKLQJ '1$ $SSO 3K\V /HWW

*XR /4 <LQ 1 1LH '' *DQ -5 /L 0- HW DO / sensor for mercury(II) ion by using carbon nanotubes to reduce background VLJQDO $QDO\VW

11. $OHJUHW 1 6DQWRV (5RGUtJXH])RUWHD $ 5LXV disruption of small double stranded DNA molecules on carbon nanotubes: A PROHFXODU G\QDPLFV VWXG\ &KHP 3K\VLFV /HWW

$NGLP % 3DFKWHU 5 'D\ 31 .LP 66 1DLN 55 ELRPROHFXODU VXUIDFH QRQERQGHG LQWHUDFWL DGVRUSWLRQ RQ VLQJOH ZDOO FDUERQ QDQRWXEH

$R =0 <DQJ - /L 6 -LDQJ 4 (QKDQFHPHQW RI JUDSKHQH &KHP 3K\V /HWW

6KXNOD 0. 'XEH\ 0 =DNDU (1DPEXUX 5 &]\]QLNR ,QWHUDFWLRQ RI QXFOHLF DFLG EDVHV ZLWK VLQ 3K\V /HWW

5DPUDM $ +LOOLHU +, 9LQFHQW 0$ %XUWRQ 1$ quantum chemical methods for calculating the interaction energy of nucleic acid EDVHV ZLWK JUDSKHQH DQG FDUERQ QDQRWXEHV

'DV $ 6RRG $. 0DLWL 3. 'DV 0 9DUDGDUDMDQ 5 ZLWK VLQJOH ZDOOHG FDUERQ QDQRWXEHV 7KHRU

17. /RQH % 6FKHLQHU 6 .DU 7 &RPSHWLWLRQ EH JURXSV IRU WKH SUHIHUUHG VLWHV DW WKH SH &DUERQ

$PLUDQL 0& 7DQJ 7 &XHUYR - 4XDQWXP PHFKD energy between DNA nucleobases and carbon nanotube: A DFT analysis. 3K\VLFD (

19. *RWKDP 6 6FKHLFKHU 5+ 3DQGH\ 5 .DUQD 63 SULQFLSOHV VWXG\ RI SK\VLVRUSWLRQ RI QXFOH FDUERQ QDQRWXEHV 1DQRWHFKQRORJ\

1HKVLDO 6 3HUL\DVDP\ * 6DPDQWD 3. 3DWL 6. binding mechanism of various chiral SWCNTs and ssDNA: a computational VWXG\ - 3K\V &KHP %

0D\R 0/ &KHQ =4 .LOLQD 69 &RPSXWDWLRQD 6HOHFWLYLW\ LQ '1$ &DUERQ 1DQRWXEH +\EULGV

0HQJ 6 0DUDJDNLV 3 3DSDORXNDV & .D[LUDV (LQWHUDFWLRQ DQG LGHQWL¿FDWLRQ ZLWK FDUERQ

4LX ; .KULSLQ &< .H) +RZHOO 6& =KHQJ 0 LQWHUDFWLRQV EHWZHHQ K\EULG '1$ FDUERQ QD

5DQMDQ 1 6HLIHUW * 0HUWL 0 +HLQH 7 :UDSSLQJ FDUERQ QDQRWXEHV ZLWK '1$ $ WKHRUHWLFDO VWXG\ $,3 &RQIHUHQFH 3URFHHGLQJV

6DUPDK $ 5R\ 5. 8QGHUVWDQGLQJ WKH ,QWHUDFWLRQ RI 1XFOHREDVHV ZLWK &KLUDO 6HPLFRQGXFWLQJ 6LQJOH :DOOHG &DUERQ 1DQRWXEHV $Q $OWHUQDWLYH 7KHRUHWLFDO $SSURDFK %DVHG RQ 'HQVLW\ )XQFWLRQDO 5HDFWLYLW\ 7KHRU\ - 3K\V &KHP &

5R[EXU\ ' -DJRWD $ 0LWWDO - 6WUXFWXUDO FKDUDFWHUL]DWLRQ RI '1$ VWUDQGV DGVRUEHG RQWR VLQJOH ZDOOHG FDUERQ QDQRWXEHV - 3K\V &KHP %

.UHVVH * +DIQHU - $E LQLWLR PROHFXODU G\QDPLFV IRU OLTXLG PHWDOV 3K\V 5HY %

9DQGHUELOW ' 6RIW VHOI FRQVLVWHQW SVHXGRSRWHQWLDOV LQ D JHQHUDOL]HG HLJHQYDOXH IRUPDOLVP 3K\V 5HY % &RQGHQV 0DWWHU

+XDQJ < =KDR 6 /LX <0 &KHQ - &KHQ =) HW DO $Q DPSOL¿HG VLQJOH ZDOOHG FDUERQ QDQRWXEH PHGLDWHG FKHPLOXPLQHVFHQFH WXUQ RQ VHQVLQJ SODWIRUP IRU XOWUDVHQVLWLYH '1$ GHWHFWLRQ

0RQNKRUVW +- 3DFN -' 6SHFLDO SRLQWV IRU %ULOORXLQ]RQH LQWHJUDWLRQV 3K\V 5HY %

/X - 1DJDVH 6 =KDQJ ; :DQJ ' 1L 0 HW DO 6HOHFWLYH LQWHUFDODWLRQ RI ODUJH RU FKDUJH WUDQVIHU DURPDWLF PROHFXOHV ZLWK PHWDOOLF VLQJOH ZDOO FDUERQ nanotubes: critical role of the molecular size and orientation. J Am Chem Soc

:DQJ 1 5DQJH ' +D 1 $ 6L ' 6LW '1$ 0L[HG 0RQR DQG GL EDVHV RI QXFOHRVLGH VROXWLRQ VHQVRUV

.\EHUW 1- /LQQHU 0% <RGK -6 3UHVL * -RKQVRQ $7& FRPSOH[YDSRU PL[WXUHV XVLQJ YHUVDWLOH '1$ FDUERQ QDQRWXEH FKHPLFDO VHQVRUV

/LX + +H - 7DQJ - /LX + 3DQJ 3 HW DO 7UDQVORFDWLRQ RI VLQJOH VWUDQGHG '1$ WKURXJK VLQJOH ZDOOHG FDUERQ QDQRWXEHV

/LX / <DQJ & =KDR . /L - :X +& 8OWUDVKRUW VLQJOH ZDOOHG FDUERQ QDQRWXEHV LQ D OLSLG ELOD\HU DV D QHZ QDQRSRUH VHQVRU

0DQRKDU 6 7DQJ 7 -DJRWD $ 6WUXFWXUH RI KRPRSRO\PHU '1$ &17 K\EULGV - 3K\V &KHP &

5DMHVK & 0DMXPGHU & 0L]XVHNL + .DZD]RH < $E LQLWLR VWXG\ RQ WKH LQWHUDFWLRQ RI '1$ QXFOHRVLGHV ZLWK VLQJOH ZDOOHG FDUERQ QDQRWXEHV $SSO 3K\V /HWW

5R[EXU\ ' 0LWWDO - -DJRWD $ 0ROHFXODU EDVLV RI QDQRWXEH UHFRJQLWLRQ E\ VLQJOH VWUDQGHG '1$

*DQJ +6 6HOHFWLYH LQWHUFDODWLRQ RI 7KHRUHWLFDO 6WXG\ RI %LQGLQJ RI 1XFOHREDVHV RQ 6LQJOH ZDOOHG &DUERQ 1DQRWXEHV ZLWK 'LR[LQ $P &KHP 6

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