

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

Results and Discussion

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

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

The corresponding binding energy for different configurations are tabulated in Table 1. In Table 1, adsorption energy (E_{ad}), equilibrium SWNT-molecule distance (d) which is defined as the shortest atom-to-atom distance, and Mulliken charge (Q) of cytosine adsorbed on metallic SWNT (6, 6) the stack configuration has a higher binding energy (-0.38 eV) than the hollow (-0.16 eV) or bridge (-0.26 eV), hence it is the most favorable adsorption configuration. Only a small charge transfer occurs in all the three configurations, which clearly shows that the interaction is physisorption. The mechanism of the interaction is attributed to π - π stacking. The calculated binding energies are close to those reported for the nucleoside/SWNT (-0.42 to -0.46 eV) [14], adenine/carbon nanotubes (-0.35 eV), [15] and interaction energy of nucleic acid bases with graphene and carbon nanotubes [16] and binding of nucleobases with single-walled carbon nanotubes systems [17].

Two atoms were used to dope the metallic SWNT (6, 6). To study the effect of metal doping in the optimized structure of SWNT-Li-Cytosine; practically there is no deformation in the geometry of SWNT and cytosine. In short, both remain near planar. Two hydrogen atoms 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 after adsorbing onto the Co-doped SWNT (Figures 3b and 3c) shows strong interaction taking place. The distance between Co and cytosine is 1.95 Å. The reported binding energies are 0.56 and -0.20 eV for Li and Co-doped single-walled carbon nanotubes which confirms that the Co-doped SWNT shows a stronger binding to the biomolecule cytosine than Li-doped SWNTs (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 overlaps, which leads to more orbital mixing and a large charge transfer. The Mulliken

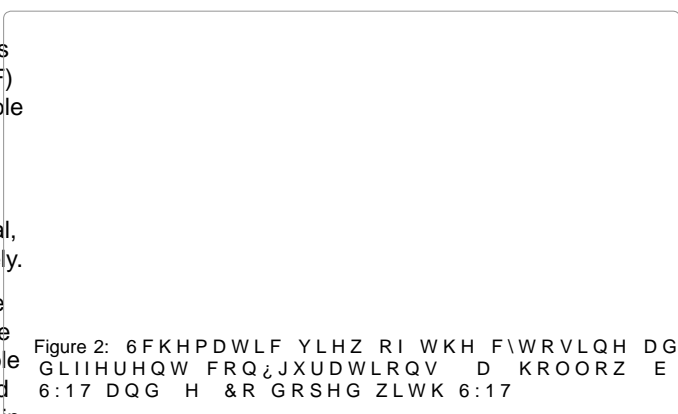


Figure 2: 6FKHPDWLF YLHZ RI WKH F\WRVLRQ DGVRUEHGLIIHUHQW FRQJXUDWLRQV D KROORZ E EULGJH 6:17 DQG H &RGRSHG ZLWK 6:17

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

Table 1: \$GVRUSWLRQH#EULXP 6:17 PROHFXOH GLDVRWKH VKRUWHVW DWRP WR DWRP GLVWDQFH DQ DGVRUEHG RQ 6:17

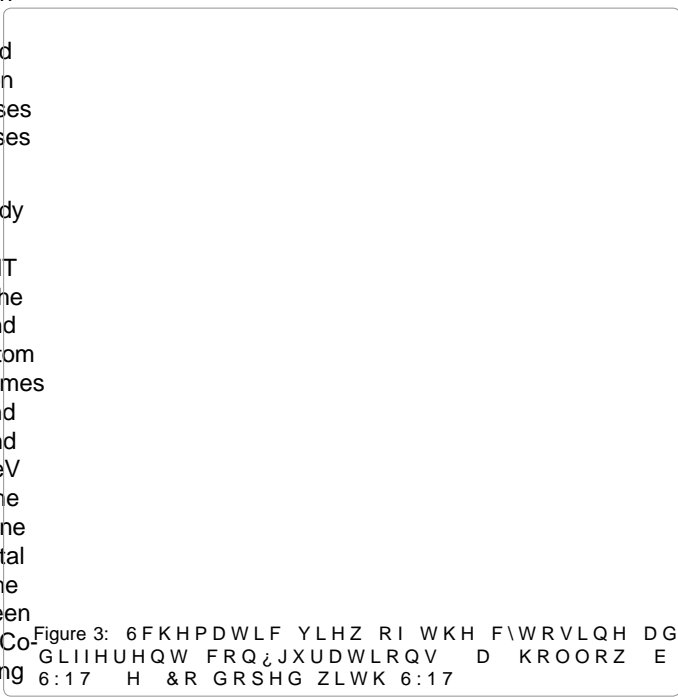


Figure 3: 6FKHPDWLF YLHZ RI WKH F\WRVLRQ DGVRUEHGLIIHUHQW FRQJXUDWLRQV D KROORZ E EULGJH 6:17 H &RGRSHG ZLWK 6:17

population analysis reveals, the Co loaded on +1.92 were considered as positively charged ion in the adsorption adduct. The 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 reflects in the Table 1.

Figure 4 indicates the total electronic charge density of states (DOS) for the stack (Figure 2c) also metal doped configurations (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

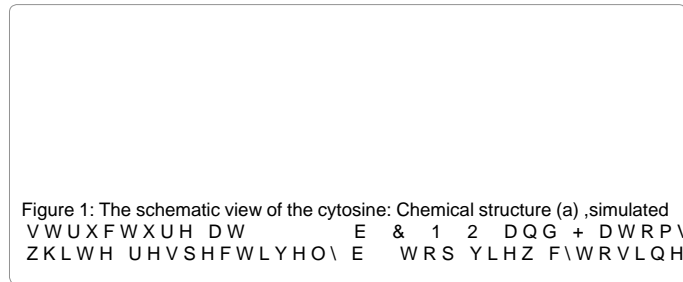
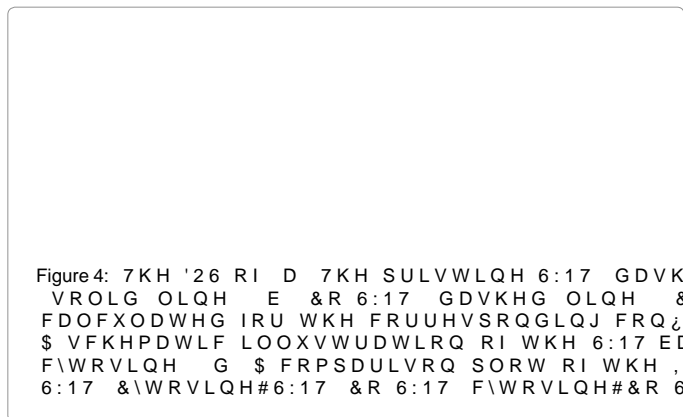


Figure 1: The schematic view of the cytosine: Chemical structure (a), simulated structure (b) on SWNT (6, 6). VWUXFWXUHDW E & 1 2 DQG + DWRPVDZKLWH UHVSHFWLYHO\ E WRS YLHZ F\WRVLRQH





there is no significant conductivity changes. The 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. Therefore 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. The 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. The simulated I-V curves for the metallic SWNT and Co-doped SWNT before and after cytosine adsorption are shown in Figure 4d.

The SWNT shows nonlinear behavior. The 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 Carbon. The DOS near the Fermi level [40]. The 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 nanotube SWNT(6-6) surface. Therefore, chemically or physically modify SWNT are required for more effective 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.

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5DQMDQ 1 6HLIHUW * 0HUWL 0 +HLQH 7 :UDS 5DQRFDUERQRQDQRWXEHV ZLW&E LQLWLR PRGHOL
 '1\$ \$ WKHRUHWLFDQ VWXG\ \$,3 &RQIHUHQFH 3URFHSURSLWLVH RI PROHFXODU HOHFWURQLF GHYLFH
 6DUPDK \$ 5R\ 5. 8QGHUVWDQGLQJ WKH ,QWHLQWLRQ-R1DQFQR6DVH - 3DUN -< HW DO
 ZLWK &KLUDO 6HPLFRQGXFWLQJ 6LQJOH :DOOHG &RQDQ 1DQRWXEHVARD\$Q\$OWHQRVGHV 6HQVRUV
 7KHRUHWLFDQ \$\$\$SURDFK %DVHG RQ 'HQVLW\)XQFWLRQDO 5HDFWLYLW\ 7KHRU\ - 3K\V
 &KHP & .EHUW 1- /HUQHU 0% <RGK -6 3UHVL * -RKQVRQ
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 5R[EXU\ ' -DJRWD \$ 0LWWDQ - 6WUXFWXUDODFKDUDFWLULWLV RI ROLJRPULF
 '1\$ VWUDQQGV DGVRUEHG RQWR VLQJOH ZDOOHG FDUERQ QDQRWXEHV - 3K\V &KHP
 % /LX + +H - 7DQJ - /LX + 3DQJ 3 HW DO 7UDQ
 '1\$ WKURXJK VLQJOH ZDOOHG FDUERQ QDQRWXEHV
 .UHVVH * +DIQHU - \$E LQLWLR PROHFXODU G\ODPLFV IRU OLTXLG PHWDOV 3K\V
 5HY % /LX / <DQJ & =KDR /L - :X +& 8OWUDVQR
 QDQRWXEHV LQ D OLSLG ELOD\HU DV D QHZ QDQRS
 9DQGHUELOW ' 6RIW VHOI FRQVLVWHQW SVHXGRSRWHQWLDOV LQ D JHQHUDOLJHG
 HLJHQYDOXH IRUPDOLVP 3K\V 5HY % &RQGHQV 0DWWHU
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 ZDOOHG FDUERQ QDQRWXEH PHGLDWHG FKHPLOXPLQHVHGH%WUHQDQYHVHQRVQFKDQGDQL \$
 SODWIRUP IRU XOWUDVHQVLWLYH '1\$ GHWHFWLRQ VLQJOH ZDOOHG &FDERQ QDQRWXEH EDVHG FKHPLO
 \$SSO 3K\V /HWW
 0RQKRUVW +- 3DQJ 6LHFLDO SRLQVW IRU %ULOORX 5RFXU\ ' 0LWWDQ DJRWD \$ 0ROHFXODU E
 3K\V 5HY % QDQRWXEH UHFRJQLWLRQ E\ VLQJOH VWUDQQGHG '1
 /X - 1DJDVH 6 =KDQJ ; :DQJ ' 1L 0 HW DO 6RQHFLYH LQWHLWLRQDO 6WVG\ RI %LQGLQJ RI C
 ODUJH RU FKDUJH WUDQVIHU DURPDWLF PROHFXOHV ZLWK PHWDOOLV VLQJOH ZDOOHG FDUERQ \$P &KHP 6
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Citation: /RQH (% \$GVRUSWLRQ RI &\WRVLQHRQ 6LQJPHZDQDQG7&DUEHQ 1DQRPHG 1DQRWHFKRO GRL

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