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Analytical Prediction of Highly Sensitive CNT-FET-Based Sensor Performance for Detection of Gas Molecules

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ABSTRACT In this study, a set of new analytical models to predict and investigate the impacts of gas adsorption on the electronic band structure and electrical transport properties of the single-wall carbon nanotube field-effect transistor (SWCNT-FET) based gas sensor are proposed. The sensing mechanism is based on introducing new hopping energy and on-site energy parameters for gas-carbon interactions representing the charge transfer between gas molecules (CO_2, NH_3, and H_2O) and the hopping energies between carbon atoms of the CNT and gas molecule. The modeling starts from the atomic level to the device level using the tight-binding technique to formulate molecular adsorption effects on the energy band structure, density of states, carrier velocity, and *I-V* characteristics. Therefore, the variation of the energy bandgap, density of states and current-voltage properties of the CNT sensor in the presence of the gas molecules is discovered and discussed. The simulated results show that the proposed analytical models can be used with an electrical CNT gas sensor to predict the behavior of sensing mechanisms in gas sensors.

INDEX TERMS Carbon nanotube, gas sensor, adsorption, field-effect transistor, *I-V* characteristics.

I. INTRODUCTION

The importance of monitoring of the gases using sensors and determining their concentrations and compositions is increasing because of the safety reasons and strict environmental regulations [1]–[5]. Depending on their type, sensors can be used in various fields such as medical and health care, food and agriculture industry, environmental monitoring, semiconductor processing, industrial safety, household security, etc. [6]–[10]. Therefore, the area of the sensors has been subject to numerous research works both in theoretical and experimental aspects. Obviously, sensors with high sensitivity and chemical stability, fast response time, and high accuracy with economical fabrication process are desirable [11]–[14].

Compared to conventional materials used as a platform for sensor fabrication, carbon nanotubes (CNTs) exhibit superior performance [15]–[17]. CNTs can be implemented for various applications such as supercapacitors, superconductors, batteries, sensors and etc. CNTs possess subtle electronic properties that enable them to improve electron transfer properties in electrochemical reactions with electroactive species when using in sensor structure [18], [19]. Offering unique structure, they have a large surface to volume ratio and are very sensitive to their environment which makes them overcome limitations of conventional devices and an ideal candidate for gas sensing applications [20]–[22]. The required temperature for sensing various gases is different and it is important that sensors can operate at room temperature. Nowadays, some metal oxide gas sensors can work and detect gas molecules at room temperature [23]. However, for

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some sensors and detection of some gases, the metal oxide gas sensors demand higher temperatures to operate [24], [25]. For example, it has been reported that for the detection of NO_2 or NH_3 gases metal oxide sensors have to operate at the temperature above 200 °C to achieve proper sensitivity [23], [26], [27]. While carbon nanotube-based gas sensors can detect numerous toxic gases at room temperature [27]. On the other hand, the high surface area of the CNT sensors provides a fast response which may also cause slow recovery of these sensors, hence some techniques such as UV radiation can be used to improve the recovery time [27], [28]. Fig. 1 shows the structure of a carbon nanotube that is formed by rolling up a graphene sheet. The structural and electrical characteristics of CNTs are affected by the diameter and helicity of the formation of graphitic rings in CNT walls that lead to semiconducting or metallic nanotubes. These properties are determined by the geometrical parameter called a chiral vector $\vec{C}_h = n\vec{a}_1 + m\vec{a}_2$, where $\vec{a}_1$ and $\vec{a}_2$ are base vectors of the unit cell and n and m are integers [29].

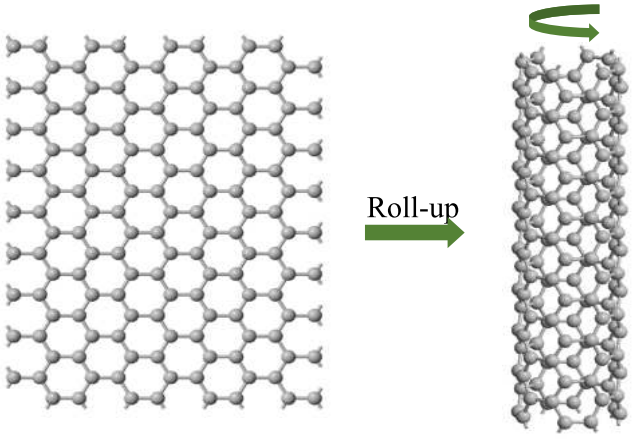

FIGURE 1. An SWCNT comprised of rolling up a graphene sheet into a cylinder.

In terms of the number of concentric cylinders, there are two types of CNTs, single-wall (SWCNT) and multi-wall (MWCNT). The number of cylinders and the length and radius of the cylinder affects both the physical and electrical properties of CNTs.

The illustration of a carbon nanotube field-effect transistor (CNTFET) based gas sensor is shown in Fig. 2. Theoretical and experimental studies have shown the superior sensitivity of carbon nanotubes when exposed to various gas molecules.

Electrically, CNT is very sensitive toward adsorption or desorption of charge and experience notable changes in its carrier concentration and electrical conductance upon molecular adsorption [30], [31]. In addition, molecular adsorption can affect physical properties, modify energy band structure, and change the CNT bandgap. Consequently, the carrier concentration and bandgap variations modulate various CNT characteristics such as the density of states (DOS), conductivity, carrier velocity and *I-V* characteristics of the CNT. In this study, this concept is used to model and study gas adsorption

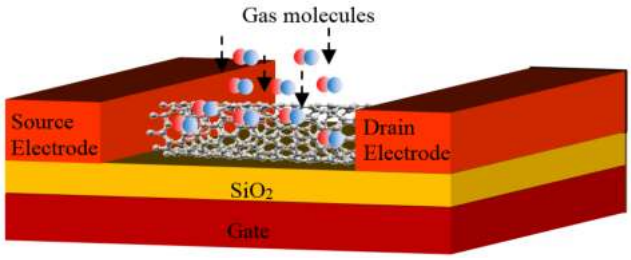

FIGURE 2. Schematics of carbon nanotube field-effect transistor (CNTFET) based gas sensor.

effects on the energy band gap, DOS, carrier velocity and *I-V* characteristics of the sensor. These parameters are important factors that can be used to monitor and detect various gases and investigate the sensing mechanism in CNT based gas sensors to design highly sensitive sensors and improve sensor performance.

II. TIGHT BINDING FORMALISM

Carbon nanotubes can be an armchair, zigzag or chiral depending on the graphene roll-up angle defined by the direction of the chiral vector. In the chiral vector, when the unit vectors n and m are equal, the CNT is an armchair type with metallic properties, and when m is zero the CNT is a zigzag nanotube that can be either metallic or semiconducting; else, it would be a chiral CNT [32], [33]. The diameter of a CNT can be determined as given.

$$d = \frac{\sqrt{3}a_{C-C}}{\pi}\sqrt{n^2 + m^2 + nm} \tag{1}$$

where n and m are the chiral numbers. Here, we use metallic zigzag CNT for the sensor modeling because its zero bandgaps provide higher sensitivity against target analytes. This is because the lower energy band gap provides higher conductivity, thus any small change in the carrier concentration of the CNT will significantly affect the *I-V* characteristics of the sensor. The impurity molecules can affect the physical and electrical properties of carbon nanotubes when adsorbed to their surface. Here, we start from the electronic band structure of the ZCNT to model and investigate its changes after gas molecules adsorption. For modeling of the electronic band structure, it is needed to solve the time-independent Schrödinger equation [14]:

$$H\psi(k, r) = E(k)\psi(k, r) \tag{2}$$

where E is the energy, H is the Hamiltonian and ψ is the wave function. The wave vector should satisfy the periodic boundary condition and Bloch's theorem [34]. To solve the Schrödinger equation, the unit vectors $\vec{a_1}$ and $\vec{a_2}$ corresponding to the graphene unit cell are given as:

$$\vec{a_1} = a\hat{x} + b\hat{y}, \quad \vec{a_2} = a\hat{x} - b\hat{y} \tag{3}$$

where $a = 3a_0/2$, $b = \sqrt{3}\, a_0/2$ and $a_0 = 1.42\dot{A}$ which is nearest neighbor carbon to carbon atom distance in graphene unit cell.

We used the tight-binding method based on the nearest neighbor approximation to solve the Schrödinger equation. For the graphene, only 2pz orbitals of each carbon atom around the Fermi energy contributes forming the conduction and valence band that are responsible for the electrical conduction. In other words, by assuming a single orbital per carbon atom the conduction and valence bands can appropriately be described. This results in a (2×2) matrix $\left[h\left(\overrightarrow{k}\right)\right]$ that can be achieved by summation of any unit-cell (n^{th} unit-cell) with its four neighbor unit-cells, which (as discussed in our previous work) results in the energy dispersion for the graphene given as [33], [35]:

$$E\left(\overrightarrow{k}\right)=\pm\sqrt{t^2+4t^2\cos\left(k_y b\right)\cos\left(k_x a\right)+4t^2\cos^2\left(k_y b\right)} \tag{4}$$

where t is the hopping energy between two adjacent carbon atoms. Once the graphene sheet is rolled up into a cylindrical shape, the value of the propagation parameter, k, is constrained by the imposition of periodic boundary condition along the chiral vector. The requirement of the periodic boundary condition for the zigzag CNT with a circumferential vector along the y-direction can be expressed as:

$$k_y=\frac{2\pi\upsilon}{2nb} \tag{5}$$

where υ is the sub-band index and n is the chiral number. Applying this condition to Equation (4), the E-k relation for the zigzag CNT is achieved:

$$E_{zc}\left(\overrightarrow{\mathrm{k}}\right)=\pm\sqrt{t^2+4t^2\cos\left(\frac{\pi\upsilon}{n}\right)\cos\left(k_x a\right)4t^2+\cos^2\left(\frac{\pi\upsilon}{n}\right)} \tag{6}$$

To investigate the sensing properties, adsorption of the target analytes in the form of gas molecules is considered as illustrated in Fig. 3. In our model, we assumed adsorption of a gas molecule in such a way that in the ZCNT the second carbon atom of each unit cell is bound to a gas molecule.

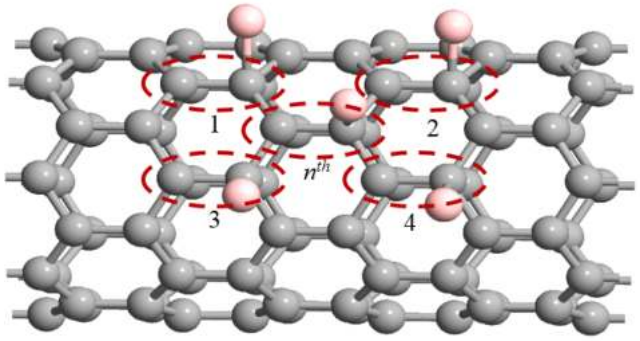

FIGURE 3. Configuration of gas molecules adsorbed on the zigzag CNT. The unit-cells 1, 2, 3, and 4 are the nearest neighbor unit-cells of the n^{th} unit-cell.

According to the tight-binding model, the Hamiltonian matrix for the unit-cell n^{th} and its four neighbors can be described as:

$$\begin{aligned}h(\vec{k})=&\begin{pmatrix}E_0 & t & 0\\ t & E_0 & t'\\ 0 & t' & E_0'\end{pmatrix}\times e^{ik(d-d)}+\begin{pmatrix}0&0&0\\ t&0&0\\ 0&0&0\end{pmatrix}\times e^{i\vec{k}a_1}\\&+\begin{pmatrix}0&0&0\\ t&0&0\\ 0&0&0\end{pmatrix}\times e^{i\vec{k}a_2}+\begin{pmatrix}0&t&0\\ 0&0&0\\ 0&0&0\end{pmatrix}\times e^{-i\vec{k}a_1}\\&+\begin{pmatrix}0&t&0\\ 0&0&0\\ 0&0&0\end{pmatrix}\times e^{-i\vec{k}a_2}\end{aligned} \tag{7}$$

where E_0 and E_0' are the onsite energy of the carbon atom and adsorbed gas, and t' is defined as the hopping energy between the adsorbate and carbon atom of ZCNT respectively.

$$\left|h(\vec{k})\right|=\left|\begin{pmatrix}E_0 & t+te^{-ika_1}+te^{-ika_2} & 0\\ t+te^{ika_1}+te^{ika_2} & E_0 & t'\\ 0 & t' & E_0'\end{pmatrix}\right| \tag{8}$$

By summation of individual matrixes over the n^{th} unit cell and its four neighbors and then calculating the determinant of the $h(k)$ matrix, and applying the periodic boundary condition for the zigzag CNT, the energy dispersion model for the zigzag CNT is achieved as:

$$E_{zc}\left(\overrightarrow{k}\right)=\begin{pmatrix}\pm\frac{\sqrt{\left(E_0+E_0'\right)^2-4E_0E_0'+4t'^2+4t^2+16t^2\cos^2\left(\frac{\pi\upsilon}{n}\right)+16t^2\cos\left(\frac{\pi\upsilon}{n}\right)\cos\left(k_x a\right)}}{2}\\ +\frac{\left(E_0+E_0'\right)}{2}\end{pmatrix} \tag{9}$$

The presented model in Equation (9) indicates the energy band structure of zigzag CNT by considering the effect of the adsorbed molecule. As shown in Fig. 4(a), the energy band structure of the zigzag CNT (12, 0) is simulated while no gas is adsorbed yet. It can be seen that zigzag CNT (12, 0) exhibits metallic properties as there is no distance between valence and conduction bands. However, in the presence of the impurity molecules, its energy band structure changes that lead to open a gap between valance and conduction bands as depicted in Fig. 4(b).

Here, the adsorption of CO_2, H_2O, and NH_3 gas molecules are considered and applied for gas detection. The main parameter that contributes to impose the adsorption effect is hopping energy (t'). Changing the value of the t' exerts some effect on both the electrical and physical characteristics of the ZCNT. For simplicity, we assumed the value of the E_0' equal to zero as the origin of the energy.

Each gas has a specific hopping energy value when binds to the ZCNT surface that can be determined through the relation given as [36]:

$$t_{\alpha\beta}\approx t_R\left(\frac{d_R}{d_{\alpha\beta}}\right)^2 \tag{10}$$

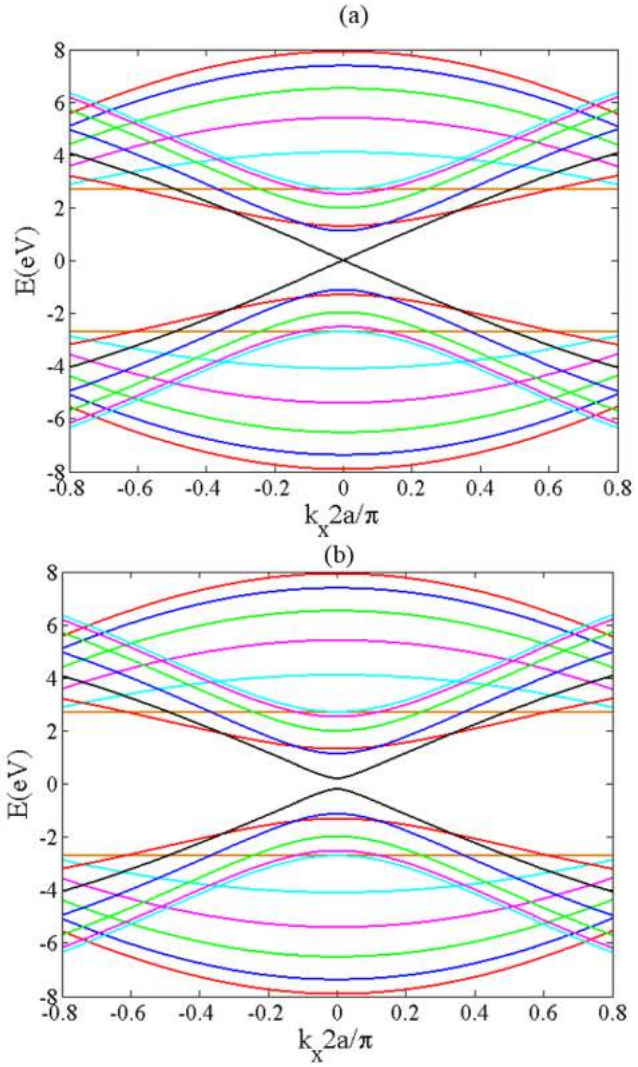

FIGURE 4. Zigzag CNT (12, 0) energy band structure: (a) without gas (b) considering molecular adsorption.

where $t_{\alpha\beta}$ is the hopping energy between ZCNT and adsorbate, t_R is hopping parameter between atoms of the ZCNT, d_R is the carbon-carbon bond length in zigzag CNT and $d_{\alpha\beta}$ represents the equilibrium ZCNT-molecule distance. The distance and orientation of each gas are assumed according to the reported study by [37]. Therefore, the hopping energy between ZCNT and molecules are presented in Table 1.

TABLE 1. The calculated hopping energies for adsorbed gas molecules.

Adsorption type	Distance (d) Å	hopping energy
CO_2	$d_{\alpha\beta} = 3.2$	$t_{C\text{-}CO2} = 0.196t_R$
NH_3	$d_{\alpha\beta} = 2.99$	$t_{C\text{-}NH3} = 0.225t_R$
H_2O	$d_{\alpha\beta} = 2.64$	$t_{C\text{-}H2O} = 0.289t_R$

The effects of the gas adsorption on the energy band structure of the zigzag carbon nanotube as a sensor substrate is presented in Fig. 5. The bare ZCNT (12, 0) shows metallic properties with zero energy band-gap. Molecular adsorption modifies the sub-bands and leads to a bandgap opening near Fermi energy. As shown in Fig. 5, each gas has a specific effect on the band structure with a different bandgap.

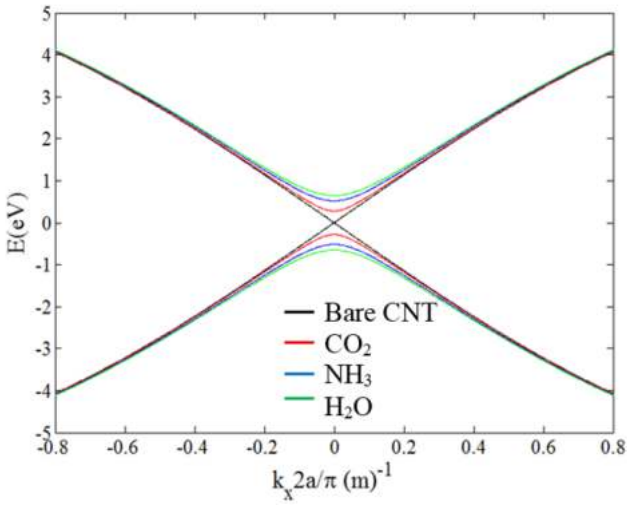

FIGURE 5. A 2D illustration of Zigzag CNT (12, 0) energy band structure variation in the presence of different gas molecules.

III. CARRIER VELOCITY MODEL

The energy bandgap variation in the ZCNT modifies other characteristics such as DOS and carrier velocity. Based on the definition, DOS describes the number of states per interval of energy that electrons can occupy. Calculating variations of the carrier density (Δn) over the variation of energy (ΔE) per length (L) of the tube gives the density of states of the zigzag CNT. Introducing the coefficients:

$$A = \left(E_0 + E_0'\right)^2 - 4E_0E_0' + 4t'^2 + 4t^2 + 16t^2\cos^2\left(\frac{\pi\upsilon}{n}\right) \quad (11)$$

$$B = \left(E_0 + E_0'\right) \quad (12)$$

$$c = 16t^2\cos\left(\frac{\pi\upsilon}{n}\right) \quad (13)$$

and applying Taylor expansion to Equation (9), the energy dispersion relation can be simplified as:

$$E = \pm\frac{\sqrt{A}}{2}\left(1 - \frac{c}{2A}\left(1 - \frac{k_x^2a^2}{2}\right)\right) + \frac{B}{2} \quad (14)$$

Now, the density of states can be calculated while the gas adsorption effect is taken into account also.

$$D(E) = \frac{\Delta n}{\Delta E.L} = \sum_{\upsilon}\frac{4A}{2\pi\sqrt{A}ca^2k_x} \quad (15)$$

where the propagation parameter along the x-direction is calculated as:

$$k_x = \pm\sqrt{\frac{2E+2}{a^2} + \frac{(B+\sqrt{A})4A}{2c\sqrt{A}}} \quad (16)$$

The simulation of the DOS for the ZCNT with and without gas molecules is carried out as illustrated in Fig. 6. It is obvious from the results that ZCNT experience notable changes

in its DOS caused by gas adsorption. Any small change in energy bandgap and DOS of the ZCNT can effectively modulate carrier transport and electronic properties such as velocity and *I-V* characteristics of the sensor that are going to be calculated. The velocity of carriers in a semiconductor is proportional to the density of states and carrier density at any time [20], [38], [39].

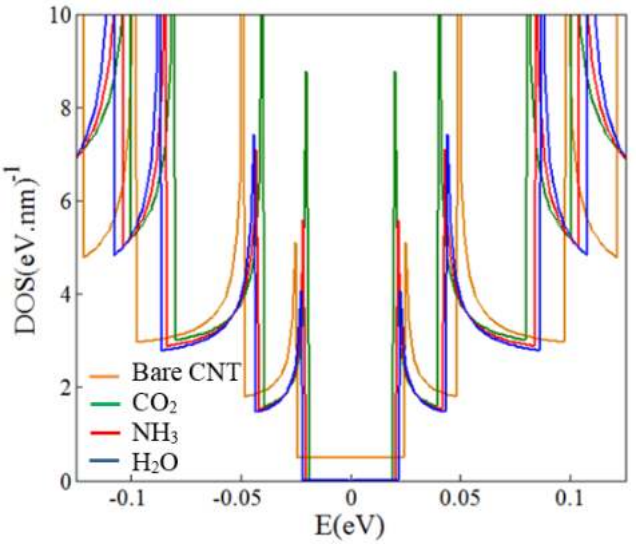

FIGURE 6. The density of states of (12, 0) Zigzag CNT in the presence of gas molecules.

Thus, carrier velocity is formulated by the accumulative velocity of electrons over carrier density [38]:

$$V_{av} = \frac{\int |v|\, D(E) f(E) dE}{\int D(E) f(E) dE} \tag{17}$$

where $f(E) = 1/\left(1 + exp(\frac{E-E_F}{k_B T})\right)$ is the Fermi function describing the probability of particles distribution over energy states and the magnitude of velocity is given as:

$$|v| = \left(\frac{2(E - E_g)}{m^*}\right)^{\frac{1}{2}} \tag{18}$$

with $x = \frac{E-E_g}{k_B T}$ and normalized Fermi function $\eta = \frac{E_F - E_g}{k_B T}$, the velocity of carriers in zigzag CNT sensor is modeled by considering gas adsorption effect as well:

$$V_{av} = \sqrt{\frac{2}{m}} \frac{\int \frac{\sqrt{x k_B T}}{k_x(1+exp(x-\eta))} dx}{\int \frac{dx}{k_x(1+exp(x-\eta))}} \tag{19}$$

While for the average velocity in Eq. (19) all subbands should be taken into account by summation over different bands. The investigation of the gas adsorption effect on the carrier velocity of the zigzag CNT based gas sensor is performed in the form of *I-V* characteristics. According to Fig. 7, the variation of the velocity versus carrier concentration is illustrated. In the gas sensing mechanism, when the gas molecules are trapped on a carbon nanotube surface, charge transfer occurs between ZCNT and gas molecules. This phenomenon changes the number of carriers on the ZCNT channel which directly affects the carrier velocity conductivity and *I-V* characteristics of the sensor. The increment of the carrier concentration increases the sensor conductivity and thus affects the carrier velocity as well.

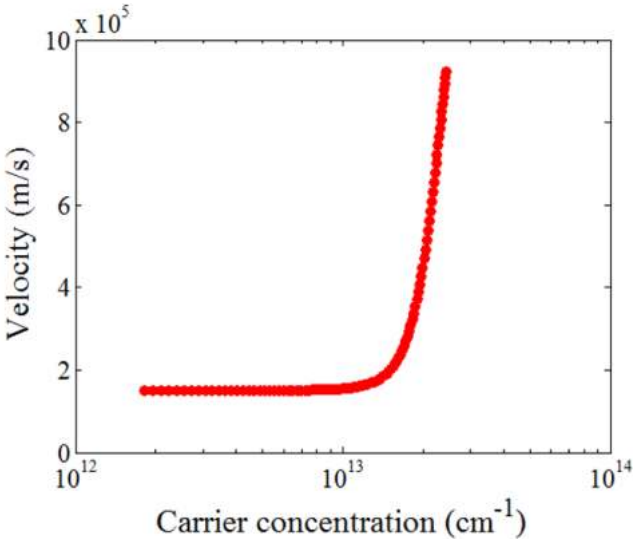

FIGURE 7. Carrier velocity of a bare zigzag single-wall carbon nanotube.

Based on the relationship between current and velocity [20], sensor *I-V* characteristics can be written as a function of the carrier velocity in the following form:

$$I_{ds} = q \times Area \times \left(\frac{2\sqrt{2} A k_B T}{\pi c a^2 \sqrt{mA}} \int \frac{\sqrt{x k_B T}}{k_x(1 + exp(x - \eta))} dx\right) \tag{20}$$

where q is the quantity of electric charge measured in coulomb. The *I-V* characteristics of the ZCNT sensor with and without considering gas molecules adsorption effect are presented in Fig. 8. According to the graph, the current increased after molecular adsorption on the ZCNT surface. This is because of electron transfer happening during gas reaction with ZCNT and due to the increased density of states after the opening of the gap. The CO_2, NH_3, and H_2O molecules act as electron-donating functional molecules and transfer an electron to ZCNT, which increases electron concentration on ZCNT, increases the conductivity of the channel, and thus increases the current of the sensor.

On the other hand, the sensor experience higher (lower) current after H_2O (CO_2) adsorption in comparison to NH_3, which means the sensitivity of the sensor toward each gas, is different as illustrated in Fig. 9 via the sensor response analysis. It can be seen that by voltage 0.25V, the slope is very sharp and after that, it becomes constant. It is because after this point the current saturates and would not increase anymore.

In Fig. 9, I_0 and I are the currents before and after adsorption. The analytical models in this work can be applied to predict the treatment of the zigzag CNT sensor toward different

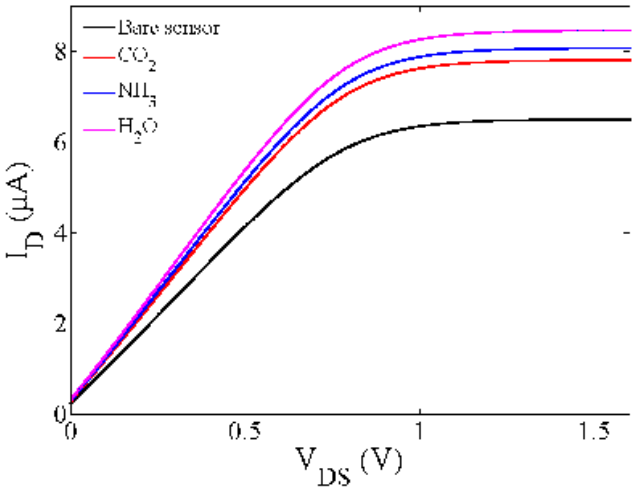

FIGURE 8. I-V characteristics of single-wall zigzag CNT-FET based sensor against various gas molecules.

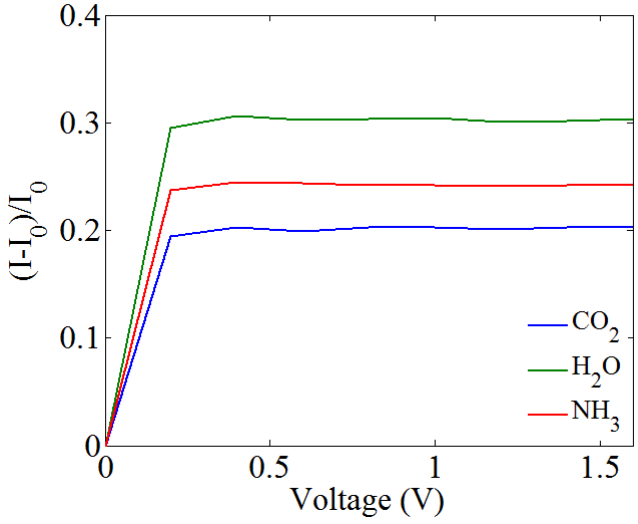

FIGURE 9. The response of the zigzag CNT-FET based sensor based on the proposed model toward various gases.

gas molecules and study sensor characteristics to develop highly sensitive sensors based on nanomaterials.

IV. CONCLUSION

The advent of nanosensors has increased the feasibility of the development of highly sensitive, fast and accurate gas sensors that are capable to detect even a single gas molecule. Carbon nanotubes possess unique physical and electrical properties with high surface to volume ratio, high conductivity and carrier mobility that enables them to surpass other nanomaterials for sensing applications. In this paper, a field-effect transistor-based gas sensor based on a single-wall zigzag CNT platform was modeled and applied for gas (CO_2, NH_3, and H_2O) detection. Therefore, the electronic band structure, density of states, carrier velocity and *I-V* characteristics of the zigzag CNTFET based gas sensor were analytically modeled by considering the molecular adsorption effects (t' and E_0'). According to the results, ZCNT experienced measurable changes in its energy band gap and density of states caused by adsorbed molecules as they change the hopping energy parameter between neighboring carbon atoms. On the other hand, due to the traveling of the electron between gas molecules and ZCNT the concentration of the charges vary on the ZCNT surface, which leads to the variation of the velocity and current. It was shown that the suggested model could simulate the deviation of the energy bandgap, DOS and *I-V* characteristics.

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