RESEARCH PAPER

Detection of Ammonia and Phosphine Gas using Heterojunction Biomolecular Chain with Multilayer GaAs Nanopore Electrode

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ABSTRACT

This paper presents Density Functional Theory and Non-Equilibrium Green's Function based First Principles calculations to explore the sensing property of Adenine and Thymine based hetero-junction chins for Ammonia and Phosphine gas molecules. This modeling and simulation technique plays an important and crucial role in the fast growing semiconductor based nanotechnology field. The hetero-junction chain has been passed through the multi layer GaAs nanopore electrodes. It has been found that Current-Voltage characteristics of the bio-molecular chain highly depend during the foreign gas molecules adsorption. This Current-Voltage sensitivity has been raised upto 40 and 9.3 times with the presence of single Ammonia and Phosphine molecules respectively under the ultra low bias voltage application. Adsorption of single molecule Ammonia and Phosphine increases the conductivity of the heterogeneous bio-molecular chain at room temperature. The quantum ballistic transmission through the direct band gap semi-conductor material GaAs nanopore increases during the Ammonia and Phosphine gas adsorption by the heterogeneous chain. In this paper we attempt to present the molecular model sensor with circuit elements. The attractive potential of conductivity modulation suggests this heterogeneous bio-molecular chain as an application in future generation bio-sensor technology.

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INTRODUCTION

The heterogeneous bio-molecular chain is made with Adenine and Thymine bio-molecules. These bio-molecules are the basic building blocks of DNA. These molecules are the protein groups. When these molecules are attached with glucose and phosphate groups then they converts themselves as nucleotides. Nucleotides are the basic backbone of single strand DNA (ss-DNA). In the world of nano-bio technology, the researchers are continuously trying to build a two-way bridge between the bio-technology and semiconductor nanotechnology [1]. GaAs is a direct band gap semi-conductor which has been used as nanopore

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electrodes for this two probe theoretical study. GaAs is one of the highly appreciable and attractive direct band gap semiconductors [2].

The various nano sensors have already been designed using Density Functional Theory (DFT) and Non Equilibrium Green's Function (NEGF). Boron nitride zigzag nano wire sensor has been designed to sense the presence of chlorine gas molecules [3]. Carbon Nano Tubes (CNTs) are sensitive towards the adsorption of foreign molecules like NO_2 gas [4]. Arm chair graphene nano ribbon is useful to sense the bio-molecule Anthracene in molecular level of foreign particle detection [5]. Detection of conformational changes in protein can be diagnosis using multi layer graphene electrodes [6]. First principle investigation has been made possible for arm chair Boron nitride nano ribbons to sense PH_3 gas molecules [7]. The gas sensing ability for graphene has been increased by introducing dopants [8]. CO gas can efficiently sense by Porphyrin bio-molecule using single wall CNT (SWCNT) as electrodes [9]. Among these sensors CNT is one of the popular bio-sensor [10]. Metalloid Porphyrin has been proven as an attractive bio-sensor for its high sensitivity towards the adsorption of CO, NO and O_2 gas molecules [11]. The Current-Voltage (I-V) characteristics are highly affected during the gas adsorption by the ZnO nano structure. This sensor has been designed using DFT and NEGF formalisms [12]. The circuit level implementation using these organic molecules can also be possible [13-15].

This proposed bio-sensor is an approach to build a bio-inspired nano sensor along with in-organic molecular nanopore electrodes. This analytical model has been designed by Atomistic ToolKit-Virtual Nano Laboratory (ATK-VNL) simulation package. The comparative study of few existing bio-sensor with the proposed bio-sensor is shown (as in Table 1).

motivation

Design of bio-inspired nano sensor at room temperature using semi-conductor nanopore electrodes is one of the challenging aspects for the researchers. The quantum-ballistic transmission ability of the heterogeneous bio-molecular chain has been visibly increased during the single Ammonia (NH_3) and Phosphine (PH_3) molecule adsorption. I-V response and bio-molecular channel conductivity has been significantly enhanced during NH_3 and PH_3 adsorption with ultra low bias i.e.0.02V.

Contributions

The bio-inspired nano sensor exhibits attractive quantum-ballistic transmission response during the adsorption of single NH_3 and PH_3 molecule adsorption at its superficial layer. The main contributions of this paper are:

1. Approximately 40 times large I-V response has been achieved during the NH_3 adsorption.
2. Approximately 9.3 times large I-V response has been achieved during the PH_3 adsorption.
3. Approximately 7.2 and 7.57 times higher conductivity has been observed after NH_3 and PH_3 adsorption respectively.
4. Large transmission co-efficient has been observed for nano bio sensor.

Table 1. Comparative study of existing and proposed bio-sensor model

Existing Bio-sensor / Features	Multi layer Graphene Nanopore [6]	Zigzag Boron nitride [3]	CNT [10]	Poposed Adenine-Thymine Heterogeneous chain
Sensing molecules	Protein	Chlorine	Amino acids	Ammonia Phosphine
Electrodes	Graphene 3 layers nanosheet with nanopore	Zigzag Boron nitride nanoribbon	SWCNT	GaAs 2 layers nanosheet with nanopore
Structural stability	stable	Less stable	-	stable
Electron mobility	high	high	-	high
Force	0.05eV/Å	0.05 eV/Å.	1 atm	0.05eV/Å
Hybridization	sp^2	-	-	MONO
Electron temperature	300K	-	300K	300K
Pore diameter	1.8 nm	-	-	1.004nm
Stress	-	-	-	$0.05eV/Å^3$
Operating Frequency	-	-	-	1000THz
Bias Voltage	0.1V	2V	-	0.02V

Table 2. Metrices for designing the proposed bio-molecular sensor

Parameters	Value
Configuration (A,B,C)	(X,Y,Z) directions
K-point sampling	1×1×100
Poisson solver	FFT2D
Self consistent function iteration method	yes
Mesh cut-off density	10Ry
Log interval	1
Maximum number of steps	200
Each step size	0.2Å
Force	0.05eV/Å
Stress	0.05eV/Å^3
Adenine density	1.9±0.1 gm/cm^3
Thymine density	1.4±0.1 gm/cm^3
Fermi level	0eV
Input voltage	0V to 0.02V
Device algorithm	Krylov
Molecular dynamics	NVE velocity Verlet
Close neighbor distance	0.01nm
Adenine- Thymine Bond length	1.05921Å
Polarization	Single zeta

computational modeling technique

This bio-inspired sensor is made with the heterogeneous chain of two Adenine and two Thymine molecules. Therefore this chain has passed through the nanopore of GaAs nanosheet. In this two probe experiment, bias voltage has been applied at the two ends of the GaAs nanosheet. This bio-molecular sensor has been constructed using DFT and NEGF based first principle approach. This analytical model has been designed using ATK-VNL, Quantumwise A/S software simulation package (ver. 13.8.0). The proposed nano sensor has the tree parts viz. left electrode and right electrode (GaAs nanosheet) and central region (body of the heterogeneous chain).

The two configuration model sensor are shown in Fig. 1(a), (b) and (c) for bared and after NH_3 and PH_3 adsorption respectively. Due to high electron mobility and the stability of GaAs nanosheet make this device attractive for future generation bio-inspired sensor applications. This nanopore has been made by drilling the small pore across the width of the nanosheet. The geometric optimization is achieved using the parameters mentioned (as in Table 2).

RESULT AND DISCUSSION

The proposed bio nano sensor exhibits its sensing capability towards the single NH_3 and PH_3 molecule when it is passing through the nanopore of the double layer GaAs nanosheet. This property has been enhanced when the ultra low bias voltage, which is applied at the both ends of the

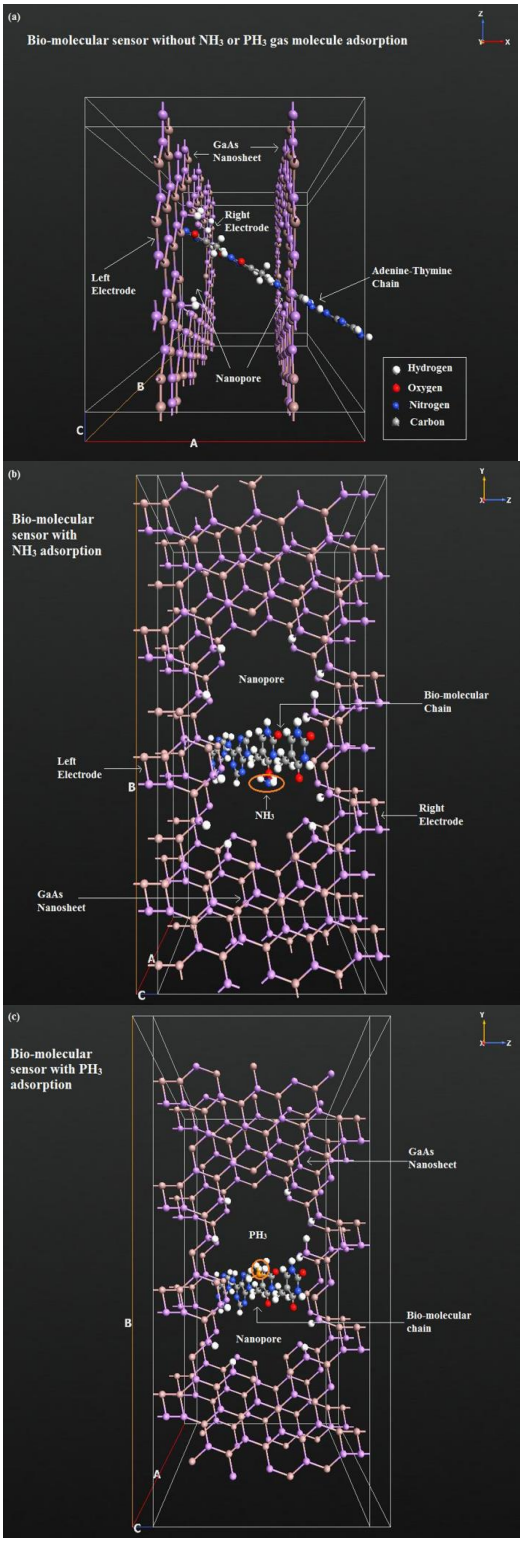

Fig. 1(a). Side view of the bio-molecular sensor using GaAs nanopore electrodes without NH_3 or PH_3 adsorption. (b) Top view of the bio-molecular sensor using GaAs nanopore electrodes after NH_3 adsorption (c) Top view of the bio-molecular sensor using GaAs nanopore electrodes after PH_3 adsorption.

GaAs nanosheet electrodes. The sensitivity of the bio-molecules are increased when GaAs nanosheet electrode has been used. Compared with other semiconductors like Silicon (Si) and Germanium (Ge), GaAs provides much significant and satisfactory result for example 2.3×10^7 times large current is obtained for GaAs nanopore electrode when simply compared with Ge. 1.51 times large current is achieved for GaAs nanopore electrode when compared with Si. Due to the high stability and electron mobility GaAs has been considered as a good choice as nanopore electrodes in this two probe theoretical study. To observe the sensing capability the subsequent properties of the nano system have been illustrated.

Transmission spectra

Quantum ballistic transmission property is the basic property of any of the atomic scale design procedure. Depending on the characteristics of quantum transmission the I-V characteristics and channel conductivity can be estimated. The potential drop generated between two electrodes, provides the driving energy to accelerate the electrons into the central bio-molecular chain. This potential drop is described as V_p in Eq. (1), where $f_L(E)$ and $f_R(E)$ are the Fermi energy levels of the left and right electrode respectively.

$$qV_p = f_L(E) - f_R(E) \tag{1}$$

Transmission spectra of any atomic scale device can be determined using Landauer-Büttiker formula in Eq. (2),

$$T(E) = \frac{2q}{e} T(E)M(E)(f_1 - f_2) \tag{2}$$

T(E) is the transmission probability defined for the intervals {0, 1}. 2q/e is the conductance of the system; f_1 and f_2 are the Fermi functions of two electrodes. M(E) is independent channels that are used by the electrons. M(E) depends on the coupling co-efficient γ and Device Density of States (DDOS), which is shown in Eq. (3).

$$M(E) = \pi\gamma D(E) \tag{3}$$

Compare with these three equations, it can be suggested that strong coupling between electrodes and the central region molecule is required to enhance significant quantum ballistic transmission [1, 12, 16]. Therefore to get more transmission the distance between the nanopore electrode and central bio-molecular chain has been kept minimal. Another way to increase quantum transmission is to increase the coupling co-efficient factor.

The transmission co-efficients which are achieved for the NH_3 and PH_3 adsorbed bio-molecular chain is larger than the bared chain, which is clearly depicted in Fig. 2. Due to ultra low bias application at the two electrodes (± 0.01V), the two Fermi levels of the two electrodes are almost merge together. The highest transmission peak is available at -1.25eV that means below the Fermi level i.e. in valance band. The dense transmission spectra have been achieved both in valence band and conduction band (above Fermi

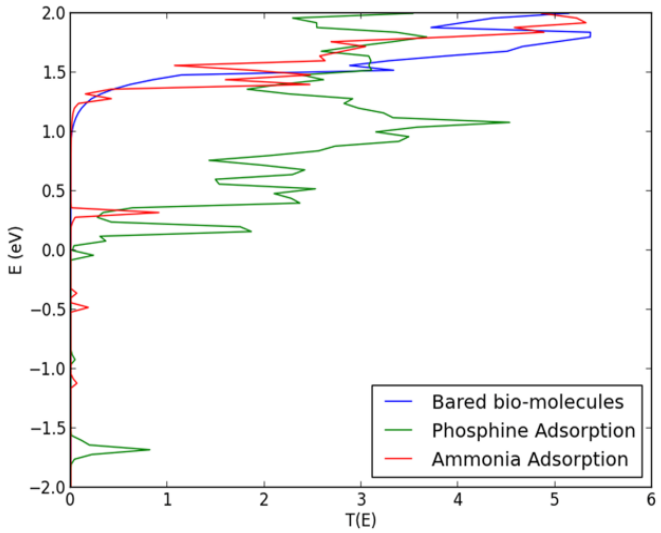

Fig. 2. Transmission spectra of the nano-bio sensor for three conditions.

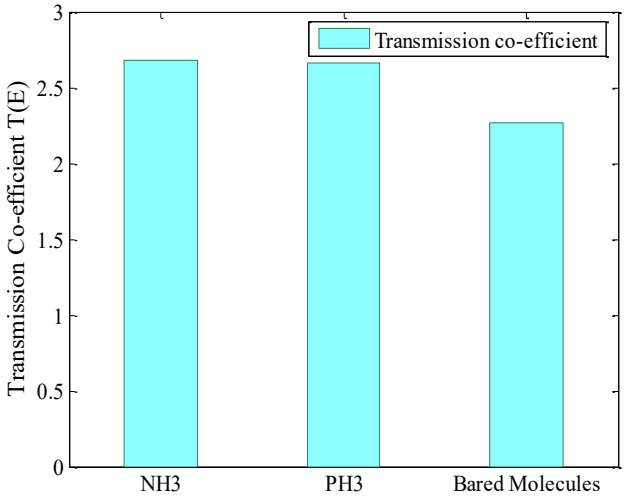

Fig. 3. Transmission co-efficients values for the nano-bio sensor.

level). Large transmission is achieved only in conduction band at the bared system level. This signifies that high transmission can be achieved when the adsorption of NH_3 molecule has been occurred. In this experiment weak coupling exists between the biomolecules and electrodes in the Coulomb-blockade region. This feature encourages incoherent transmission which results in sequential tunneling. During foreign molecules adsorption the tunneling capability is increased which results in strong quantum transmission [16, 17].

Fig. 3 shows the transmission co-efficients observed during the three conditions at constant bias voltage 0.02V. It has been observed that highest transmission co-efficient is achieved during the adsorption of NH_3 molecule. Almost same transmission co-efficient is also found after PH_3 molecular adsorption. The difference of transmission co-efficient observed for the two foreign molecules are very close to each other. But for all the cases these transmission co-efficients are observed above Fermi level that means in conduction band. This illustrates that due quantum-ballistic excitation maximum quantum transmission is happened at conduction band.

Device Density of states

Device Density of States (DDOS) is the atomic level description of the central region. The variation in DDOS is achieved within the bias window, i.e., -2eV to +2eV. DDOS determines the concentration of energy states within the bias window. Highest Occupied Molecular Orbital (HOMO) is the maxima of valence band and Lowest Unoccupied Molecular Orbital (LUMO) is the minima of conduction band. Thus HOMO reclines above Fermi level and LUMO has been found below Fermi level. The HOMO-LUMO gap signifies the thermodynamic stability of the nano scale device. Large gap signifies thermodynamic stability of the molecular system. The HOMO-LUMO gap which is obtained for the nano sensor (after NH_3) adsorption is quite large compared with the bared molecule. This gap is significantly large due to the degeneracy of the highest populated molecular orbital which are not filled up fully. This effect is known as Jahn-Teller effect [1, 18].This signifies that the nano system is quite stable even after the adsorption of NH_3. The comparative models for DDOS and HOMO-LUMO plot are shown in Fig. 4. The observed HOMO and LUMO for the proposed device is shown (as in Table 3).

Table 3. HOMO-LUMO for the proposed bio-molecular sensor

Prime Molecules	HOMO (eV)	LUMO (eV)	$G_{HOMO-LUMO}$ (eV)
Bared AA-TT Chain	-1.58 (H_1)	0.9 (L_1)	2.48
Ammonia	-1.72 (H_2)	0.08 (L_2)	1.8
Phosphine	-0.49 (H_3)	0.42 (L_3)	0.91

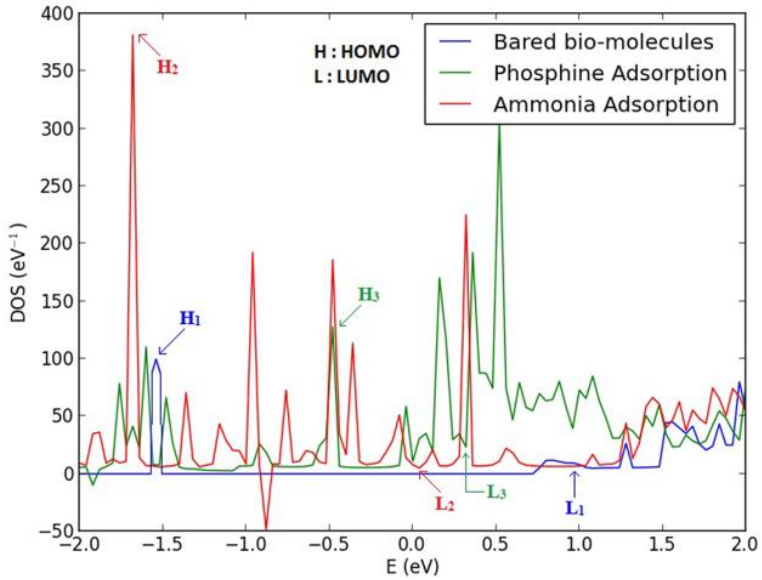

Fig. 4. DDOS and HOMO-LUMO plot for the bio-molecular sensor with GaAs nanopore electrodes.

Current – Voltage Characteristics

The I-V response is very crucial and interesting phenomenon for any nanoscale system. The nature of this graph signifies the trend of electronic transmission for any atomistic model. Due to the Broaden effect (Γ), electron will stay long time on the molecule for long period of time. The lifetime of electron is represented as τ_c, which is much less than 1/Γ (τ_c<<1/Γ) for in-coherent transmission. Thus the electron is responsible for sequential tunneling. This type of in-coherent transmission is thus applicable for those molecules which are weakly coupled with the electrodes. But the results show that after adsorbing single foreign gas particles (NH_3 and PH_3) enhance the ability of in-coherent transmission. Henceforth the amount of sequential tunneling has also been improved. This quantum ballistic in-coherent transmission maintains strong tunneling current conduction through the bio-molecular chain [16, 17].

The comparative diagram for current transmission after the adsorption of foreign gas molecules and the bared bio-molecular chain is shown in Fig. 5. This figure emphasis that 40 times better current is achieved during the adsorption of NH_3. After the adsorption of single PH_3 molecule at the superficial layer of the bio-molecule, the I-V response increases upto 9.3 times.

Conductivity

The significant change has been observed in the channel conductivity for the proposed bio-sensor when foreign gas molecules are adsorbed at the superficial layer of the bio-molecular chain. After adsorption of gas molecules, channel conductivity has been increased tremendously, which is shown in Fig. 6. This reflects that the sensing capability of the bio-molecular chain has been increased due to the adsorption of NH_3 and PH_3. Channel conductivity depends on the transmission co-efficients as shown in Eq. (4). This equation reflects that channel conductivity increased with the increment of T(E).

$$G = \int_{-\infty}^{\infty} dET(E)\left(-\frac{\delta f}{\delta t}\right) \quad (4)$$

In Eq. (4), T(E) is the transmission co-efficient, f is the Fermi level of the electrodes [19]. So it is evident that as the quantum ballistic transmission is large enough for the foreign gas molecules thus the channel conductivity increases tremendously after the gas molecules adsorption.

Adsorption energy

Adsorption energy is one of the essential metric to calculate the relative stability of the molecular sensor devices. To investigate the effect of adsorption of guest particles it is essential to calculate the adsorption energy for the proposed sensor. The adsorption energy is calculated using the total energy of the adsorbed guest molecules and bared bio-molecular chain using relation

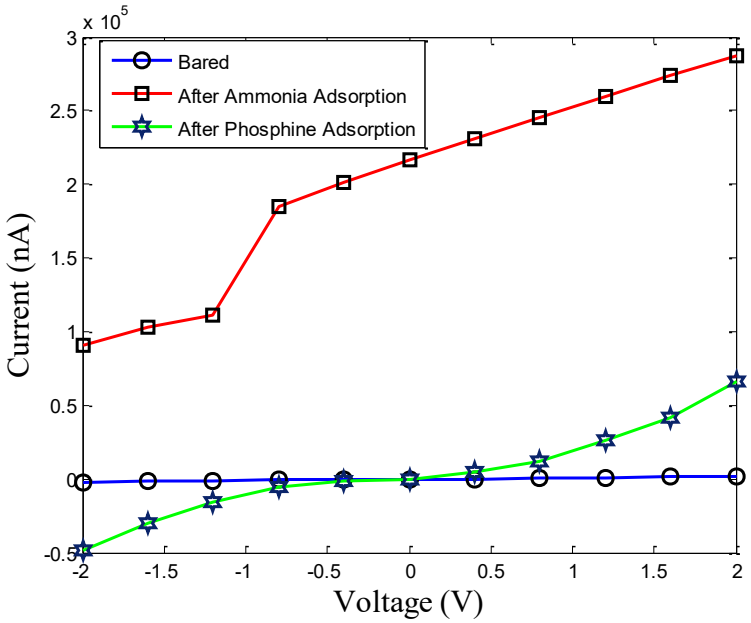

Fig. 5. I-V response of the bio-molecular sensor.

shown in Eq. (5). The adsorption energy is the key parameter that emphasis the affinity of the guest molecules towards the bio-molecular chain. If the energy is increased that means the proposed sensor device is thermodynamically stable even after the adsorption of guest molecules. Table IV indicates the calculated bond-lengths and the adsorption energy of the respective gas molecules. The values of adsorption energy show that the device is even more stable after the adsorption of guest molecules. Thus no such structural deformation occurs during the adsorption of gas molecules [20-24]. It has been observed from (as in Table 4) that the adsorption energy of the bio-molecular sensor has been increased even after the adsorption of NH_3 and PH_3. Thus it can be stated that the proposed sensor is energetically more stable even after the adsorption of foreign molecules. The values of high adsorption energy shows that the device is thermo dynamically stable even after the adsorption of guest molecules. Thus no such structural deformation occurs due to adsorption effect. Moreover it is evident that the device demands more thermodynamic stability after the adsorption of NH_3 and PH_3 gas molecules.

$$E_{Ad}^{NH_3} = E(Adenine + Thymine + NH_3) - E(Adenine) - E(Thymine) - E(NH_3) \quad (5)$$

Chemical potential

Partially free molar energy is referred as chemical potential of the atomic scale device. During any chemical synthesis or adsorption of any guest particles this chemical potential energy is released. Channel current conductivity and transmission spectra depend on chemical potential of the electrodes. This phenomenon can be depicted well using Eq. (6).

$$I = \frac{2e}{h} \int dET(E)[f_L(E) - f_R(E)](E - \mu) \quad (6)$$

From Eq. (6), it can be seen that quantum ballistic transmission depends on chemical potential which is represented with (E-μ) term. T(E) is the transmission co-efficient, I is the current through the bio-molecular chain, 2e/h represents channel conductivity, $f_L(E)$ and $f_R(E)$ are the Fermi levels for the left and right electrodes respectively . Moreover high conductivity has been observed when chemical potential moves deep into conduction band or the valence band of transmission spectra. If the energy difference between the transmitting electron and the chemical potential is small this specifies the movement of chemical potential deep into the conduction band [25]. The chemical potentials for the three conditions are shown in Fig. 7. It is observed that chemical potential is high

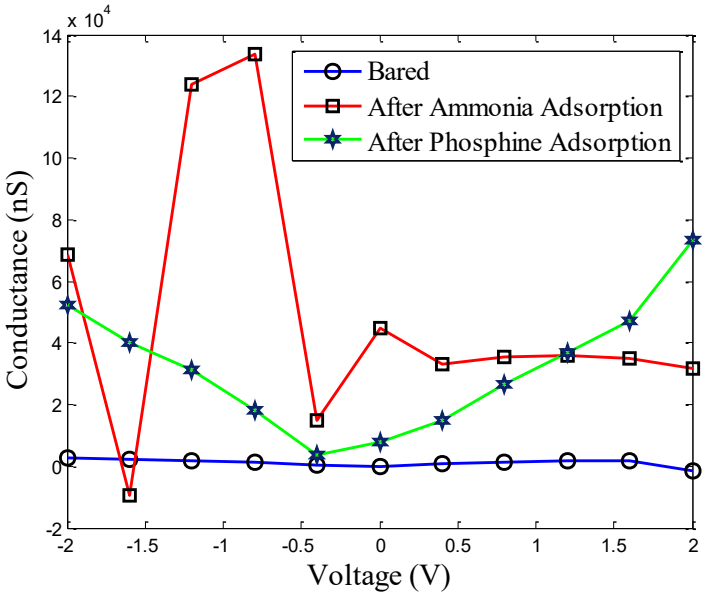

Fig. 6. Conductivity with different bias voltages for the nano-bio sensor.

enough for NH_3. It remains moderate during PH_3 adsorption. For bared Adenine- Thymine bio-molecular chain the observed value is low. These results signify that high chemical potential has been achieved during the adsorption of guest molecules. Channel conductivity as well as channel transmission increases to a large extent due to the large value of chemical potential of the electrodes. As a result large current is observed for NH_3 and PH_3 compared to bared bio-molecular chain. High chemical potential has been observed for the GaAs nanosheet electrodes.

Mathematical Modeling of the Asymmetric Adenine-Thymine Molecular Sensor

Analytical model of any nanoscale device is important due to their feasibility aspect. In this section the mathematical model of this bio-inspired sensor has been illustrated. From the I-V characteristics graph, it is clearly viewed that the device acts as diode sensor. Fig. 8 shows the sensor device and its corresponding circuit level modeling [13].

According to the circuit level designing process at reverse bias the condition of current flow has been stated in Eq. (7) [13].

$$V_{ds} = \frac{V_{t,0}}{\beta} + 2V_t \tag{7}$$

At forward bias the condition for current flow is stated in Eq. (8)[13].

$$V_{sd} = V_{t,0} + 2V_t \tag{8}$$

The $V_{sd/ds}$ is the applied bias voltage and $V_{t,0}$ is the threshold voltage at no bias condition. The employed n-MOSFET model has been designed with typical parameters such as $K_p = 5 \times 10^{-7}$, $V_t = V_{th}$, lambda = 0, gamma = 0.586. The calculated values of β for NH_3 and PH_3 are 0.056 and 0.75 respectively. Based on the circuit level analytical design of this model sensor, one can conclude that the rectification effect for the sensor can be observed at room temperature operation [13].

Finally, the cross-tick table shown (as in Table 5), which explores the satisfactory contributions and novelty of the proposed nano-bio-molecular sensor when compared with some other existing sensors.

Table 4. The calculated bond-lengths and adsorption energies of the respective particulars

Particulars	Bond Length (Å)	E_{ad} (eV)
Adenine-NH_3	1.14988	-1.23×10^4
Adenine-PH_3	1.92278	-1.31×10^4
Adenine-Thymine	1.05921	-8.45×10^3
H-C	1.090	-
H-N	1.020	-
H-O	1.05921	-
Adenine-H	1.4128	-
Thymine-O	1.01926	-

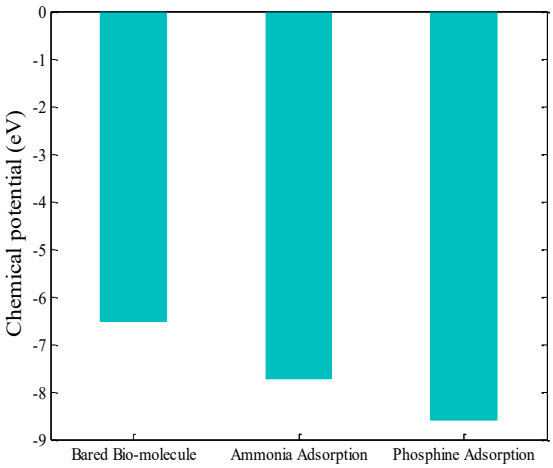

Fig. 7. Chemical potential of bio-molecular sensor.

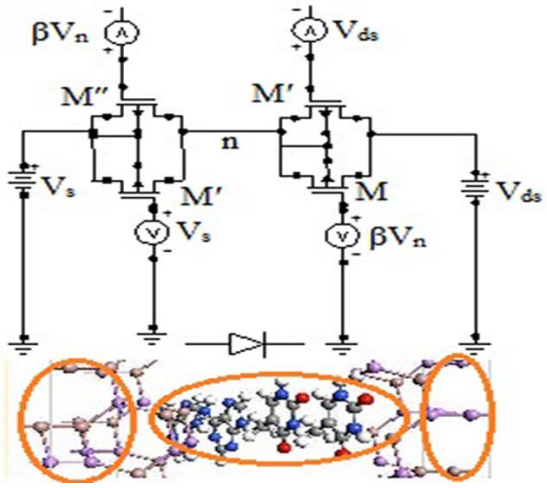

Fig. 8. Proposed circuit model for the sensor.

Table 5. Cross-Tick table for existing sensor and proposed sensor

Different types of Sensor	Existing Approach				Proposed Approach
	BN Nano ribbon $COCl_2$ Gas [20]	CNT Mechanical [26]	ZnO Nanowire NH_3 Gas [27]	ss-DNA based Lead ion Detection [28]	Bio molecular H_2 and NH_3 Gas
Based on / Features	DFT + NEGF+ First Principle Approach	MEMS+ VHDL-AMS and System C-AMS	Electro-Chemical Approach	Electro-Chemical impedance spectroscopy	ATK+DFT+EHT
Reduced Force	√	√	×	×	√
Reduced Stress	×	×	×	×	√
Ultra Low Bias Voltage	√	×	×	√	√
Satisfactory current signal after adsorption	×	√	√	√	√
Room Temperature Operation	×	√	×	×	√
Reduced Mesh cut-off density	×	×	×	×	√
Reduced Device Active area	×	×	×	×	√
Ultra High Operating frequency	×	×	×	×	√
Bio compatibility	×	×	×	√	√
High Adsorption energy	√	×	×	×	√
Optical sensitivity	×	×	×	×	√

CONCLUSION

The system level investigation for the proposed Adenine-Thymine chain based nano sensor has been carried out using DFT and NEGF based First Principle approach to detect the presence of NH_3 and PH_3 gases in room temperature. The reported results for transmission spectra along with channel conductivity and I-V response are the evident of high sensitivity of the proposed sensor towards these guest molecules. DDOS and HOMO-LUMO of the model sensor also shows the significant thermodynamic stability for the sensor. Chemical potential satisfies the significant response of the bio-molecules during the adsorption of NH_3 and PH_3 gases. This efficient high frequency bio-molecular sensor can be operated under mid-UV range. These remarkable electronic transport properties of the proposed sensor towards the sensing of $NH_3$and PH_3 gases consider this device as a one step ahead for future generation bio-molecular sensor.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publicaton of this manuscript.

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