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Theoretical Study of Carbon Nanotube toward Adenine Sensing: DFT Study

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***Abstract*— As a due of its electronic and physical properties, the carbon nanotube (CNT) is utilized in the production of accuracy sensors. In this paper, the thickness utilitarian hypothesis Density Functional Theory (DFT) with the B3LYP level, and by utilization of the Gaussian 09 arrangement of projects, were used to explore the adsorptive and detecting ability of Adenine on the unblemished CNT. The detecting capacity of these structures was determined as far as a variation of band hole vitality after cooperation among CNT and Adenine. Due to counts, it was found that the electronic properties of CNT are firmly delicate to the nearness of Adenine. In this way, we accept that GNRs can be utilized in sensor gadgets**

I. INTRODUCTION

Analysts have used adenine to explore life in earlier events. The adenine is a general crucial the proximity of life where are in general living animals, the examination proposes sense the adenine molecule by using one of the nanomaterials.

Nanostructures accept a noteworthy activity in the movement of consistent and structuring advancements at the nanoscale. Over late years, nanostructures have propelled a great deal of interest by their specific characteristics that sway physical, electrical, substance, common, and optoelectrical properties. The bit of nanostructures, for instance, monometallic, bimetallic, alluring, metal oxide, semiconductor, cream, composite, etc., have been used routinely as the purpose behind their portrayal. This area studies the different types of nanostructures and nanomaterials, for instance, nanowires, nanofibers, nanotubes, nanobelts, nanofluids, nanoribbons, nanosprings, nanocapsules, quantum touches, nanosheets, nanocomposites, and nanoparticles, pondering their different bearings, morphologies, and characteristics. Nanostructures, in the aggregate of their structures, build up a working zone of creative work in the fields of nanotechnology and nanoscience.

One of the huge nanostructures is the carbon nanotube, which is used in clinical and current applications,
Carbon nanotubes (CNTs) have pulled in light of a legitimate concern for researchers and architects since their revelation in 1993 [1], because of their one of a kind auxiliary, mechanical, and electronic properties, just as huge application potential[2-5]. These tale materials have a wide scope of potential applications, extending from the field of nanoelectronics to nanoscale biotechnology. For instance, they might be utilized in adenine [6]. Graphene is the name given to a level monolayer of carbon molecules firmly stuffed into a two dimensional (2D) honeycomb cross-section and is an essential structure hinder for graphitic materials of every single other dimensionality. It tends to be wrapped up into 0D fullerenes, folded into 1D nanotubes or stacked into 3D graphite[2, 7]

Sensors are a contraption that recognizes the modifications in the physical improvement with changes over them into a measurable sign which can be recorded or evaluated. It gets a physical sum and changes over it into a sign proper for planning (for instance optical, electrical, mechanical1)[8]. Nanosensors are a part of sensor systems in which a nanoscale joint effort is abused as the reason for perceiving the closeness of a known analyte[8]. Electrochemical nanosensor has starting late found wide applications in biomedical organizations with certain central focuses, for instance, lower area limits, increasingly broad straight response expands, affectability, incredible security, and reproducibility when differentiated and various sensors and procedures. Nowadays, an assortment of some method that is used in characteristic, or clinical research communities and different business motivation behind consideration devices work by using nanosensors [8].

In this work, we examine the carbon nanotube with 8 Angstrom (Å) length as a nanobiosensor for Adenine atom by utilizing the thickness utilitarian hypothesis (DFT) technique. At that point, we utilized the variety in the basic and electronic properties, that are coming about because of the connection between CNT with Adenine particle to utilize CNT as a nanobiosensor for Adenine atom.

II. COMPUTATIONAL METHODS

We picked a CNT (8,0) with 8 A° as a model nanosensor, which are contained of 64 C atoms and in which the end particles have been drenched with 32

hydrogen atoms to diminish the breaking point impacts, see Fig. 1. It all depends on the CNT that was performed using the thickness practical hypothesis (DFT) technique with the crossover useful B3LYP [9] and 3-21G basis set as implemented in the Gaussian 09W package [10]. The DFT method with this level have been chosen because of the accuracy associated[11-19], where the DFT method focuses on the electron density function instead of wavefunction were used to study the interaction between CNT and the Adenine and calculation of global reactivity indexes by the Koopmans theory-based quantities [16, 20, 21] This hypothesis depends on the contrasts between the most noteworthy involved sub-atomic orbital Highest Occupied Molecular Orbital (HOMO) and least empty sub-atomic orbital Lowest Unoccupied Molecular Orbital (LUMO) energies for the impartial particle[22, 23], the electronic properties of carbon nanotube are shown in Fig. 2.

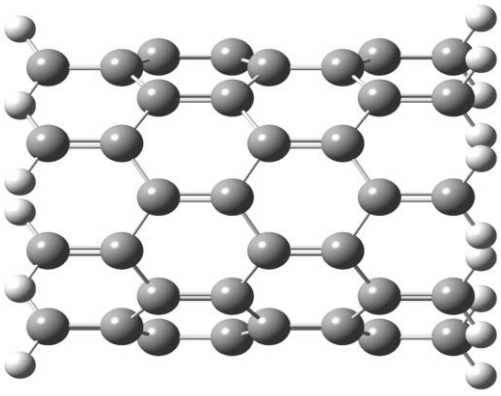

Fig.1. The Chemical structure of pristine graphene nanoribbon.

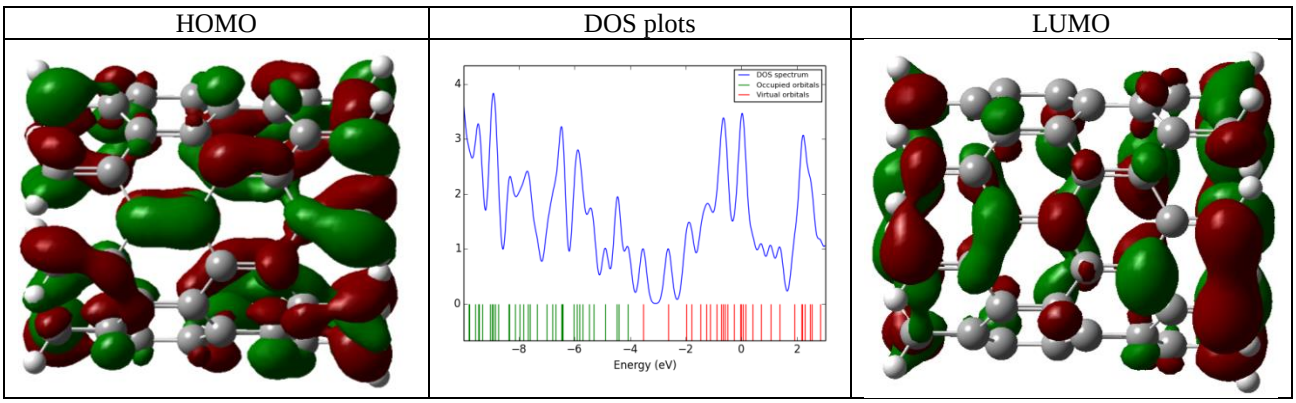

Fig.2. The density of states as well as HOMO – LUMO distribution of carbon nanotube

The nitrogenous base (Adenine) is composed of aromatic rings with spaced base pairs 3.4 A˚ in the double helix [24], see Fig. 3.

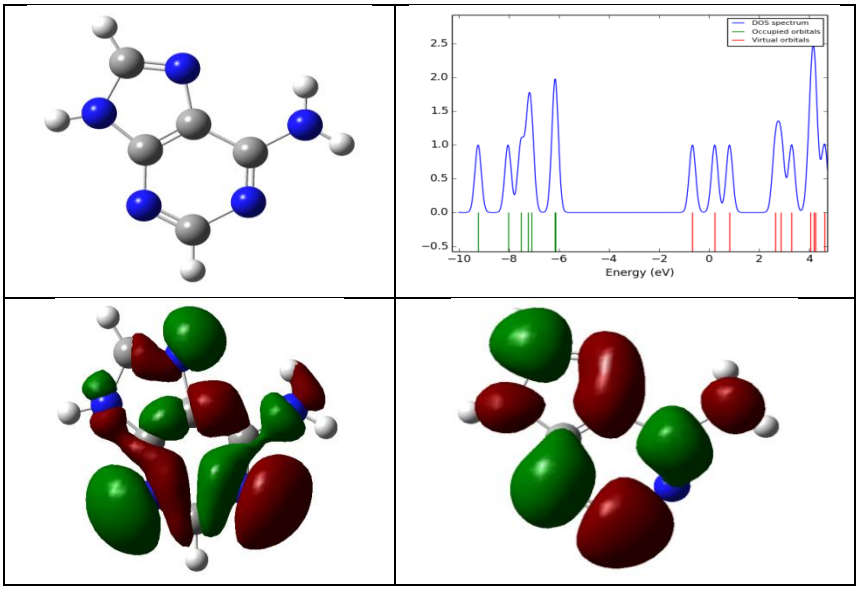

Fig.3. The optimized structure and the density of states as well as HOMO – LUMO distribution of Adenine

To evaluate the reactivity and the stability of the nano sensor, DFT-based descriptors were calculated[21, 25]:

$$\mu = (\partial E/\partial N)_{V(r),T} \quad (1)$$

$$\eta = 1/2(\partial^2 E/\partial N^2)_{V(r),T} \quad (2)$$

$$S = \frac{1}{2\eta} \quad (3)$$

$$\omega = \mu^2/2\eta \quad (4)$$

where μ, η, S and ω are the chemical potential, chemical hardness, chemical softness, and electrophilicity, respectively. While *E*, *N*, and *V(r)* are the total electron energy, the number of electrons, and external potential, respectively[26]. Using Koopman's theorem the above equations can be given as :

$$\chi = (E_{HOMO} + E_{LUMO})/2 \quad (5)$$

$$\eta = (E_{HOMO} + E_{LUMO})/2 \quad (6)$$

GaussSum program[27] was used to obtain the density of states (DOS)results, it is worth mentioning that the adsorption energy (E_{ads}) between adenine on CNT was defined as [28-32]:

$$E_{ads} = E_{adenine/CNT} - (E_{adenine} + E_{CNT}) \quad (7)$$

Where $E_{adenine/CNT}$, $E_{CNT,}$ and $E_{adenine}$ are total energy of the adenine/CNT, the total energy of CNT, and adenine molecules in relax geometry, respectively. negative adsorption energy refers to the stable formed systems and the positive adsorption energy indicates the local minima, i.e. through this explanation when $E_{ads} < 0$ leads to a stable structure, which corresponds to exothermic adsorption, Sees Fig. 4. [21, 32],

Variation of the conductivity of each structure which determines the performance in adenine sensing is determined in terms of variation bandgap energy through Eqs. [29, 33]:

$$\%\Delta E_g = \frac{E_g\ (without\ adenine) - E_g\ (with\ adenine)}{E_g\ (without\ adenine)} \times 100 \quad (8)$$

where, E_g (with adenine) and E_g (without adenine) represent the band gap energy of the substrate after and before interaction with adenine molecule, respectively.

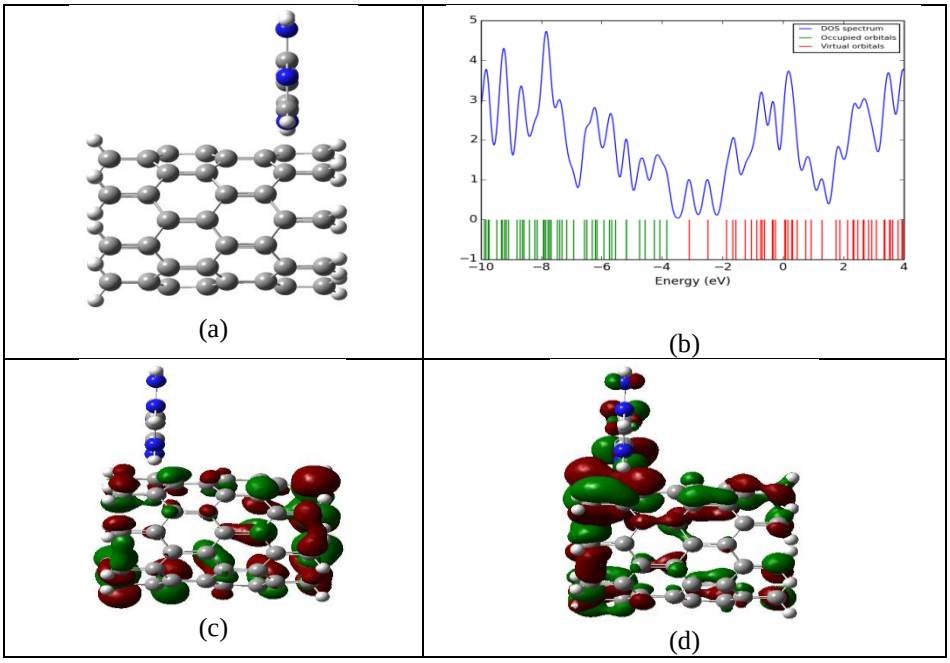

Fig. 4: a) Geometrical optimization of CNT, b) DOS, c) HOMO distribution and d) LUMO distribution

As shown in Fig. 4. the HOMO of CNT is generally confined on the C–C bonds and its LUMO on the clashing site. After interacting with adenine, LUMO shifts on adenine molecule which corresponds to the reduction in the gap of energy (E_g).

III. Results and Discussions

In our result, the interactions between adenine and CNT are studied using DFT calculations. After full structure relaxation, the adenine molecule was added to pristine CNT and study the sensing and adsorption capability.

A. *Adsorptive capability*

Adsorption vitality is the primary marker of structures' capacity in adenine adsorption, where, minimal estimation of ΔE_{ads} infers the higher liking of CNT structure upon adenine adsorption. From Table 1, the adsorption vitality estimations of the association Adenine with CNT are 3.40287 eV.

It is qualified to refer to that the presence of a solid collaboration among the adsorbed particle and adsorbent surface isn't attractive. The large E_{ad} just an as solid connection between the adsorbed atom and the adsorbent sheet reason solidify the desorption procedure with draw out recuperation time. In any case, it is qualified to refer to again that the positive estimation of Eads shows the exothermic character of the CNT. The customary change state hypothesis shows that the recuperation time (τ) is characterized by[34]

$$\tau \propto v_0^{-1} \exp(-E_{ads}/(K_B T)) \quad (8)$$

where v_0 is the attempt frequency which in many investigations is taken to be of the request for 109^{s-1} [23, 35], K_B and T are the Boltzmann's constant and the

temperature in Kelvin. As indicated by the above condition, the expansion in E_{ad} worth will draw out the recuperation time in an exponential model.

B. Sensing capability

The detecting capacity of CNT was concentrated by considering the variety of E_g after the expansion of adenine. From Table 1, sees that the $\%\Delta E_g$ esteem is negative; the negative estimations of $\%\Delta E_g$ express the hole vitality of structures declines from unique estimations of CNT because of adsorption adenine consequences for the surface it, bringing about higher conductivity for these structures. While, the synthesis with the most elevated $|\% \Delta E_g|$ show up better sensor execution. nA simple change in the E_g of CNT causes modify the amount of electrons that called conduction electrons. This adjustment in conductivity can be gone to a discernible electrical signal[31]. In any case, it is qualified to make reference to that changing the bandgap E_g can adjust the electrical conductivity for the framework as per the condition [36-38]:

$$\sigma \propto \exp\left((-E_g)/(2K_B T) \right) \quad (9)$$

T: temperature, σ: conductance, and k_B: Boltzmann's constant.

From TABLE 1, we notice that the estimation of %ΔEg is 37.81. So, the CNT is a good sensor for adenine.

TABLE1. The electronic properties of CNT with Adenine

Structure	E_{HOMO}	E_{LUMO}	E_g (eV)	ΔE_g	E_{tot} (eV)	E_{ad} (eV)
CNT	-4.07947	-3.53607	0.543404	–	-66466.5964	–
Adenine	-6.13336	-0.66776	5.465602	–	-12644.0567	–
CNT/Adenine	-3.85362	-3.10478	0.748847	-37.81	-79107.2502	3.40287

IV. Conclusion

In summary, we study the interaction between CNT and adenine molecules by using DFT in terms of the energetic data of the CNT. It was observed that adsorption energy values of the interaction Adenine with CNT are 3.40287 eV. So, the interaction between GNR and Adenine is stronger.

Also, we notice that the value of $\%\Delta E_g$ is 37.81. So, it can be concluded that the CNT is a good sensor for adenine molecules.

Refrences

1. Biercuk, M.J., et al., *Electrical transport in single*-wall *carbon nanotubes*, in *Carbon Nanotubes*. 2007, Springer. p. 455-493.

2. Omidvar, A., M. Anafcheh, and N. Hadipour, *Computational studies on carbon nanotube–graphene nanoribbon hybrids by density functional theory calculations.* Scientia Iranica, 2013. **20**(3): p. 1014-1017.

3. Liu, L., F. Liu, and J. Zhao, *Curved carbon nanotubes: From unique geometries to novel properties and peculiar applications.* Nano Research, 2014. **7**(5): p. 626-657.

4. Zhou, O., et al., *Materials science of carbon nanotubes: fabrication, integration, and properties of macroscopic structures of carbon nanotubes.* Accounts of chemical research, 2002. **35**(12): p. 1045-1053.

5. Baughman, R.H., et al., *Carbon nanotube actuators.* Science, 1999. **284**(5418): p. 1340-1344.

6. Gao, H., et al., *Spontaneous insertion of DNA oligonucleotides into carbon nanotubes.* Nano Letters, 2003. **3**(4): p. 471-473.

7. Newson, R.W., et al., *Ultrafast carrier kinetics in exfoliated graphene and thin graphite films.* Optics express, 2009. **17**(4): p. 2326-2333.

8. Kurbanoglu, S. and S.A. Ozkan, *Electrochemical carbon-based nanosensors: A promising tool in pharmaceutical and biomedical analysis.* Journal of pharmaceutical and biomedical analysis, 2018. **147**: p. 439-457.

9. Stephens, P., et al., *J. Baker, J. Andzelm, M. Muir, PR Taylor.* Chem. Phys. J. Phys. Chem, 1994. **98**: p. 11623.

10. Taylor, D.E., et al., *Blind test of density-functional-based methods on intermolecular interaction energies.* The Journal of chemical physics, 2016. **145**(12): p. 124105.

11. Rad, A.S. and V.P. Foukolaei, *Density functional study of Al-doped graphene nanostructure towards adsorption of CO, CO2, and H2O.* Synthetic Metals, 2015. **210**: p. 171-178.

12. Rad, A.S., et al., *DFT study on the adsorption of dimethyl, ethyl methyl, and dimethyl ethers on the surface of gallium doped graphene.* Applied Surface Science, 2017. **401**: p. 156-161.

13. Mohammed, M.H., *Controlling the electronic properties of the graphene nanoflakes by BN impurities.* Physica E: Low-dimensional Systems and Nanostructures, 2018. **95**: p. 86-93.

14. Mohammed, M.H., *Designing, and engineering electronic bandgap of graphene nanosheet by P dopants.* Solid State Communications, 2017. **258**: p. 11-16.

15. Al-Abood, M.H., F.N. Ajeel, and A.M. Khudhair, *Influence of oxygen impurities on the electronic properties of graphene nanoflakes.* Physica E: Low-dimensional Systems and Nanostructures, 2017. **88**: p. 1-5.

16. Mohammed, M.H., F.N. Ajeel, and A.M. Khudhair, *Adsorption of gas molecules on graphene nanoflakes and its implication as a gas nanosensor by DFT investigations.* Chinese journal of physics, 2017. **55**(4): p. 1576-1582.

17. Ajeel, F.N., *Engineering electronic structure of a fullerene C20 bowl with germanium impurities.* Chinese Journal of Physics, 2017. **55**(5): p. 2134-2143.

18. Ajeel, F.N., M.H. Mohammed, and A.M. Khudhair, *Tuning the electronic properties of the fullerene C 20 cage via silicon impurities.* Russian Journal of Physical Chemistry B, 2017. **11**(5): p. 850-858.

19. Ajeel, F.N., M.H. Mohammed, and A.M. Khudhair, *Effects of lithium impurities on electronic and optical properties of graphene nanoflakes: A DFT–*

TDDFT study. Chinese Journal of Physics, 2019. **58**: p. 109-116.

20. Khudhair, A.M., F.N. Ajeel, and M.H. Mohammed, *Theoretical Study of the Electronic and Optical Properties to Design Dye-Sensitivity for Using in Solar Cell Device.* Russian Journal of Physical Chemistry B, 2018. **12**(4): p. 645-650.

21. Ajeel, F., et al., *DFT Investigation of Graphene Nanoribbon As a Potential Nanobiosensor for Tyrosine Amino Acid*. Russian Journal of Physical Chemistry A, 2019. **93**(4): p. 778-785.

22. Cramer, C.J., *Essentials of computational chemistry: theories and models*. 2013: John Wiley & Sons.

23. Ajeel, F.N., M.H. Mohammed, and A.M. Khudhair, *SWCNT as a Model Nanosensor for Associated Petroleum Gas Molecules: Via DFT/B3LYP Investigations.* Russian Journal of Physical Chemistry B, 2019. **13**(1): p. 196-204.

24. Arnold, A.R., M.A. Grodick, and J.K. Barton, *DNA charge transport: From chemical principles to the cell.* Cell chemical biology, 2016. **23**(1): p. 183-197.

25. Li, S., et al., *Biosensor nanomaterials*. 2011: John Wiley & Sons.

26. Li, J. and N. Wu, *Biosensors based on nanomaterials and nanodevices*. 2013: CRC Press.

27. NM, O. and A. Boyle, *Tenderholt, and KM Langner*. J. Comput. Chem, 2008. **29**: p. 839.

28. Pandey, S.K., K.-H. Kim, and K.-T. Tang, *A review of sensor-based methods for monitoring hydrogen sulfide.* TrAC Trends in Analytical Chemistry, 2012. **32**: p. 87-99.

29. Yousefian, Z., et al., *Theoretical studies on B, N, P, S, and Si-doped fullerenes toward H2S sensing and adsorption*. Physica E: Low-dimensional Systems and Nanostructures, 2019. **114**: p. 113626.

30. Velázquez-López, L.-F., et al., *DFT study of CO adsorption on nitrogen/boron doped-graphene for sensor applications.* Journal of molecular modeling, 2019. **25**(4): p. 91.

31. Rouhani, M., *DFT study on adsorbing and detecting the possibility of cyanogen chloride by pristine, B, Al, Ga, Si, and Ge doped graphene*. Journal of Molecular Structure, 2019. **1181**: p. 518-535.

32. Oftadeh, M., M. Gholamian, and H.H. Abdallah, *Investigation of interaction hydrogen sulfide with (5, 0) and (5, 5) single-wall carbon nanotubes by density functional theory method.* International Nano Letters, 2013. **3**(1): p. 7.

33. Chen, S., et al., *The adsorption and dissociation of H2S on Cu (100) surface: a DTF study*. Surface Science, 2014. **620**: p. 51-58.

34. McNaught, A. and A. Wilkinson, *Compendium of Chemical Terminology, Volume 1669*. 1997, Blackwell Science Oxford Oxford, UK.

35. Vallejo-Fernandez, G., et al., *Measurement of the attempt frequency in antiferromagnets.* Applied Physics Letters, 2010. **97**(22): p. 222505.

36. Ajeel, F.N., M.H. Mohammed, and A.M. Khudhair, *Energy bandgap engineering of graphene nanoribbon by doping phosphorous impurities to create nano-heterostructures: A DFT study*. Physica E: Low-dimensional Systems and Nanostructures, 2019. **105**: p. 105-115.

37. Xu, S., et al., *Real-time reliable determination of binding kinetics of DNA hybridization using a multi-channel graphene biosensor.* Nature communications, 2017. **8**: p. 14902.

38. Rastegar, S.F., A.A. Peyghan, and N.L. Hadipour, *Response of Si-and Al-doped graphenes toward HCN: a computational study*. Applied surface science, 2013. **265**: p. 412-417.

V.