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Adenine Adsorption on Ag Doped Graphene : A Theoretical Insight

Baliram Lone[1, a*]

[1]Nanomaterials Research Laboratory, Department of Physics, Vinayakrao Patil Mahavidyalaya, Vaijapur-423701, Dist. Chhatrapati Sambhjinagar, Maharashtra, India

[a*] *drbglone@gmail.com*

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ABSTRACT

The adsorption phenomenon of Adenine on silver (Ag) doped graphene extensively studied by using density functional theory (DFT) method to insight the role of DNA nucleobase adenine as adsorbent. Our theoretical findings suggest that the structural and electronic properties of the complex system of graphene-adenine (Gr-Ade) strong depends on Silver (Ag) atom. The DNA base adenine molecule is adsorbed on pristine graphene, while there is strong chemisorption phenomenon is observed on Ag-doped graphene. We successfully reported the Dipole moment, HOMO-LUMO and density of states (DOS). The complex biomolecular system (Gr-Ag-Ade) studied could be used to assemble DNA based biosensors in different fields as well.

Keywords : Adenine, Silver, Graphene, DFT, HOMO-LUMO

I. INTRODUCTION

Deoxyribose nucleic acid (DNA) [1] play a crucial role to carry genetic information in next generation of biologically live entity. It can detect disease diagnosis and treatment, detection of cancer, forensic sciences, environmental monitoring, food safety and agriculture [2]. The DNA molecule consists of a monosaccharide sugar, a phosphate group, and four kinds of nitrogen-containing nucleobases, Viz. Cytosine (C), guanine (G), adenine (A), and thymine (T) [3-4]. The interaction of DNA nucleobase and the graphene surface, based on the signal that the device detected during the DNA nucleobases biosensors classified into electrochemical DNA sensors [5-6], electronic sensors [7] and optical DNA biosensors as well [8]. The high sensitivity, high specificity and fast responding signifies emerging potential in DNA based diagnostics. The adsorbent capability of graphene can be increased predominantly by modification of its surface using [9-10] doped or decorated atoms. In recently published work the interaction of biomolecules (Alanine) with nanomaterials (SWNT), the physical adsorption of mechanism of Alanine molecules on surface of Pristine semiconducting zigzag single walled carbon nanotubes (8,0) studied. The results are useful for targeted drug delivery of L-Alanine besides to this the biosensors can

be used to check concentration level of alanine in patients to avoid delay in treatment as well [11].

we investigated the adsorption properties of complex system i.e. DNA nucleobase Adenine with Graphene sheet doped by silver atom (Gr-Ag-Ade). The DNA nucleobase adenine molecule is adsorbed on pristine graphene. Our findings suggest that strong chemisorption phenomenon is observed on Ag-doped graphene. We successfully reported the charge transfer, HOMO-LUMO and density of states (DOS) of the complex biomolecular system Gr-Ag-Ade.

II. COMPUTATIONAL METHODS

Using DFT method the basis set B3LYP was applied for relaxation of Graphene –Silver (Gr-Ag) and complex system of graphene-Silver-Adenine (Gr-Ag-Ade) with split basis sets (except Ag atom, for all atoms basis set was 6-31G (d,p). We utilized basis set lanl2dz available in Gaussian09 [12].

All the quantum chemical investigations including charge transfer, highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), adsorption energy and density of states (DOS) were computed by using above mentioned basis set.

The adsorption energy (E_{ads}) upon DNA nucleobase adenine on Gr-Ag was calculated as follows

$$E_{ads} = E_{GrAg-Adenine} - \left(E_{GrAg} + E_{Adenine}\right)$$

Where $E_{GrAg\text{-}Ade}$ is complex system of graphene with doped silver atom coupled with DNA base adenine (Ade), the adsorbed system of GrAg atom. The E_{GrAg} gives energy of GrAg and E_{Ade} gives isolated energy of DNA nucleobase adenine.

We used GaussView 5.0 [13] for modeling the structure of pristine graphene, Ag doped graphene and DNA nucleobase cytosine.

III. RESULT AND DISCUSSIONS

Figure 1 shows the chemical structure of DNA base Adenine Fig.1.(a) and fig.(b) simulated structure of DNA base adenine at 6-31++ basis set.

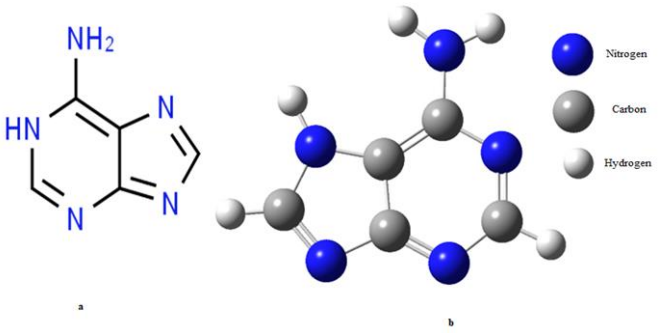

FIGURE 1. *The schematic view of the Adenine: (a) Molecular structure. (b) The simulated structure of adenine at 6-31G(d,p) basis set within WB97XD using DFT method (b) N, C, and H atoms are shown as blue, grey and white respectively.*

We have optimized the geometries of DNA nucleobase adenine molecule with pristine graphene and Ag doped graphene sheet as well. We know that pristine graphene has a planer surface with sp^2 hybridization, replacing one carbon atom by Ag in graphene results deformation of its surface because of larger bond lengths of Ag C (1.51 Å) than C- C (1.43 Å), to decrease the stress doped atom have to place on graphene sheet which consists of 43 carbon atoms of the composed system.

The deformation was taking place with change in hybridization of Gr from SP2 to sp3 at doped (Ag atom dopant) site atom.

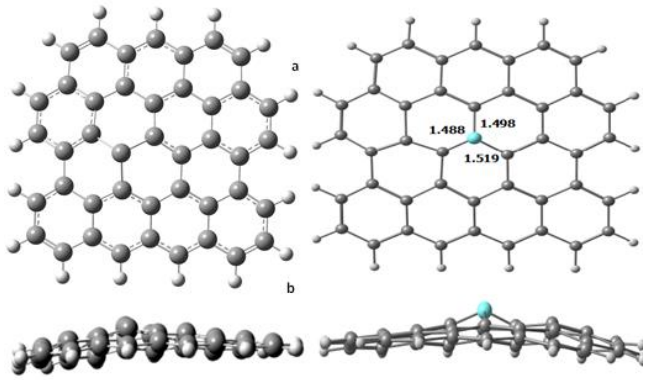

FIGURE 2. *Pristine Graphene sheet with C-43 and hydrogen 17 atoms top (a) side (b) view, Figure c & d indicates top and side view with Ag doped graphene sheet respectively.*

The above figure 2 (a) shows the top view of pristine graphene and fig.2 (b) shows side view of pristine graphene the calculations performed at 6-31G.

The silver doped graphene figure 2(c, d) top and side view signifies the dopant atom changed the bond distance from 1.43 Å (C- C) to 1.51 Å (Ag- C) as well. The lanl2dz basis set was utilized from Ag atom in complex system.

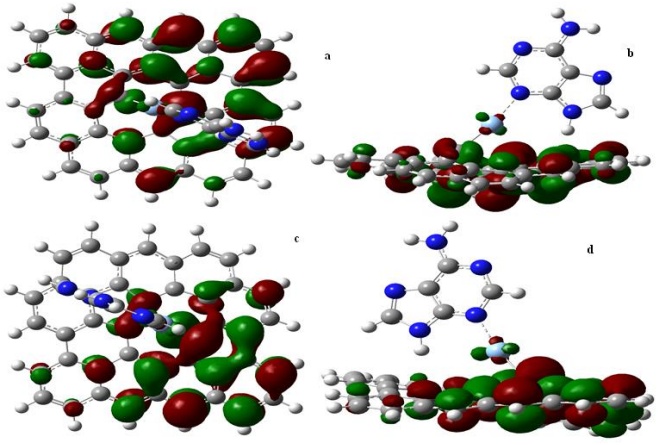

FIGURE 3. *Adenine adsorbed on pristine Graphene surface top (a) side (b) view distance in A.U., Figure c & d indicates top and side view with Ag doped graphene with adenine adsorbed on its surface.*

The Pristine Graphene (Gr@C43) sheet and DNA nucleobase adenine nucleobase were successfully performed simulation within DFT frame work of Gaussian 09 suit. The adenine and graphene N and C distance were measured 1.347 A.U.

Whereas Ag doped graphene with adenine adsorbed found 1.547 A.U., furthermore, it implies the deformation is taking place due to addition of Ag atom with adenine adsorbed on graphene surface of a bimolecular complex system.

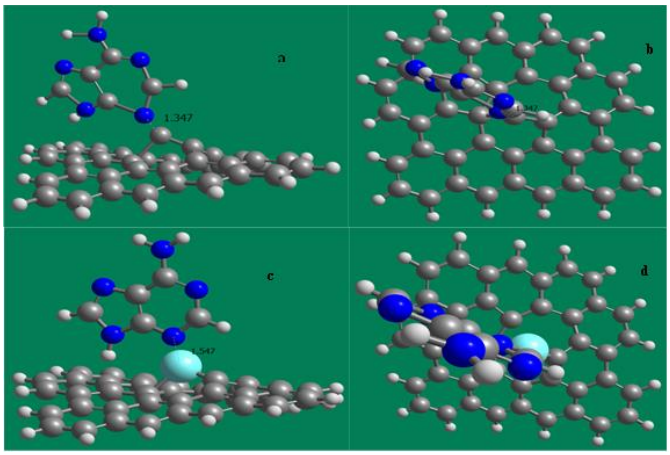

FIGURE 4. *The complex bimolecular system Gr-Ag-Ade HOMO (MO=179= -0.176392 a.u.) top view (a), side view (b) , LUMO (MO=180= -0.178390 a.u.) top view (c) and side view (d) respectively.π-MO (contour value=0.025 a.u.) of Gr-Ag-Ade, Eigenvalues of this π-MO are -0.4770 a.u.)*

Charge density analysis: The highest occupied molecular orbital (HOMOs) of Gr-Ag-Ade is shown in fig.4 a, fig.4 b with contour value 0.025 Å and HOMO (MO=179=-0.176392 a.u.). The lowest unoccupied molecular orbital (LUMOs) of the complex biomolecular system Gr-Ag-Ade shown in fig.4c, fig.4d with eigen values of π-MO are -0.178390 Å.

The HOMO-LUMO gap play a crucial role to evaluate the parameters including kinetic stability, chemical stability and electrical conductivity of the cluster [14]. HOMO-LUMO gap signifies the energy gap between highest occupied orbit and lowest unoccupied orbit of the cluster.

A higher value of HOMO–LUMO gap corresponds to a high energy required for electrons jump from the occupied orbit to unoccupied orbit. In a word, a smaller value of HOMO–LUMO gap represents a higher chemical reactivity, whereas a higher value of HOMO–LUMO gap indicates a weaker chemical reactivity.

The analysis data for HOMOs and LUMOs distribution shows the structural stability and strength of the complex biomolecular system Gr-Ag-Ade as well.

Table 1. Physical parameters DNA nucleobase adenine molecule adsorbed on Pristine Gr sheet and Ag. doped Gr sheet adsorption energy, NBO charge transfer and binding distance (d) in A.U.

System	E_{ad} in Hartree	d (Å)	Polarizability-α (A.U.)	μ in Debye
Adenine	-464.7063400	……	70.154220	7.607106
Gr-Ag	-1736.435255	1.347	…….	4.931340
Gr-Ag-Ade	-2197.753130	1.547	…….	4.716954

Note: We calculated all values theoretically tabulated in table 1.

From table 1, it is clear that the complex system of Gr-Ag-Ade to have more adsorption energy, same trend is followed for natural bond orbital and distance. The bond distance between Gr-Ag and Ade is a crucial parameter to evaluate the adsorption energy n complex system. The complex with short bond distances between Gr-Ag and Ade shows higher adsorption energy. All values of adsorption energy have negative values it infers that the molecules of adenine attract to the Gr-Ag surface due to this energy is released and the heat of adsorption is negative in nature. The adsorption phenomenon is always exothermic it confirms from the Gr-Ag -Ade complex system.

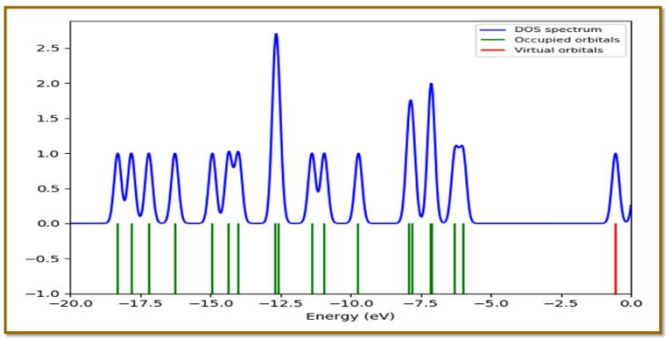

FIGURE 5. *a) The density of states (DOS) of DNA nucleobase Adenine*

To understand the chemical bonding through electronic structure, we have calculated the density of states of the biomolecular complexes system. Figures 7.a.,7. b and7. C, represents the plot of density of states of the DNA nucleobase adenine, graphene-silver and graphene-silver-adenine biomolecular complex system obtained by using Gaussian broadening 0.1 eV of the one-electron Kohn-Sham electronic energies. A comparison of the electronic energy spectrum indicates that the energy levels of the DNA nucleobase adenine-Ag undergo an overall red shift when the Ag was bound it. A maximum shift is shown in fig 7.b, was found in the energy spectrum when Ag was bound to the graphene.

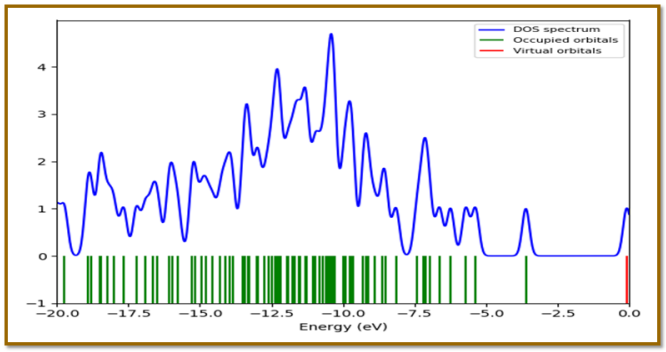

FIGURE.5 *b) The density of states of Graphene-Silver (Gr-Ag) system.*

The degree of shift of E_F of Gr-Ag complex varies as function of polarizability is 70.154220 A.U. of Ag molecules as shown in table 1. The DOS data shown in fig.5.b shows the number of allowed electrons states

per unit volume at a given energy of the Ag with graphene(C-42).

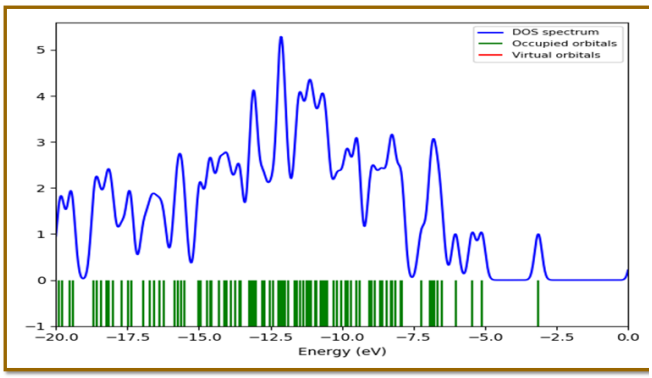

FIGURE.5 *c) The density of states of Graphene-Silver-Adenine (Gr-Ag-Ade) biomolecular complex system.*

The density of states of Gr-Ag-ade complex biomolecular system shown in fig.5.c. This shows the number of allowed electrons states per unit volume at a given energy of the DNA nucleobase Adenine (-NH2) with silver (Ag-1) doped -graphene(C-42) of the complex system.

IV. SUMMARY AND CONCLUSIONS

The adsorption of DNA nucleobase Adenine molecules on surface of graphene-silver investigated using density functional theory calculations in gas phase. The adsorption energy infers that it is suitable surface for Gr-Ag-Ade complex system. The electronic changes studied through HOMO-LUMO gap. Our theoretical findings suggest that the structural and electronic properties of the complex system of graphene-adenine (Gr-Ade) strong depends on Silver (Ag) atom. The DNA base adenine molecule is adsorbed on pristine graphene, while there is strong chemisorption phenomenon is observed on Ag-doped graphene. We successfully reported the dipole moment, HOMO-LUMO and density of states (DOS). The complex biomolecular system (Gr-Ag-Ade) studied could be used to assemble DNA based biosensors in different fields as well.

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Note: The authors declare no competing financial interest.

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