RESEARCH ARTICLE

Adenine molecule interacting with golden nanocluster: A dispersion corrected DFT study

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ABSTRACT

The interaction between nanoparticles and biomolecules such as protein and DNA is one of the major instructions of nanobiotechnology research. In this study, we have explored the interaction of adenine nucleic base with a representative golden cluster (Au13) by using dispersion corrected density functional theory (DFT-D3) within GGA-PBE model of theory. Various active sites as and ways of the approach as well as several affecting parameters on the interaction nature of interacting molecules such as adsorption energy, binding distance, solvent effect and, electronics structure were investigated. Our first-principles results indicated that adenine forms a stable complex with the golden cluster with interaction energy of −42.84 kcal/mol and binding distance of 2.139 Å. Charge transfer analysis with Hirshfeld approach demonstrated about 0.52 e was transferred from adenine to golden cluster skeleton. It was found from the obtained interaction parameters that there is strong interaction (chemisorption) between adenine and golden cluster. The type and strength of interaction have been also confirmed by hybrid functional B3LYP level of theory. This finding is very promising for potential medicinal and pharmaceutical applications of golden clusters.

INTRODUCTION

Drug-delivery systems (DDSs) are tools to enhance the efficiency of pharmaceutical payloads owing to poor solubility, limited stability, biodistributions and pharmakinetics of payloads rather than the free ones. Thus, DDSs have been designed and practically employed, which one of the most important of them are based on nanomaterials. Nanomaterials because of their unique specifications have been considered as potential carriers for drug and gene. Broad range of surveys have been done by many researchers that some of them concentrate on kind of materials that used for drug delivery and some others discuss the experimental and theoretical methods of studies. Materials that have been used as carrier are polymers, dendrimers, liposomes and recently nanomaterials such as nanotubes (1, 2) nanorods (3) and nanoparticles (4, 5).

Inorganic nanoparticles have represented various advantageous features such as tunable size, specific surface properties, multifunctional capabilities, and their abilities to result in synergistic properties of metal core. Amongst these nanoparticles, gold nanoparticles (AuNPs) due to their physical and biological properties, including chemical stability, compatible with biological media, non-toxicity, and satisfied interactions with biological species, can be examined as an attractive candidate to deliver some payloads, such as nucleic acids of DNA, RNA, proteins and free amino acids, into intended targets. For instance, it was found AuNPs can play an effective role as carrier and insulin-loaded (6). As AuNPs act well in drug delivery, for gene transfer would also

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be appropriate and this claim is proved by some researchers. In a research, delivery applications of AuNPs like drug and nucleic acid delivery were studied simultaneously (7). In other work, delivery of nucleic acid and its challenges such as endosomal entrapment/escape and active delivery/ presentation in the cell were discussed (8). More recently, in a novel work siRNA delivery has been assessed by AuNPs as a promising strategy (9).

On the other hand, nucleic acids can also provide promising tools for therapeutic targets, including pathways and molecules involved in cancer and genetic disorders. In addition, the efficient release of these therapeutic agents is a prerequisite for an impressive therapy. This releasing process may be affected by some internal and external functions including glutathione (GSH), pH, temperature, light, and interference species in accordance with the related drug and gene. Moreover, in contrast with small-molecule therapeutics, nucleic acids require delivery vehicles for protection from nucleases and other environmental agents and to facilitate entry into the cell. Hence, the preference of these carriers should be previously studied at *in vitro* and also *in vivo* conditions.

Accordingly, since the experimental studies are so complicated, time consuming and costly, the theoretical ones have been more interested. The modern theoretical approaches based on quantum chemistry such as dispersion-corrected DFT (DFT-D) represented a good compromise between computational findings and accuracy. In the present work, the potential application of gold nanocluster as nanocarrier was investigated by using DFT-D calculations. The main goal of this project was theoretically identification whether gene delivery based on gold nanostructures is appropriate regarded to biological aspects. Here, the molecular structures according to their length and angle of bonds were modeled. After that, the DFT calculations were performed to calculate the interaction parameters of complex including nucleobase and nanocluster.

COMPUTATIONAL DETAILS

All calculations were carried out on the basis of DFT method to study the interaction between the considered adenine nucleobase and Au13 golden cluster. DFT is the main computational technique, which extensively utilized in this research. Quantum-based designs were conducted using ORCA (3.0.3) (10, 11) and all electrons

DFT calculations were investigated in accordance with the Perdew–Burke–Ernzerhof (PBE) (12) functional and generalized gradient approximation (GGA). To achieve this objective, geometry of designed structures was optimized and total energy calculations were respectively carried out for all atoms utilizing split-valance polarization (def2-SVP) and triple-ζ plus polarization basis set (def2-TZVP) in accordance with the method suggested by Ahlrichs et al. (13, 14). In addition, the [SD (60, MDF)] effective core potential (ECP) for Au atom (15, 16) was utilized in this study within the nucleus effective charge method. In order to consider the electrostatic interaction of molecular systems within the solvent, the solvent effect was described by conductor-like screening models (COSMO) (17).

Accordingly, the normal optimization convergence criteria have been satisfied using ORCA and this process was considered to thoroughly optimize all structures for SCF iterations set to VeryTightSCF to diminish the contaminating of noise in the gradient calculations. In order to examine the long-range dispersion interactions, Grimme's atom pair-wise dispersion corrections, 3rd version, with Becke–Johnson damping, called D3-BJ, were combinational employed (18-20). The influence of imperfect nature of the basis set in non-covalently bonded systems was reduced whereas the basis set superposition error (BSSE) is decreased utilizing counterpoise correction (21). On the other hand, the complex systems were investigated when the optimized structures were subjected to single point energy calculations on the basis of def2-TZVP basis set until the energies were approached to the basis set limit. Energies of adsorption were calculated by the following equation:

$$E_{ads} = E_{Au13}\text{-}_{NB} - (E_{Au13} + E_{NB}) - \sigma_{BSSE} \qquad (1)$$

Where $E_{Au13}\text{-}_{AA}$, E_{Au13}, and E_{NB} are respectively related to the total energies of the complex, golden cluster Au13, and nucleobases. The compatibility between the utilized method amongst the basis set and the experimental results have been validated in the next section.

The molecular properties including gap energy (E_g), hardness (η), and softness (s) for the related species and their interactions were calculated utilizing the following equations (22).

$$I = - E_{HOMO} \qquad (2)$$

$$A = - E_{LUMO} \qquad (3)$$

$$E_g = E_{LUMO} - E_{HOMO} \tag{4}$$

$$\eta = 1/2 \ (I-A) \tag{5}$$

$$S = \eta^{-1} \tag{6}$$

Where the HOMO and the LUMO are related to the highest occupied molecular orbital and the lowest unoccupied molecular orbital states of energy transitions.

RESULTS AND DISCUSSION

In this study, the interaction between the adenine nucleobase and the gold cluster nanostructure was investigated by the DFT-D3 method and the GGA-PBE model of theory. As mentioned, the main objective of this work was practical examination of golden nanocluster (Au13 in the present work) for drug nanovector and use it for other biomedical applications such as DNA sequencing and bio-functionalized materials. Hence, the molecular structures of nucleobases as

well as Au13 nanocluster were first modeled and then optimized with SVP basis set. The optimized structure of Au13 and nucleobase are shown in Fig. 1. The obtained geometries parameters with the PBE-D3/SVP are in good agreement with reported theoretical and experimental values in literatures (23-27). For more evaluation of the accuracy of the current method, we have also optimized the adenine molecule with high-level quantum chemistry method at the MP2 level of theory. MP2 considers electron correlation effects on the Hartree–Fock method which improves molecular properties of system under study such as polarized group in molecular system (28, 29). The optimized structure obtained with the same basis set is demonstrated in Fig. 1(c). As it can be seen from the figure, the PBE functional is in good consistence with the MP2 method indicating the validity of selected theory model for optimization procedure.

Several orientations have been considered
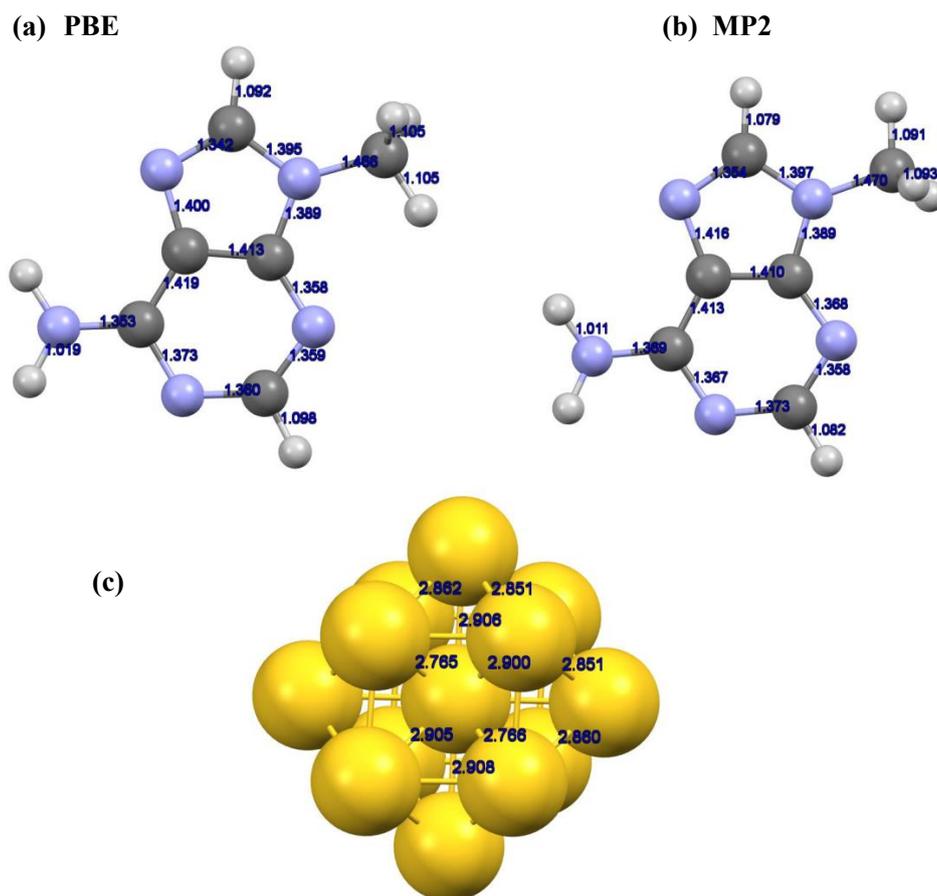

(a) PBE

(b) MP2

(c)

Fig. 1: The schematic representation of optimized structure of (a) adenine with PBE, (b) adenine with MP2 and, (c) Au13 gold cluster with PBE.

Fig. 2: The optimized structure of most stable configuration for adenine-Au13 with PBE: (a) bond length in Å and (b) the orientation angle of adenine attached to Au13 cluster. Calculated isosurface of (c) the total electron density and (d) the HOMO/LUMO states for most stable adenine-Au13 complex (iso-value of 0.02 and 0.07 were considered, respectively). The calculated PDOS for bonded Au–N atoms from adenine and Au13 cluster ((e) and (f)).

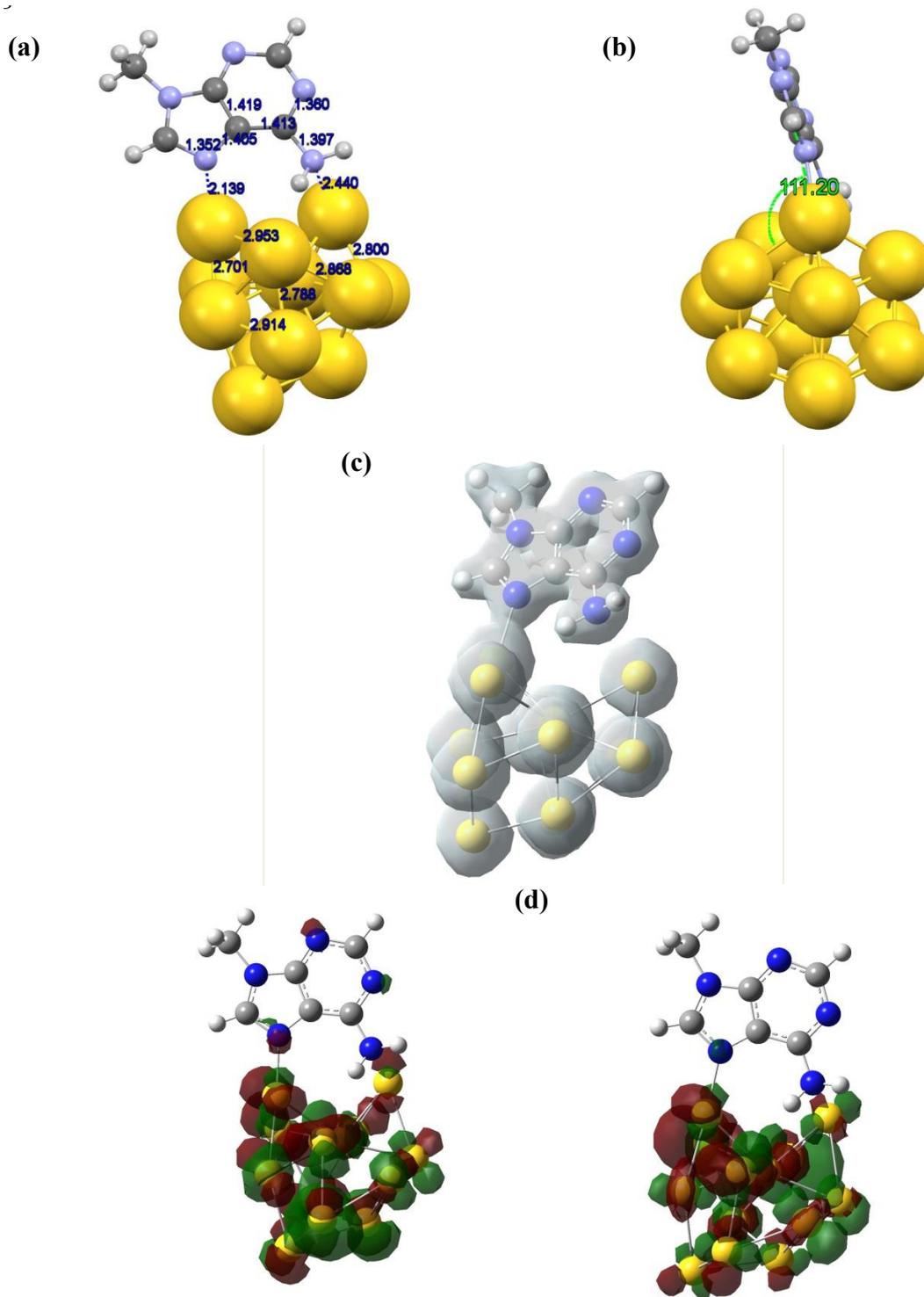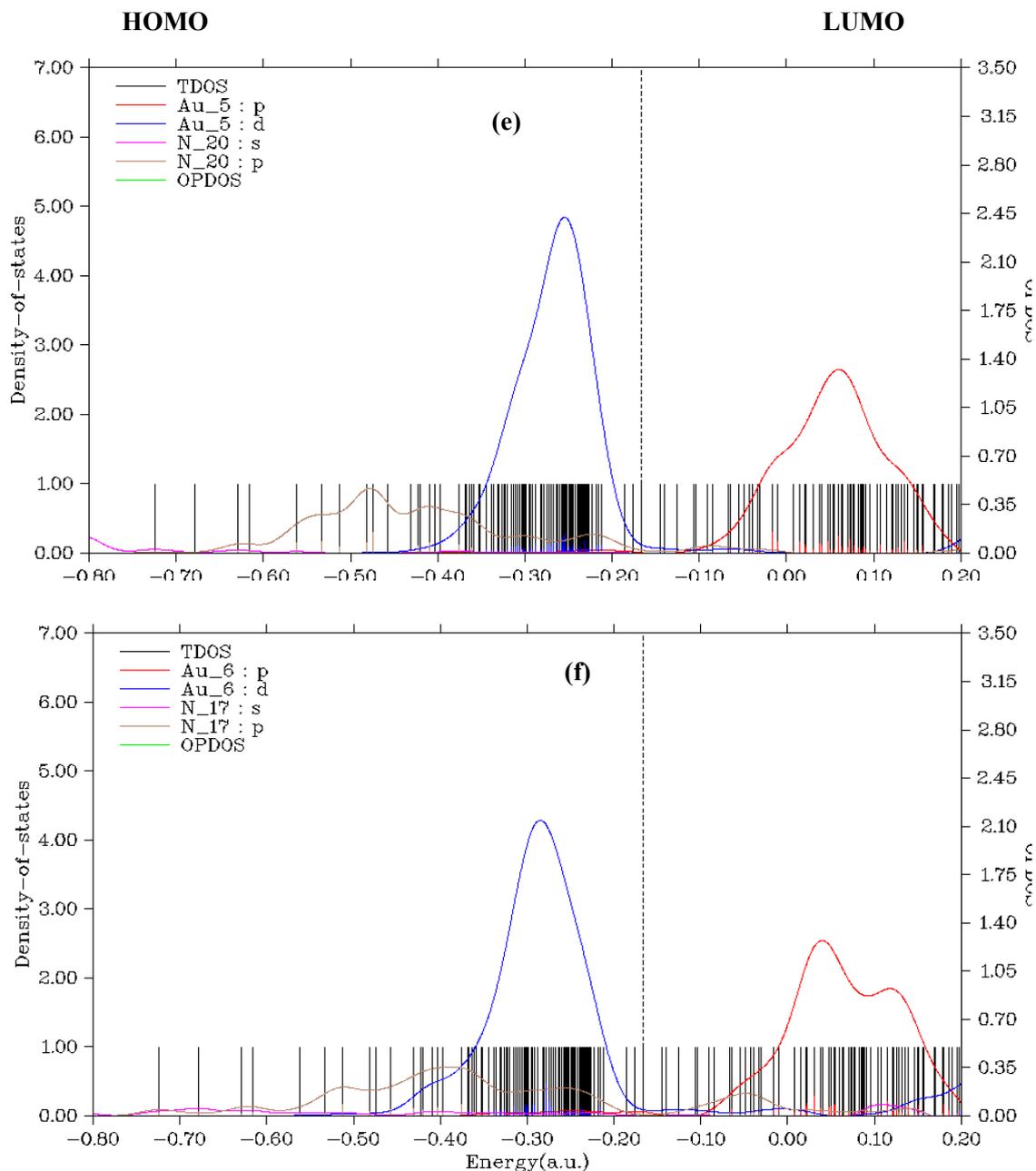**HOMO**   **LUMO**

Fig. 2: The optimized structure of most stable configuration for adenine-Au13 with PBE: (a) bond length in Å and (b) the orientation angle of adenine attached to Au13 cluster. Calculated isosurface of (c) the total electron density and (d) the HOMO/LUMO states for most stable adenine-Au13 complex (iso-value of 0.02 and 0.07 were considered, respectively). The calculated PDOS for bonded Au-N atoms from adenine and Au13 cluster ((e) and (f)).

for interacting adenine molecule with Au13 including various active sites such as N atoms as well as pentagon and hexagon rings of nucleobase approaching to gold atom of nanocluster (Aden/Au13 (I)-(III), respectively). According to this

scheme, three orientations have been evaluated as shown in Fig 2. The *first-principles* calculations data have been obtained when the nucleobase is separately investigated and also in the situation of them interacted with the nanocluster. The corresponding

Table 1. The adsorption energy for the interaction between nucleobases and golden cluster Au13 and also the related molecular properties.

System	Interaction energy (eV)			Charge Transfer (e)	
	Aqueous (vdW)	Gas (vdW)	Aqueous (non-vdW)	Mulliken	Hirshfeld
Aden/Au13 (I)	-1.858	-1.784	-1.366	+0.489	+0.477
Aden/Au13 (II)	-1.696	–	–	–	–
Aden/Au13 (III)	-1.625	–	–	–	–

computational calculations including adsorption energies of geometry optimized structures with the BSSE correction between interacting molecules have been calculated and listed in Table 1.

As the interaction of adenine and nanocluster Au13 was studied, the resulting data represented that adenine preferred to bound to Au13 with the interaction energy of -1.858 eV (-42.841 kcal/mol). In this configuration, the adenine binds to gold atoms of nanocluster through its NH_2 and N atom of 5-membered ring with equilibrium distances between the nearest atoms of 2.440 and 2.139 Å, respectively. Our obtained interaction properties are in agreement with reported experimental and theoretical values for adenine molecule interacting with similar gold clusters (30-32). Comparison of calculated bonding distance of our DFT-D3/PBE with experimental and theoretical (MP2) values for similar molecular systems (33-35) indicates the existence of covalent bond between Au and N atoms. As consequence, the obtained interaction energy and bonding distance reveal that there is a strong interaction (typical for the chemisorption) (36-40) between adenine and gold cluster and the complex is energetically stable in aqueous media. It should be noted that the obtained structural geometry of adenine was slightly changed after complexation while golden cluster skeleton deviates significantly from the sphere. This is important for gene delivery and bio-functionalization technology where the structure of selected biomolecule remains harmless. We have also calculated the interaction energy of complex under study with high-qualified hybrid B3LYP-D3 functional and the result (-1.754 eV) indicate good agreement between two employed approaches.

To give deeper intuition into the interaction nature of respective complex charge analysis based on the popular Mulliken as well valuable Hirshfeld methods was carried out and it was found that about 0.489 and 0.477 charges, respectively, have been transferred from the adenine to the Au13 cluster.

This high amount of charge transfer confirms the strong interaction between interacting entities. As evidence from the electronics structure point of view, total charge density has been also obtained for the complex and represented in Fig. 2 (c). As it is clearly found there is a charge accommodation between N atom of 5-memberd ring while no localization of charge was observed between N of amine group and gold cluster. This is expected from the obtained bonding distance of these two N atoms in the complex (see Fig. 2(a)). The calculated molecular orbitals related to the highest occupied and lowest unoccupied states (HOMO and LUMO, respectively) demonstrated that the majority of both HOMO and LUMO states are localized on the golden cluster moiety while the HOMO is slightly located on the adenine atoms (see Fig. 2(d)). This is in line with the observed charge transfer where adenine tends to give charge to the golden cluster. Further insight into the interaction nature of molecular systems can be gained by analyzing the projected density of states (PDOS) onto the involved orbitals in the formation of complex. The calculated PDOS plots for two bonded N and Au atoms in the Aden/Au13 complex was depicted in Fig. 2(e, f). It was found that in energy range of about -0.3 a.u. the overlap between the $2p$ orbitals of the N atoms and $3d$ orbitals of the Au atoms was happen which indicates the formation of Au–N bond in the complex.

In order to evaluate the influence of dispersion forces in system under consideration we have also carried out similar optimization procedure without considering the vdW forces for most stable complexes. The optimized geometry with the same model of theory indicates that no significant change was observed for the formed complex as shown in Fig 3. However, the calculated interaction energy (-1.366 eV) reveals an underestimation with respect to the original system (PBE-D3 method). Furthermore, the estimated dispersion forces for considered complex was found to be about
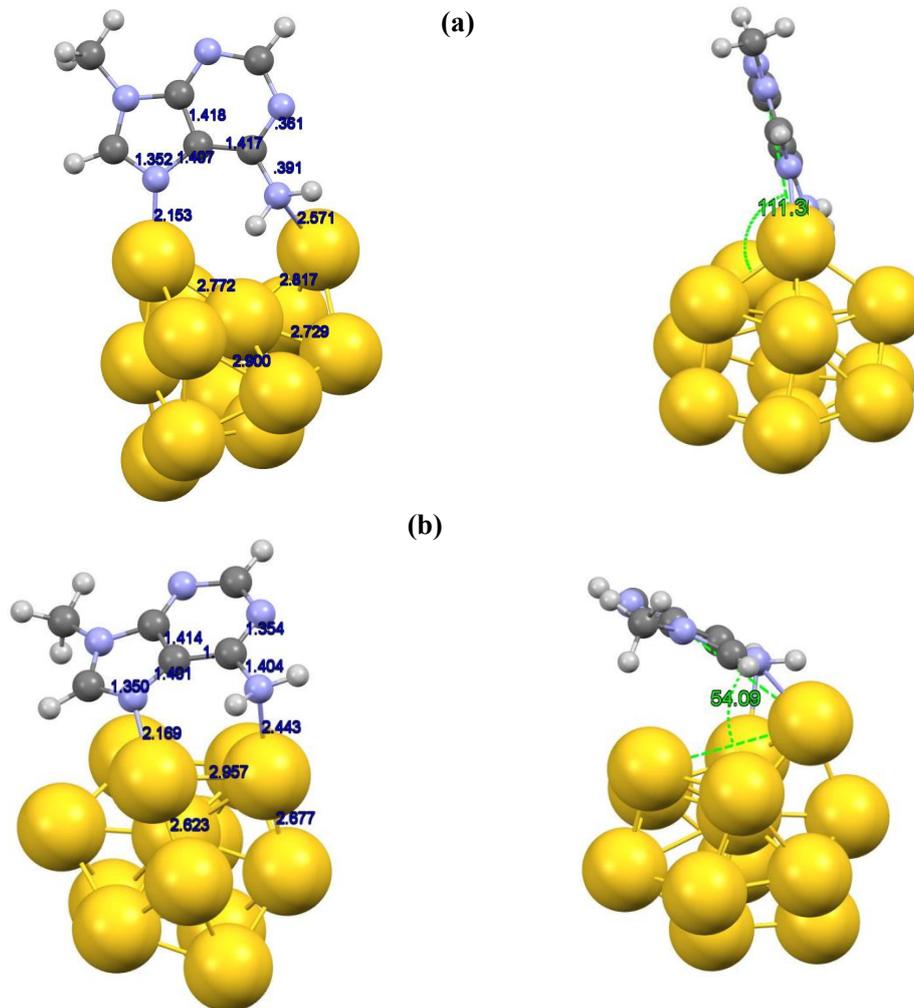
Fig. 3: The optimized structure of most stable configuration for adenine-Au13 with PBE: (a) without vdW forces and (b) gas phase (left: bond length and right: orientation angle of adenine attached to the Au13 cluster).

Table 2 The values of molecular properties (HOMO-LUMO states, gap energy, softness, hardness and dipole moment) of adenine, Au13 and adenine/Au13 complex in aqueous solution with DFT-D3/TZVP model of theory.

Molecule	E_{HOMO}	E_{LUMO}	Hardness (η)	Softness (S)	Dipole momentum (µ)	Gap Energy (E_g)
				Molecular properties		
Adenine	−5.475	−1.764	1.885	0.539	3.562	3.711
Au13	−4.925	−4.313	0.312	3.208	0.019	0.624
Adenine/Au13	−4.755	−3.938	0.197	5.084	16.819	0.393

−3.013 eV. Hence, the vdW forces play a key role in exploring the interaction nature of such molecular systems.

We next investigate molecular properties of systems, which provides beneficial information about chemical reactivity of adenine/Au13 complex. The calculated energy gap, softness and dipole moment of adenine, Au13 and most stable state of adenine/Au13 complex are given in Table 2. It was found that both adenine and golden cluster have a large gap leading to small softness value indicating low chemical reactivity of individual molecules. However, the calculated gap/softness value for the complex is smaller/higher than its individual

entities. This reveals higher chemical reactivity of adenine/Au13 complex in comparison with the adenine molecule. In addition, the obtained dipole moment of molecular systems shows a larger dipole for the adenine/Au13 system which causes the complex to be more soluble in water than adenine.

We finally determined the solvation energy of complex under consideration by re-optimization of more stable state of adenine/Au13 system. Similar optimization procedure has been carried out in gas phase and the solvation energy was determined to be about −0.749 eV (−17.278 kcal/mol) which is in consistence with the obtained dipole moment for considered complex. It should be noted that interaction energy (−1.784 eV) and bonding distance (2.153/2.571 Å) are similar to the aqueous media which indicates the small influence of aqueous solution to interaction properties of molecular systems. Optimized structure of adenine/Au13 complex in gas phase is represented in Fig. 3(c). As it can be observed from the figure, the adsorbed adenine was located in a different situation compared to one in aqueous media (see the calculated angle between two molecules).

Our *first-principles* findings reveal that Au13 cluster can be considered as suitable nanocarrier for efficient drug and gen delivery application. Moreover, the performed studies improved our knowledge against the formation of probable complexes between biomolecules and golden nanostructures. This fact can be further studied in the fields of drug and gen delivery and relevant subjects based on nanomaterials.

CONCLUSION

In summary, we have investigated the interaction of adenine nucleic base with Au13 golden cluster, using the DFT-D3 calculations with the GGA-PBE model of theory. We have found that the interaction of adenine through its N atoms (N atom at amine group and 5-member ring) with the gold atoms is strong. The interaction energy at the equilibrium distance has a value of −1.858 eV (−42.841 kcal/mol), implying a chemisorption process. The charge transfer analysis revealed a large amount of charge transferred between interacting molecules. Charge density of complex showed accommodation of charge in contact region of adenine with gold cluster indicating strong interaction of two species. Our DFT based results for the magnitude and type of interaction look promising for a detailed modeling of possible biological applications of Au13 cluster because the functionalization can be applied in large category of golden clusters.

CONFLICT OF INTEREST

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

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