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RESEARCH PAPER

A Density Functional Theory Study on the Effects of Silver Clusters on the α-Glucose Molecule

Nagham M. Shiltagh [1*], ***Walaa S. Sarhan*** [2]

[1] *Department of Physics, College of Science, University of Kerbala, Karbala 56001, Iraq*

[2] *Department of Physics, College of Applied Medical Sciences, University of Kerbala, Karbala 56001, Iraq*

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ABSTRACT

Glucose is a naturally occurring monosaccharide that possesses multiple hydroxyl groups capable of coordinating with metal ions. Due to its biocompatibility, non-toxicity, and ability to stabilize metal species, glucose has attracted considerable interest with regard to biomedical and industrial applications, particularly in the synthesis and stabilization of silver-based materials. In the current study, density functional theory (DFT) calculations were employed to investigate the electronic properties and stability of the Glucose/2Ag complex's structure. The results obtained confirmed the formation of stable Ag–O coordination bonds, with an Ag–O bond length of approximately 2.4 Å, indicating a relatively strong interaction between the oxygen donor atoms of glucose and the silver centers. The calculated global reactivity descriptors revealed an electronegativity of 4.5715 eV, chemical hardness of 1.823 eV, and softness of 0.5485 eV. Furthermore, the HOMO–LUMO energy gap of the complex was found to increase compared with free glucose, demonstrating enhanced electronic stability, increased chemical hardness, and reduced chemical reactivity. These findings suggest that coordination with silver l allows for the significant stabilization of the electronic structure through charge redistribution between glucose and the silver atoms. According to the HSAB principle, this stabilization supports the formation of a chemically stable complex with increased resistance to electronic perturbation. Overall, the theoretical results indicate that the Glucose/2Ag complex exhibits favorable stability and electronic characteristics, making it a promising candidate for potential biomedical applications such as antimicrobial materials, drug-delivery systems, and biosensors, as well as industrial applications such as catalytic processes and antimicrobial coatings.

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INTRODUCTION

Nanotechnology is amongst the industries that are currently showing the quickest rates of growth. In particular, metal nanoparticles exhibit potentially promising physical and chemical characteristics. They have shown an interesting degree of promise in the diagnosis and treatment of cancer, and have been utilized in a variety of

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* *Corresponding Author Email: nagam.altememi@uokerbala.edu.iq*

applications [1] including the administration of medications, amino acids, and antimicrobials [2, 3]. Recently, attention has turned to nanomaterials in general, and to silver nanoparticles in particular, due to their important physical properties in terms of molecular structure and cross-sectional area for interaction. Therefore, they have been incorporated into many biomedical industries [4]. Silver nanoparticles are characterized by their small size, which endows them with potentially useful chemical and physical properties [5], a characteristic that has been exploited in their use as antimicrobial agents and in nanoparticle preparations [6]. Silver nanoparticles can be synthesized using glucose as a reducing agent and strong blocking agent under alkaline conditions, with a molecular geometry can be improved through the use of density functional theory [7]. Nanosilver exhibits strong adsorption onto the surfaces of various chemical species, as measured by surface-enhanced Raman scattering, indicating a physical adsorption type [8]. Gonzalez *et al.* used Raman spectroscopy to study α-D-glucose and D-gluconate adsorption on surfaces as capping agents, both experimentally and conceptually (DFT) [7]. Previous studies have shown that there is compatibility between silver nanoparticles adsorbed on carbohydrate surfaces, with the related calculations suggesting an increase in the energy gap with the appearance of active groups in the infrared spectrum [9]. Zahra Jamshidi et al. investigated the interaction of α-D-glucose with metallic clusters of silver, gold, and copper atoms using density functional theory, demonstrating that gold has the highest electron affinity among them [10]. On the other hand, a study was conducted on the interaction of silver nanoparticles with monosaccharides to determine the most suitable fraction as a reducing agent in applying the green synthesis approach, with the engineering optimization carried out using the functional density of individual silver atoms (1,3,5) with the α-D glucose molecule [11]. In recent years, the use of hybrid nanomaterial interactions to enhance properties or induce synergistic effects has become increasingly widespread. The adsorption of silver nanoparticles with α-D-glucose is a hybrid reaction used to determine glucose levels in human tissue using an inert surface to improve physical properties such as fluorescence [12]. The time-dependent density functional theory of silver nanoparticles adsorbed onto the glucose surface contributed allowed the calculation of absorption spectra in the ultraviolet and visible regions and the determination of adsorption energy values at the COOH and COO carbon points, with the latter proving to be the most effective [13]. Furthermore, computational procedures offer accurate scales in chemical interactions, electronic structure, and combination processes, where a number of theoretical DFT calculations have been used or otherwise taken into consideration in practical uses [14]. Density functional theory plays an important role in exploring the electrolytic properties of silver nanotubes as good sensors for glucose and hydrogen peroxide due to their charge-accepting surface, an effect that can be studied through molecular orbital analysis [15]. Previous studies have demonstrated reasonable agreement between experimental and theoretical results regarding the stability of silver nanoparticle adsorption on carbohydrate surfaces, and have shown that this behavior is beneficial for osteoblasts [16]. Researchers have turned their attention to the use of hybrid nanomaterials by combining carbohydrates with carbon quantum atoms and silver nanoparticles. Both theoretical and experimental results have been found to be in good agreement with regard to the associated infrared spectra, particularly at high absorption energies, through bond analysis and charge distribution [17]. This research methodology investigated the pair values of silver nanoparticles (AgNPs) and their effects on the α-D-glucose molecule, taking into account the adsorption energies and stability energies between molecular levels as hybrid nanomaterials, through studying the surface charge distributions, and analyzing molecular levels and all associated physical parameters through computer modeling.

COMPUTATIONAL MODELS

This work utilizes the B3LYP functional, a variation of the DFT approach that uses the Becke three-parameter functional DFT exchange terms, related to the gradient-corrected correlation functional of Lee, Yang, and Parr (LYP). For C, O, and H atoms, the B3LYP and 6–311+G* functional set were utilized in the DFT theory. LANL2DZ set was used for the silver (Ag) atom [18, 19]. All geometrical variables were optimized without symmetrical restrictions to determine the geometry of all carbohydrates under investigation. Minimal energy structures were indicated by the absence of imaginary frequencies. Water was used as a solvent, taking into account the self-consistent reaction field. Gaussian 09 and GaussView 6.0 were used for all of the computations and operations [20]. The first stage in creating a stable molecule with reduced energy convergence thresholds was to optimize the molecules geometrically. As shown in Fig. 1, a geometric optimization was performed for the isolated α-D-glucose structure ($C_6H_{12}O_6$). The silver nanoparticles were optimized using two silver nanoparticles with one glucose molecule, and their adsorption onto the glucose surface was evaluated. This design showed good agreement with previous studies through calculations of adsorption energy, isostatic properties, analysis of empty and filled molecular levels, and certain physical parameters related to molecular structural stability.

RESULTS AND DISCUSSION

The geometric optimization of a glucose molecule with paired silver nanoparticles was performed, the result of which is shown in Fig. 2. This is the most stable molecular form, achieved by meeting the criteria for geometric optimization on the one hand, and by avoiding the appearance of imaginary frequencies on the other.

This fact allowed us to obtain the optimal

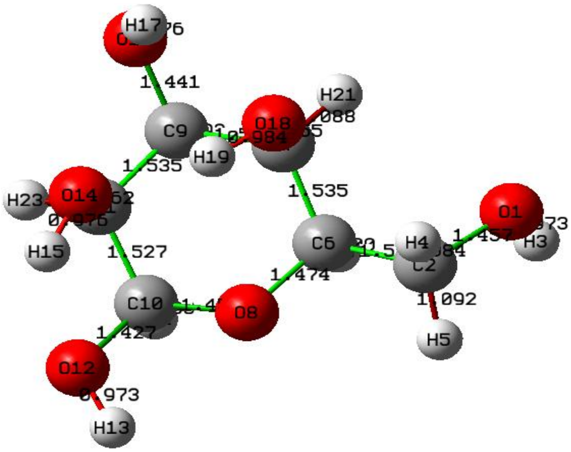

Fig. 1. The final geometric optimization of the α-D-glucose molecule – where red indicates oxygen atoms and white and gray indicate hydrogen and carbon atoms, respectively – was performed using the 6–311+G* basis

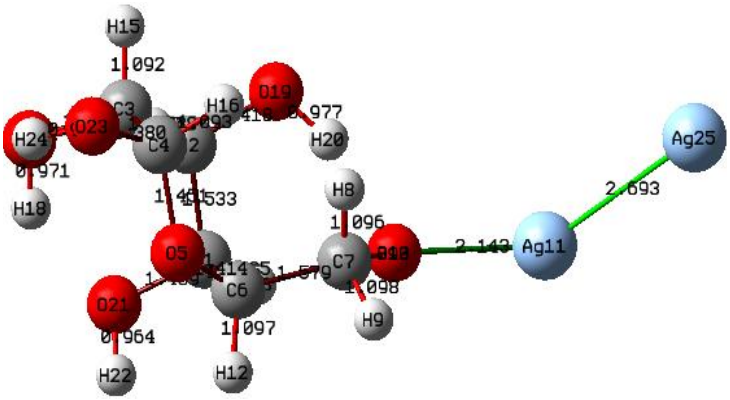

Fig. 2. The final optimized geometric structure of the α-D-glucose molecule including two sliver nanoparticles, where red indicates oxygen atoms and white, gray, and blue indicate hydrogen, carbon, and sliver atoms, respectively. Optimization was performed using the 6–311+G* and LAN2DZ for AgNPs.

stabilization energy of the molecular species along with the adsorption energy, resulting in negative values, as reported in Table 1.

In Fig. 2, it can be seen that the oxygen atoms effectively control the charge distribution of the molecules that make up the carbohydrate. Because they are able to provide the silver atoms electron density, these sites are thought to be the most active. In this way, one electron might be moved to the silver atom in order to go from an Ag$^+$ cation to Ag^0, filling the 5s^2 and 4d^6 [21, 22]. The distance between the silver cluster atoms and the carbohydrate molecule is crucial as this process requires both atoms to be in contact. Distances play a significant role in complex formation and reveal the nature of relationships. A typical oxygen-silver bond (silver oxide) distance is around 2.31 Å [23].

The bond between the oxygen O10 atom and the silver nanoparticle Ag11 is 2.143 Å, as shown in Fig. 2, which is consistent with previous studies.

All distances between silver nanoparticles and the glucose molecule were determined from functional theory with hybrid functions, and are reported in Table 2. The results show that the best proximity is between silver and oxygen atoms in the complex [24].

After incorporating the most important properties of the engineering improve- ments and comparing them with previous studies, the optimal molecular stability of the α-D-glucose compound was achieved after adding the double atoms of silver nanoparticles.

Frontier molecular orbital (FMO) theory states that the interacting species' HOMO and LUMO levels determine the chemical reactivity [26].

EHOMO is a quantum chemical parameter related to the molecule's electrodonatability. A high EHOMO is likely indicative of a molecule's propensity to donate electrons to the an acceptor molecule with low-lying empty molecular orbitals [27]. The molecule's capacity to accept electrons can be determined by the energy of the lowest unoccupied molecular orbital, or ELUMO [28] The inhibitor's binding capacity to the nanoparticle's surface improves with increasing EHOMO and reducing ELUMO energies. The lower the value of ELUMO, the more easily the molecule is able to act as an electron acceptor [29]. The values of such calculated for glucose were compared to determine the type of reaction by calculating the energy gap between the donor and acceptor

Table 1. Comparison of electronic energy and adsorption energy before and after adding silver nanoparticles to the alpha- D glucose molecule.

Structure	Stability energy (Hartree)	Adsorption energy (Hartree)
Glucose	-687.143809	----
Glucose/2 Ag	- 978.269115	-1956.53823

Table 2. Calculated bond lengths in Angstroms and bond angles in degrees for D-glucose /2Ag NPS using 6–311+G* and LAN2DZ basis functions.

Bond	Bond Length Å [25]	Angle θ	Value [9]
C(2)-C(1)	1.535	C(2)-C(1)-H(13)	28.29
C(3)-O(17)	1.427	C(3)-O(17)-H(18	105.84
O(19)-H(20)	0.977	C(2)-O(19)-H(20)	109.54
C(3)-H(15)	1.092	C(4)-C(3)-H(15)	107.66
Ag(11)-O(10)	2.143	Ag(11)-O(10)-C(7)	123.48
Ag(11)-Ag(25)	2.593	O(10)-Ag(11)-Ag(25)	142.29

Table 3. The energy gap for glucose before and after the addition of silver nanoparticles, as determined via density functional theory.

Structure	ELUMO (eV)	EHOMO (eV)	Eg = ELUMO – EHOMO (eV)
Glucose	-7.130	-10.398	3.267
Glucose/2Ag	-2.749	-6.394	3.645

levels, as reported in Table 3.

Table 3 shows an increase in the energy gap when silver nanoparticles interact with a glucose molecule. The reason for this is the interconnection of two silver atoms with the glucose molecule increase the HOMO–LUMO energy gap from 3.267 eV to 3.645 eV. This increase indicates enhanced electronic stability and chemical hardness of the associated complex. The interaction between Ag atoms and the oxygen-containing functional groups of glucose redistributes the electron density and modifies the frontier molecular orbitals, resulting in a less reactive and more stable electronic structure.

In Fig. 3, the HOMO of the glucose/2Ag complex is mainly localized around the silver atom with minor contributions from the glucose framework. This localization indicates charge redistribution upon adsorption and suggests that silver atoms significantly contribute to the frontier molecular orbitals. The limited overlap between the Ag and glucose orbitals leads to enhanced electronic stabilization, which is consistent with the observed increase in the HOMO–LUMO energy gap [30]. Fig. 3 shows the HOMO and LUMO orbitals of two species. (A) represents a-D-glucose before the addition of silver nanoparticles, and (B) shows a-D-glucose after the addition of the silver nanoparticles via the hybrid function.

For these species, calculations were performed to determine the energies of the HOMO and LUMO orbitals (EHOMO and ELUMO), the energy gap (ΔE), the hardness (η), the softness (σ), the proportion of transferred electrons (ΔN), and the electrophilicity index (ω). Molecular orbital theory states that the inhibitor molecules' EHOMO and ELUMO are related to the ionization potential, I, and electron affinity, A, respectively, according to the following formulae:

I = -EHOMO, A= -ELUMO

The electrostatic potential map shown in Fig. 4 reveals a significant redistribution of electron density after the incorporation of silver atoms into the glucose structure. The negative electrostatic potential (ESP) is mainly localized around oxygen atoms, indicating their role as electron-rich centers. The distortion of the ESP contours around the Ag atoms suggests charge transfer and electronic interaction between silver and oxygen atoms. This redistribution stabilizes the electronic structure and contributes to the observed increase in the HOMO–LUMO energy gap, indicating enhanced molecular stability [31].

Among the most important physical parameters that depend primarily on the energy of the HOMO and LUMO orbitals are electronegativity, X, absolute hardness of the inhibitor, η, and the softness, σ, as shown below [32].

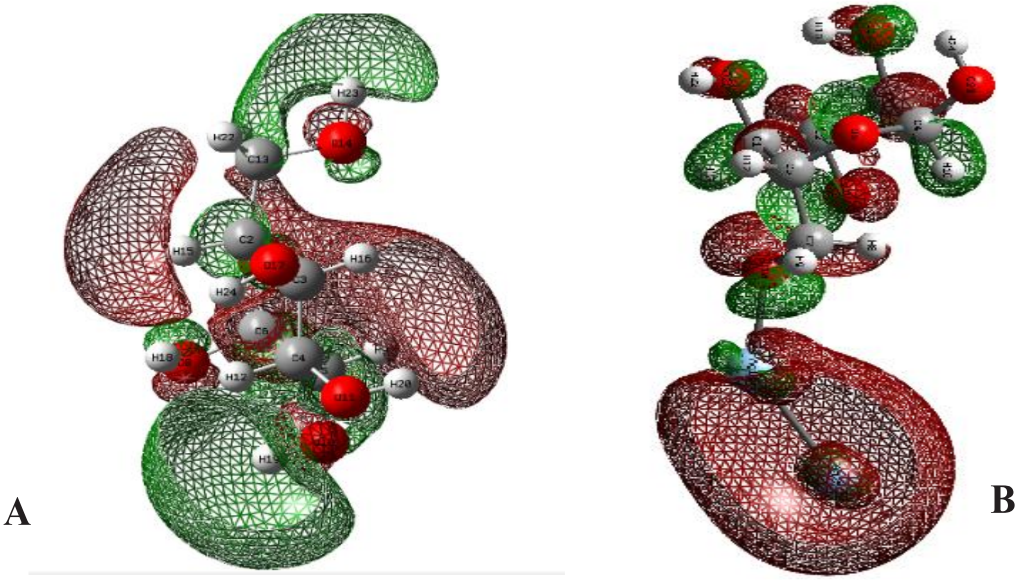

Fig. 3. The HOMO and LUMO levels of (A) represents a-D- glucose before the addition of the silver nanoparticles, and (B) a-D- glucose after the addition of the silver nanoparticles.

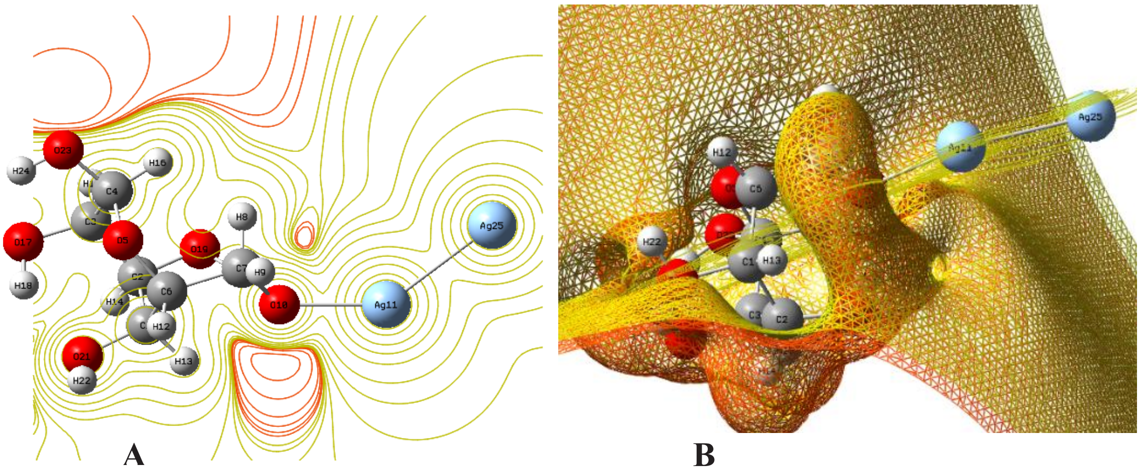

Fig. 4. (A) Molecular electrostatic potential (MEP) contour surface for (A) a-D- glucose/2Ag and (B) the MEP isosurface diagram of the MEP, in 3D, for D- glucose/2Ag.

Table 4. Chemical parameters of the glucose molecule with silver nanoparticles, as determined via density functional theory.

Structure	Chemical parameter	value
Glucose/2Ag	I (eV)	6.394
	A (eV)	2.749
	X(eV)	4.5715
	η (eV)	1.823
	σ(eV)	0.5485

$$X = \frac{I+A}{2}., \eta = \frac{I-A}{2}, \sigma = \frac{1}{\eta} \quad (1)$$

Table 4 examines the effects of the glucose molecule bonding with the silver nanoparticles as inhibitors more precisely by measuring electronegativity, chemical hardness, and softness. The Hard-Soft Acid-Base (HSAB) and frontier-controlled interaction concepts can be used to describe the bonding inclinations of the inhibitors with regard to the metal atom [33]. Hard acids tend to coordinate with hard bases, whereas soft acids tend to coordinate with soft bases, according to the broad ideas proposed by the HSAB principle. Metal atoms are classified as soft acids. Soft molecules have a small HOMO-LUMO gap, while hard molecules have a large one [34].

The increase in the HOMO–LUMO energy gap subsequent to silver coordination is indicative of the enhanced electronic stability of the glucose–silver complex. The larger energy gap reflects increased chemical hardness and reduced charge-transfer capability, suggesting that the Ag–O coordination bond stabilizes the electronic structure of the complex [35].

CONCLUSION

The calculated global reactivity descriptors reveal that the coordination of glucose with silver atoms significantly modifies its electronic properties. The increase in the HOMO–LUMO energy gap and chemical hardness accompanied by a decrease in softness indicates enhanced electronic stability and reduced chemical reactivity of the Glucose/2Ag complex compared with free glucose. According to the HSAB principle, the formation of Ag–O coordination bonds leads to stabilization of the electronic structure through charge redistribution between the oxygen donor atoms and silver centers. Therefore, the glucose–silver complex exhibits greater resistance to electronic perturbation and higher kinetic stability than the isolated glucose molecule.

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CONFLICT OF INTEREST

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

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