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RESEARCH ARTICLE - PHYSICS

Simulation of Structural, Electronic and Pharmacodynamics Properties of Developed Zeolite Docking with Hemoglobin

1*Mohamed A. Abdulrahman, 2Bahjat B. Kadhim, 3Mohamed A. Dawooda
1* Department of Physics, College of Science, Mustansiriyah University, IRAQ
* Corresponding author Email: **sci.phy.bbk@uomustansiriyah.edu.iq**

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Abstract

The study involved simulating the preparation of zeolite with its natural square structure in its simplest form, as well as the structure of a modified zeolite. The modification was achieved by adding one atom of copper or iron to the square zeolite. Additionally, the study included the preparation of cubic zeolite. Simulation of the structural and electronic properties of zeolite and developed zeolite structures was studied, using density functional theory at the B3LYP level and the 6 – 311G(d,p) basis set. The above properties of non-oxidized and oxidized hemoglobin were also simulated, for the purpose of making a comparison between it and the coalescence of developed zeolite with non-oxidized hemoglobin, to know the effect of the developed zeolite structures on hemoglobin as a pharmacodynamics property. The Gibbs free energy was calculated for the docking of oxygen with non-oxidized heme, which was (-51.624 eV) as well as for the zeolite structures developed after docking with non-oxidized heme, which was (94814.14175 eV) for Fe - zeolite with DHB and (4107.871817 eV) for Cu - zeolite with DHB. Through the thermodynamic results, it was shown that the docking process of the developed zeolite structures with non-oxidized hemoglobin is non-lethal and harmless and is similar to the docking process of oxygen with heme. It can be concluded from this, that the developed zeolite structures can be used in medical applications, such as participating in treatment, delivering medications, or carrying medications inside the human body.

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Keywords*:* Zeolite, density functional theory, simulation, thermodynamic, hemoglobin, Gibbs energy.

1. Introduction

Nano materials are a new science that enters into many fields and diverse applications. As is known, nanomaterial has unique properties that differ from the properties of the same material in conventional size (bulk). The size of nanomaterials starts from the molecular limit up to 100 nanometers, and one of the most important unique properties that nanomaterials have is the ratio of surface area to volume, which is very large, which increases the effectiveness of their interaction with the surroundings or other materials with which they can combine[1][2]. The use of nanomaterials inside the human body is considered one of the new challenges that deserves study in terms of the safety of its health use and the reliability of its activity and effectiveness in medical applications, such as treatment, drug delivery and transportation to different areas in the human body[3]. In our current study, crystalline zeolite was chosen to be the material under physical simulation tests represented in calculating the optimal structural properties[4], effective electronic properties, and thermodynamic properties to determine the effect of zeolite on the human body. Zeolite possesses several unique characteristics that make it valuable in various industrial and scientific applications like; high surface area, ion exchange capability, molecular sieving, thermal stability, acidic properties, hydrophilicity / hydrophobicity and structural versatility. These characteristics enable zeolites to be widely used in industries such as catalysis, adsorption, ion exchange, and environmental protection. Generally, zeolites have a general formula $[(SiO2)(AlO2)x]M\ x/n\ n+ \cdot w\ H2O$. M is a cation with positive charge equal to n. It is usually a group I or II metal ion. The silicon and aluminum oxide part of the substance provide the framework of interconnected tetrahedral structures[5]. Zeolites are microporous crystalline aluminosilicates with high surface area and uniform pore size[6]. Natural and synthetic zeolites have been used to adsorb organic and inorganic compounds in human body due to their physicochemical properties and the low cost of the process. While zeolites are microporous crystalline aluminosilicates with a large surface area and uniform pore volume, it is important to clarify that their use directly within the human body is not common due to safety concerns and pharmaceutical considerations. However, they have been studied for various medical and pharmaceutical applications, including drug delivery systems and in vitro models for studying drug interactions with biological tissues[7] . There are some key points to consider regarding the potential use of zeolite in medical applications, including its adsorption properties, as zeolite is known for its ability to absorb molecules due to its porous structure. This property has been explored for applications such as wound healing, as zeolite can absorb excess fluids and toxins from wounds, creating an environment conducive to healing. Zeolites are also used in drug delivery systems, where zeolites have been studied as carriers for controlled drug delivery. Drugs can be encapsulated within the zeolite structure and released in a controlled manner, improving drug efficacy and reducing side effects. Synthetic zeolites have been used as components of in vitro models to mimic biological environments to study drug and toxicological interactions and metabolic processes. These models help researchers understand how drugs behave inside the body and evaluate their potential effects on human health[8]. However, there are medical safety concerns. While zeolite is generally considered safe for many industrial and environmental applications, its use in medical contexts requires rigorous safety evaluation. Concerns include potential cytotoxicity, tissue damage, and the release of ions or other substances that could have adverse effects on human health [9]. Regulatory medical considerations any medical application of zeolite must comply with regulatory standards for safety and effectiveness. This includes extensive testing in preclinical studies, including in vitro and animal studies, before potential clinical trials in humans[10]. In summary, while the zeolite structure has properties that make it attractive for medical applications such as drug delivery and in vitro modeling, its direct use within the human body is not common due to safety and regulatory considerations. However, ongoing research continues to explore its potential in various medical and pharmaceutical contexts. For these reasons, it is necessary to resort to simulation for the purpose of evaluating and avoiding any harm that zeolite may cause to human health.

2. Theoretical Considerations

The theoretical basis for this study, which deals with simulating structural, electronic and pharmacokinetic properties, is based on a set of scientific foundations and principles. The current study requires knowledge of quantum mechanics, through the Schrödinger equation, for the purpose of calculating the total energy of the system under study, through which a wide range of electronic properties can be calculated. This is done by employing solid state physics for the structure of the materials under study, in terms of the location of atoms, bond lengths, triple angles and quadruple angles, for the purpose of obtaining the optimal structure of the materials under study.The Schrödinger equation, through which the total energy of the system is calculated, is described by the equation[11]:

$$E = E_T + E_v + E_J + E_{XC} \qquad (1)$$

E_T: Electronic kinetic energy, E_v: Electronuclear interaction energy, E_J: Electron-electron repulsion energy, E_{XC}: exchange correlation term.

One of the most important electronic properties, that must be calculated after obtaining the total energy at its lowest value, is the energy gap, which is calculated from the difference between the lowest un occupied molecular orbit (LUMO) in the conduction band and the highest occupied molecular orbit (HOMO) in the valence band[12]:

$$E_g = (\varepsilon_{LUMO} - \varepsilon_{HOMO}) \qquad (2)$$

The amount of energy required to release an electron from the system at the ground state reference geometry called ionization potential (*IP*)[13]:

$$IP = -\varepsilon_{HOMO} \qquad (3)$$

electron affinity (*EA*) is known as the amount of energy released when an electron is related to the system[14]:

$$EA = -\varepsilon_{LUMO} \qquad (4)$$

The Fermi level was had as the energy of the highest occupied molecular orbital (HOMO) in the valence band at (0 K). Nevertheless, some studies have utilized the mid gap level, calculated from the HOMO and LUMO, as the Fermi energy[15] :

$$E_F = -(IP + EA)/2 \qquad (5)$$

$$E_F = E_{HOMO} + (E_{LUMO} - E_{HOMO})/2 \qquad (6)$$

Work function symbolized to the minimum energy desired to take out an electron from the Fermi level and it's computed as the energy variance between vacuum level (LUMO) and the Fermi level (chemical potential)[16].

$$\Phi_m = LUMO - E_F \qquad (7)$$

Electronegativity means compute of the inclination of system to pull a bonding two of electrons. Electronegativity is describing the escape inclination of the electrons from the equilibrium system[17].

$$\chi = (E_{HOMO} + E_{LUMO})/2 \qquad (8)$$

Also electronegativity can be written with the formula:

$$\chi = (IP + EA)/2 \qquad (9)$$

Electrophilicity index measures the stabilization in energy when the system acquires an additional electronic charge from the environment[18].

$$\omega = [\chi^2 / (2\eta)] \qquad (10)$$

The chemical hardness is a measure of the impedance to transports charge. Chemical hardness can it known theoretically, the second derivative of electronic energy with relative to electrons number, when the potential external is constant Chemical hardness can be computation immediately from the equation[19], [20]:

$$\eta = (IP - EA)/2 \qquad (11)$$

The global chemical softness, Sr, can be defined as a property of molecules that measurement the range of chemical reactivity. It is the inverted of the chemical hardness[21]:

$$S_r = (1 / 2\eta) \qquad (12)$$

In thermodynamics, the Gibbs free energy (or Gibbs energy as the recommended name; symbol *G*) is a thermodynamic potential that can be used to calculate the maximum amount of work, other than pressure-volume work, that may be performed by a thermodynamically closed system at constant temperature and pressure. It also provides a necessary condition for processes such as chemical reactions that may occur under these conditions. The Gibbs free energy is expressed as[22]:

$$\Delta G = \Delta H - T\Delta S \qquad (13)$$

Where H is the enthalpy of the system, S is the entropy of the system, T is the temperature of the system.

It has also been considered the pharmacodynamics (drugs effect on human body) proprieties via the docking as a coupled physical quantity and from the perspective of thermal stability, where it is possible to have a thorough grasp of how drugs and nanomaterial's are dependent on binding energy E_B and interaction energy E_{int}, where E_B is the fundamental electron binding energy that has been determined for both the pre-and post-docking processes[23], [24]:

$$E_B = [(N\,E_X + M\,E_Y) - E_{XY}]/(N + M) \tag{14}$$

Where, E_{XY} stands for the total energy considered for XY docking atoms, E_X, E_Y energy of X and Y atoms respectively. N and M are the number of X and Y atoms present in the system structure respectively.

The residual forces on the surface diminish as the adsorption and reaction energies are computed, and as a result, so does the surface energy, which manifests as heat. This is also one of the causes of the exothermic nature of interaction energy as given by the following equation[25], [26]:

$$E_{int} = E_{Docking} - \left(E_{DHB} + E_{Drug}\right) \tag{15}$$

Where E_B, E_{int}, $E_{Docking}$, E_{DHB} and E_{Drug}, are the binding energy, the total energies of the interaction, DHB, and drug molecule respectively. Also stands for the total energy required to docking DHB with the drug.

3. Materials and Methodology

There are now multiple specializations that overlap with each other through the preparation of new materials in thin films, superconductivity, semiconductors, complexes, single and multiple crystals, and materials science in general [27]. For the developed nano-zeolite, a single atom of copper or iron with multiple structures: square structure and cubic structure were used. The structures of the nano zeolite for different types and for nano zeolite under study are built through simulation using the Gauss View 6 program by employing density functional theory at the level (B3LYP) with basis set (6 – 311G(d,p). B3LYP stands for "Becke, 3-parameter, Lee-Yang-Parr" and is a widely used hybrid functional in density functional theory (DFT) calculations, particularly in computational chemistry [28]. It is implemented in various quantum chemistry software programs, including Gaussian. Here's a breakdown of B3LYP:B: Becke exchange functional.3: Refers to three empirical parameters introduced by Becke. LYP: Lee, Yang, and Parr correlation functional. In essence, B3LYP combines the Hartree-Fock exact exchange functional with the Becke exchange functional and the Lee-Yang-Parr correlation functional, along with some empirical parameters to improve the accuracy of the calculations. This combination often provides a good balance between computational cost and accuracy, making it a popular choice for a wide range of molecular systems and properties. In the Gaussian program, the basis set 6-311G(d,p) is a specific type of split-valence basis set with polarization functions. Here's a detailed breakdown of its components:6-311: This indicates the composition of the basis functions:6: Six Gaussian functions are combined to form a single basis function for the core (inner-shell) electrons.3: Three Gaussian functions form one basis function for the valence electrons.1: One Gaussian function for the valence electrons.1: Another single Gaussian function for the valence electrons. The notation "6-311" signifies that the valence shell is described by a triple-zeta basis set (three sets of functions: 3, 1, and 1).G: This denotes that the basis functions are Gaussian-type orbitals.(d,p): These are polarization functions added to the basis set to allow for more flexibility in the molecular orbitals. d: Polarization functions for heavy atoms (usually transition metals and heavier elements), which are d-type Gaussian functions. These help to describe the shape of orbitals more accurately. p: Polarization functions for hydrogen atoms, which are p-type Gaussian functions. These allow for a better description of bonding and molecular geometry. So, 6-311G(d,p) is a triple-zeta valence basis set with polarization functions added to improve the accuracy of calculations, particularly in describing electron distribution and molecular geometries. This makes it a commonly used basis set in computational chemistry for a variety of molecular systems. The developed nano zeolite structure were tested on hemoglobin with chemical formula ($C_{42}H_{45}FeN_7O_5$) to determine the effect of the developed nano zeolite structures on hemoglobin[28], [29]. The simulation was carried out using Gaussian 16 software to obtain the optimal structural, electronic and thermodynamic properties[29], [30],

[31].

4. Results and Discussion

All the computations of simulation have performed using density functional theory (DFT) implemented in the Gaussian 16 version running and visualized by Gauss View 6 program. DFT is very successful approach for the description of ground state properties of metals, semiconductors, and insulators. In this paper B3LYP level coupling with (6-311g (d,p)) basis set were used, in all calculations to find electronic and thermodynamic as well as pharmacodynamics proprieties. The geometry optimization for normal zeolite (square and cubic) and the two developed structures of zeolite by add (Fe atom) or (Cu atom)) were found. The optimized structure is obtained when the structure has the minimum total energy. Figure 1 shows the optimized structure of normal nano zeolite, as well as Figure 2, which is shown the optimization results for DHB and OHB respectively.

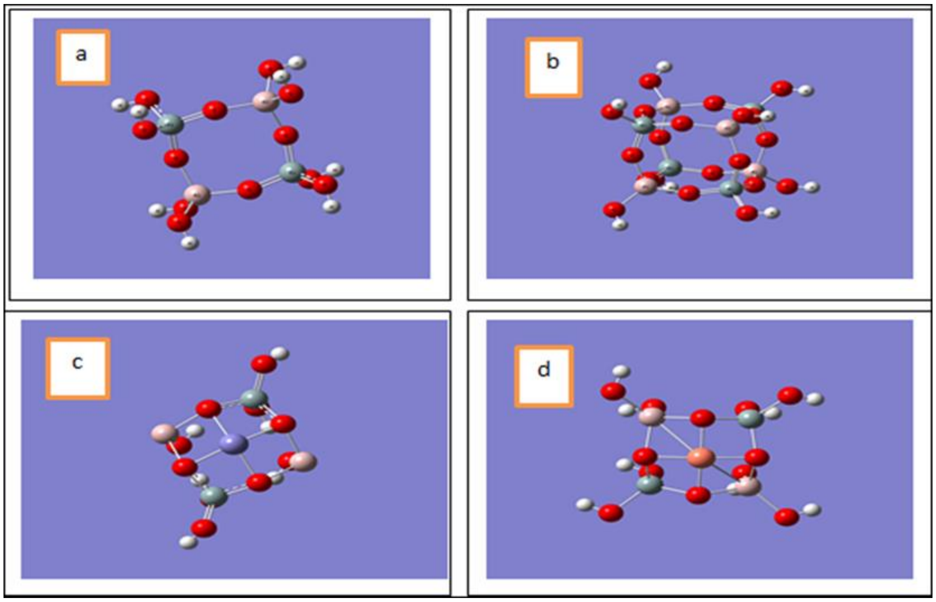

Fig. 1 Optimized structure for zeolite: (a) Square, (b) Cube, (c) zeolite-Fe, (d) zeolite-Cu.

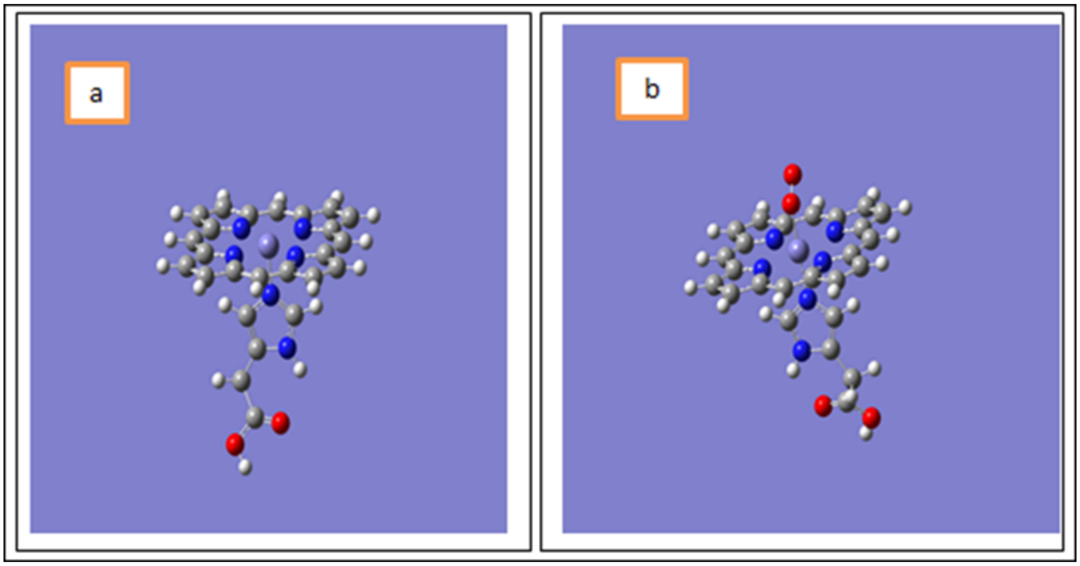

Fig. 2 Optimized structure For, (a) Deoxyhemoglobin, (b) Oxyhemoglobin.

Obtaining the optimal structures in Figures (1 and 2) gives an indication that the use of DFT theory according to the B3LYP level and the basis set 6 – 311G(d,p) was compatible to obtain these structures at the lowest total energy, whose results were according to what is listed in Table 1, where in the case of not obtaining at the lowest total energy of the system under study, this will lead to not obtaining the optimal structures, which are very important for obtaining electronic, thermodynamic and pharmacodynamics properties. This is consistent with research published in[27], [32], [33], [34], [35]. Figures 3 and 4, show the optimal structures for the docking process of deoxygenated hemoglobin with square nano-zeolite, cubic nano-zeolite, zeolite-copper developer, and zeolite-iron developer. Obtaining these optimal structures after the docking process with deoxygenated hemoglobin demonstrates the success of using density functional theory at the level (B3LYP) with the basis set (6-311G(d,p)), which is agreed with many references[36], [37], [38], [39], [40]. By simulating the optimized structures, the electronic and thermodynamic properties were obtained for square zeolite, cubic zeolite, zeolite-iron developer and zeolite-copper developer as shown in Tables 1 and 2, respectively.

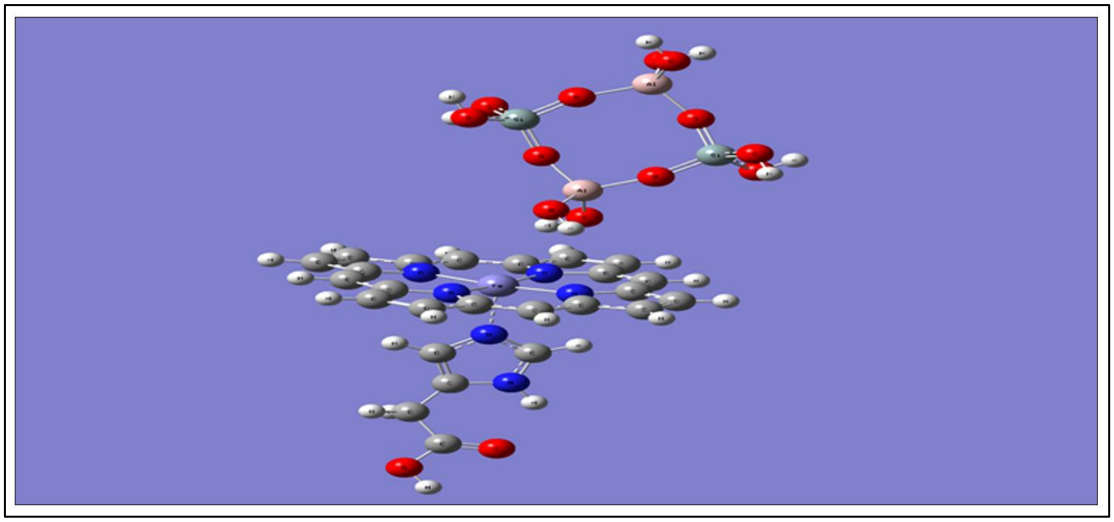

Fig. 3 Optimized structure for square – zeolite docking with Deoxyhemoglobin.

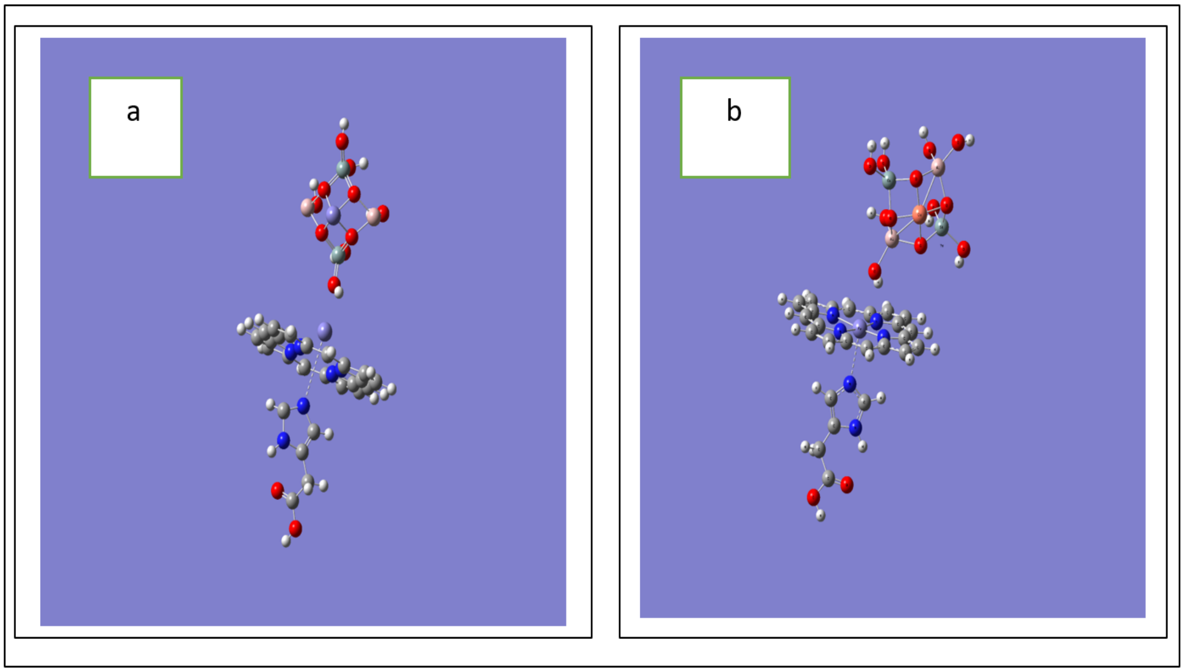

Fig. 4 Optimized structure for developed zeolite docking with Deoxyhemoglobin: (a) Fe-zeolite (b) Cu-zeolite.

Table 1 The electronic proprieties in (eV).

Properties	zeolite Cube	zeolite Square	zeolite - Fe	zeolite - Cu
HOMO	-17.932049	-8.07704113	-4.4680462	-5.14804909
LUMO	-15.96959168	-7.38887494	-3.60382484	-1.69932695
IP	17.932049	8.07704113	4.4680462	5.14804909
EA	15.96959168	7.38887494	3.60382484	1.69932695
$E_{.g.}$	1.96245732	0.68816619	0.86422136	3.44872214
E_f	-16.95082034	-7.732958035	-4.03593552	-3.42368802
Φ_m	0.98122866	0.344083095	0.43211068	1.72436107
χ	-16.95082034	-7.732958035	-4.03593552	-3.42368802
Hard	0.98122866	0.344083095	0.43211068	1.72436107
S	377.3017194	1075.958877	856.7695214	214.6993846
ω	0.190384973	0.013894267	0.004752963	0.013648898
SCF	-98983.39878	-53664.71898	-83916.69778	-94184.88286

Table 2 Thermodynamic proprieties.

Structure	Gibbs, eV	Enthalpy, eV
zeolite Cube	-99195.52112	-99192.56786
zeolite squarer	-53785.31156	-53783.23958
zeolite - Fe	-84097.19448	-84095.472
zeolite - Cu	-94387.33853	-94385.55698

Table 3 shows the effect of square zeolite, cubic zeolite, zeolite - iron developer, and zeolite - copper developer on non-oxidized hemoglobin, through comparison with oxidized hemoglobin, through the thermodynamic properties represented by Gibbs free energy, enthalpy and entropy, in addition to binding, interaction, and total energies, which is dealing with simulated pharmacodynamics properties.

Table 3 Thermodynamic and pharmacodynamics proprieties.

Energies eV	**DHB**	**OHB (O_2 with DHB)**	**Zeolite with DHB**	**Fe - zeolite with DHB**	**Cu - zeolite with DHB**
G	-73593.730	-77735.800	-127318.896	-66839.988	-167814.517
H	-73591.270	-77733.304	-127315.380	-66837.241	-167811.244
ST	1540743.400	1565070.968	2205330.959	1723126.917	2051621.528
ΔG	-	-51.624	4087.821	94814.142	4107.872
ΔH	-	-52.190	4086.773	94812.674	4106.870
ΔST	-	-355181.909	-656486.452	-919969.799	-628436.813
SCF	-73602.350	-77744.678	-127330.729	-66851.117	-167825.702
E_{Bin}	-	-69588.098	-68705.563	-78582.454	-80111.228
Ei_{nt}	-	-52.384	4086.951	94813.682	4107.320

5. Conclusions

Through the results of the simulation of the optimal structural properties obtained, it can be concluded that the theory DFT according to the function B3LYP and in combination with the basis set (6 – 311G(d,p)) was suitable and successful for the purpose of completing the simulations to calculate the electronic and thermodynamic properties. Through the results of simulating thermodynamic properties, it can be concluded the possibility of developing zeolite crystals through the process of docking with atoms of metallic elements such as a copper atom or an iron atom. It can be concluded from simulating the process of docking the developed, square and cubic zeolites with non-oxidized hemoglobin, and after comparing with oxidized hemoglobin, that there are no negative or harmful effects on human health, and thus it can be used in many medical applications such as delivery, loading, and treatment.

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