Original Research Article

A Comparative Study of Corrosion Inhibition Properties of Amoxicillin on Al(110), Fe(111) and Cu(110) Surfaces using Computational Method

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ABSTRACT

One of the most important areas of research to address the deterioration of metal surfaces in various settings is corrosion inhibition. The effectiveness of amoxicillin as a corrosion inhibitor on Fe(111), Al(110), and Cu(110) surfaces was investigated in this work using simulation techniques and density functional theory (DFT). Using extensive computer simulations, we identified the key chemical reactions and energy processes that control the inhibitory pathway. Our results highlight the critical roles that the electrophilic site O22 and the Fukui nucleophilic site C2, S7 play in mediating the inhibitory pathway. Furthermore, the binding energies of -50.65, -38.97, and -43.24 for the Fe(111), Al(110), and Cu(110) surfaces, respectively, demonstrate the high affinity of amoxicillin for these substrates. In addition, the energies of -5.608 HOMO and -1.873 LUMO provide information on the electrical properties that support the inhibition process. When taken as a whole, these findings provide light on the molecular mechanisms by which amoxicillin inhibits corrosion, providing important information for the development of new materials and corrosion-resistant techniques. Interestingly, the Fe-amoxicillin interaction shows more potential than the Al-Cu interaction. In conclusion, the molecule amoxicillin had a mild inhibition in the order Fe(111)>Al(110)>Cu(110) also inhibiting a physisorption on both surfaces of Fe(111), Al(110), and Cu(110).

Introduction

Metal corrosion is still a major problem in many different sectors, resulting in large financial losses and environmental issues. The hunt for efficient corrosion inhibitors has been more intense in recent years, with an emphasis on sustainable and eco-friendly materials [1-3]. Because of their multiple chemical functions, organic molecules have become attractive options for corrosion inhibition, assisting in lessening the impact of corrosion on metals.

The commonly used antibiotic amoxicillin has demonstrated remarkable promise because of its molecular structure, which includes heteroatoms—functional groups that may build protective coatings on metal surfaces (Scheme 1). Corrosion is the term used to describe the deterioration of materials due to chemical processes, which usually include oxidation in the presence of air and water [4-5]. In addition, it happens when materials come into contact with acidic or basic corrosive chemicals [1]. The impacted material's physical characteristics change as corrosion worsens. Corrosion is sometimes referred to as erosion and may occur in materials other than metals, including plastic and wood [6]. Certain materials have a strong corrosion resistance, such as stainless steel [7]. On the other hand, aluminum oxide quickly coats the metal when it comes into contact with air. Although this oxide layer is usually just a few nanometers thick, it offers some corrosion protection by acting as a barrier to more oxidation. Compared to the passive oxide layers that develop on corrosion-resistant metals like stainless steel, it is not as durable. As a result, aluminum is prone to corrosion in some conditions, especially those with a lot of moisture or acidic environment [8-9]. Therefore, metals that are prone to corrosion can be shielded by protective techniques like plating and coating. Moreover, compressed oxide layer glazes produced by high-temperature corrosion may, under some circumstances, lessen metal wear [10]. DFT is a commonly utilized approach in materials research because it provides an accurate research study by explaining the corrosion study of Al, Fe, and Cu. The study of materials science has undergone a revolutionary transformation because of DFT, which offers a strong foundation for comprehending the atomic-level electrical structure and characteristics of materials. DFT provides an effective method for examining the adsorption behavior of molecules on metal surfaces in the context of corrosion prevention, allowing predictions of adsorption energies, charge transfer, and surface reactivity [11,12]. The dynamic behavior of molecules on metal surfaces under realistic environmental circumstances, such as variations in temperature and pressure, is captured by

molecular dynamics (MD) simulations, which are a useful tool to supplement DFT computations. We hypothesize that amoxicillin molecules will adsorb on the metal surfaces via specific functional groups, forming protective barriers against corrosive materials. The adsorption behavior and effectiveness of amoxicillin are expected to vary among the three metal surfaces due to differences in surface properties of the metals. Understanding the corrosion inhibition properties of amoxicillin on metal surfaces holds significant implications for the development of novel corrosion protection strategies. By elucidating the underlying mechanisms governing the interaction between Amoxicillin molecules and metal surfaces. This study is aim to contribute to the design of environmentally friendly and sustainable corrosion inhibitors with enhanced performance and stability. Also, it aims to clarify amoxicillin's potential as a corrosion inhibitor and offer insightful information on how it adsorbs on various metal surfaces. We hope to improve knowledge of interactions between organic molecules and metal surfaces by fusing theoretical calculations with molecular simulations. This will help create corrosion techniques that work in corrosion inhibition. In their independent investigations, Boyuan *et al.* and Ayaba *et al.* [1,13] found that the mild steel surface and the molecule had a moderately high inhibition efficiency. They also achieved a moderate corrosion inhibition of expired amoxicillin in HCl concentration. In addition, Eddy *et al.* and Abdulfatai *et al.* used the DFT approach to study the molecule and determine the locations of electrophilic and nucleophilic assaults [1,8-10]. The study's gap revealed that mild steel (Fe) has always been the focus of research, rather than the molecule being examined and theoretically or empirically compared with other surfaces like Cu and Al. In this study, using a computational approach, a comparative analysis of the corrosion inhibition properties of amoxicillin on Al(110), Fe(111), and Cu(110) surfaces will be conducted. The goal is to determine which surface amoxicillin tends to be effective on and, using Fukui functions, to illustrate the molecular mechanism.
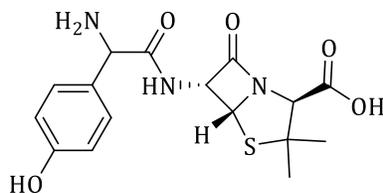
Scheme 1: Structure of amoxicillin

Theoretical Methods

Sketching of the studied molecules

The 2D Amoxicillin molecular structure was sketched using Chem Draw Ultra 7.0.3 from CambridgeSoft and was optimized using DMol³, a tool included in the BIOVIA Materials Studio 8.0 program from Accelrys, Inc. This is to ensure that the molecules had a stable geometry and obtained minimum amount of energy possible. Before establishing the stable geometry of the Amoxicillin, the molecule imported from ChemDraw Ultra 7.0.3 CambridgeSoft to BIOVIA Materials studio 8.0 (Accelrys, Inc.) was optimized through the local density function B3LYP utilizing DFT under restricted spin polarization DNP basis in gas phase [12,13].

Quantum chemical parameters calculations

The quantum chemical calculation was performed using a DMol³ module in the BIOVIA Material Studio 8.0 program (Accelrys, Inc.) with underlying fundamentals of DFT. The B3LYP function was used to calculate the parameters with the basis set to "double-numeric polarization" (DNP) in the gas phase model [13-16]. The ionization energy (IE), electron affinity (AE), and other functions that characterize the molecule's reaction behavior as well as other aspects of its global and local reactivity were calculated, as shown by Equations 1-11, in line with the expanded theorem of Koopman. The initial electron distribution in the molecule and the local reactivity computation of the Fukui function f(r) from ab-initio quantum chemistry are described by the following Equations [17-20]:

$$IE = -E_{HOMO} \tag{1}$$

$$AE = -E_{LUMO} \tag{2}$$

ΔE_g: Energy gap (eV) $\qquad \Delta E_g = E_{LUMO} - E_{HOMO} \tag{3}$

χ: absolute electronegativity (eV) $\qquad \chi = \dfrac{IE+AE}{2} = -\dfrac{(E_{HOMO}+E_{LUMO})}{2} \tag{4}$

η: global hardness (eV) $\qquad \eta = \dfrac{IE-AE}{2} = \dfrac{(E_{LUMO}-E_{HOMO})}{2} \tag{5}$

σ: global softness (eV)$^{-1}$ $\qquad \sigma = \dfrac{1}{\eta} = -\dfrac{2}{E_{HOMO}-E_{LUMO}} \tag{6}$

ω: global electrophilicity index (eV) $\qquad \omega = \dfrac{\mu^2}{2\eta} = \dfrac{\chi^2}{2\eta} \tag{7}$

μ: chemical potential (Debye) $\qquad \mu \approx -\dfrac{1}{2}(IE+AE) = \dfrac{1}{2}(E_{LUMO}+E_{HOMO}) \tag{8}$

ε: nucleophilicity(eV)$^{-1}$ $\qquad \varepsilon = \dfrac{1}{\omega} \tag{9}$

$\Delta E_{b\text{-}d}$: Energy of back donation $\qquad \Delta E_{b-d} = -\dfrac{\eta}{4} = \dfrac{1}{8}(E_{HOMO} - E_{LUMO}) \tag{10}$

ΔN: Fraction of electron(s) transfer $\qquad \Delta N = \dfrac{\chi Fe - \chi Inh.}{2(\eta Fe + \eta Inh)} \tag{11}$

The absolute hardness, represented by ηFe, ηAl, ηCu, and ηinh, is also the inhibitor molecule's, on the other hand, the χ of Fe, Al, Cu, and the inhibitor molecule's Eigen values are represented by χFe, χAl, Cu, and χinh. According to theory, the η of the surfaces of iron, aluminum, and copper is $\eta Fe = 0$ eV, $\eta Al = 5.6$ eV, and $\eta Cu = 4.5$ eV, respectively, and the χ of bulk iron is Fe = 7.0 eV, Al = 5.6 eV, and $\eta Cu = 4.5$ eV, assuming that the metallic bulk has a higher density than neutral metallic atoms [21-24]. The distinction between nucleophilic and electrophilic local Fukui functions is the definition of the Fukui second function (f2), another global descriptor that is also known as the dual descriptor $\Delta f(k)$. According to the Fukui behavior of the atoms, these functions also determine the electrophilicity $(1/\omega)$ or ε of molecules [25]. If $f2(r) > 0$, site k favors a nucleophilic attack; if $f2(r) < 0$, site k favors an electrophilic attack. Accordingly, $f2(r)$ serves as a selectivity index for attacks that are electrophilic or nucleophilic (Equations 12-15).

$$f(k)^+ = qk(N + 1) - qk(N) \text{ (for nucleophilic attack)} \tag{12}$$

$$f(k)^- = qk(N) - qk(N - 1) \text{ (for electrophilic attack)} \tag{13}$$

$$f(k)^0 = \frac{qk(N+1) - qk(N-1)}{2} \text{ (for radical attack)} \tag{14}$$

$$\Delta f(k) = f^+ - f^- = f^2 \text{ (Fukui function)} \tag{15}$$

Where, N is the number of electrons in the molecule, N+1 is an anion with an electron added to the LUMO of the neutral molecule, and N-1 is a cation with an electron removed from the HOMO of the neutral molecule, qk is the gross charge of atom k in the molecule, which is the electron density at a point r in space around the molecule. The ground state geometry served as the basis for all calculations. Using an atomic charge partitioning scheme, such as Mulliken population analysis in Equations, these functions were condensed to the nuclei of the atoms [26,27].

Molecular dynamic simulations

A high stability quench adsorption approach was used to replicate the studied Amoxicillin molecule on a surface composed of closely spaced Fe(111), Al(110), and Cu(110) atoms. The FORCITE tool package, integrated inside the BIOVIA Materials Studio 8.0 software (Accelrys, Inc.), was utilized in the simulation process. The condensed-phase optimized molecular potentials for atomistic simulation studies (COMPASS) force field tool and the Smart algorithm approach were used in a simulation box measuring 17Å × 12Å × 28Å to execute computations in order to model a representative area of the surface [28]. The Fe crystal was cleaved across by the (111) plane at a fractional depth of 3.0 Å. The bottom layers' form was constrained before the surfaces were optimized to avoid edge effects caused by the sizes of the molecules. A 5 × 4 supercell was then created by enlarging the surfaces. By maintaining the temperature at 350 K, a compromise was achieved between a system with excessive kinetic energy, in which the molecule desorbs from the surface, and a system with inadequate kinetic energy, in which the molecule is unable to travel across the surface [13,23]. With a simulation length of 5 ps and a time step of 1 fs, the temperature was set using the NVE (microcanonical) ensemble. It was envisaged that the process quenches every 250 steps for a total of 5000 cycles to ascertain the statistical values of the energies on the surfaces of the Fe(111) crystal. The lowest energy interactions of the molecules were found using FORCITE geometry optimized geometries of the molecules and the Fe(111) surfaces [3,4,10,14,23]. Equations 16-17 were used to determine the adsorption and binding energies between the pyrimidine derivatives and the Fe(111) surface.

$$E_A = E_T - (E_I + E_S) \qquad (16)$$

$$E_B = -E_A \qquad (17)$$

Where, E_A is the adsorption energy, E_T is the combined energy of the molecule and the iron surface, E_S is the energy of the iron surface, E_I is the energy of the inhibitor molecule without the iron surface and E_B is the binding energy [23,29].

Result

Geometry optimization involves finding the arrangement of atoms that minimizes the total energy of the system according to the laws of quantum mechanics. This process typically involves iteratively adjusting the positions of atoms until the forces on each atom become sufficiently small, indicating that the structure has reached a stable configuration [10,12,23]. The optimized geometry obtained from DFT calculations provides valuable insights into molecular structure, reactivity, and properties, enabling researchers to make predictions and interpretations that guide experimental investigations in fields ranging from chemistry to materials science [30]. Based on the result, the electron density of the molecule amoxicillin cover the entire molecule which indicated that the reaction of the molecule can occur at all points within the molecule [15-19]. The Homo orbital occurs at amino and hydroxyl-phenyl group and the LUMO occurs at dimethyl-6-methylamino-7-oxo-4-thia-1-aza-bicyclo acid

part of the molecule (Figure 1). This is equivalent to a study by Belghiti, *et al.* on some of the organic molecules [30].

Quantum energies

In quantum chemistry, the idea of the highest occupied molecular orbital (HOMO) energy is crucial, especially when considering DFT. It stands for the energy of the maximum energy orbital that an electron in a solid or molecule may occupy [31]. For example, in organic chemistry, it is frequently associated with a molecule's capacity to donate electrons and its inclination to participate in chemical processes. The HOMO energy is associated with charge transport characteristics and electronic structure in materials science [32]. In DFT computations, the electronic structure of the system is obtained by solving the Kohn-Sham equations, which leads to the HOMO energy. It helps with the interpretation of experimental data and the creation of novel materials with desired features by offering insights into the behavior of electrons and their interactions inside the material [12,13].

HOMO energy and IE

Although the particular context of the system under study heavily influences the relevance of the HOMO energy and its threshold, the following general principles apply:
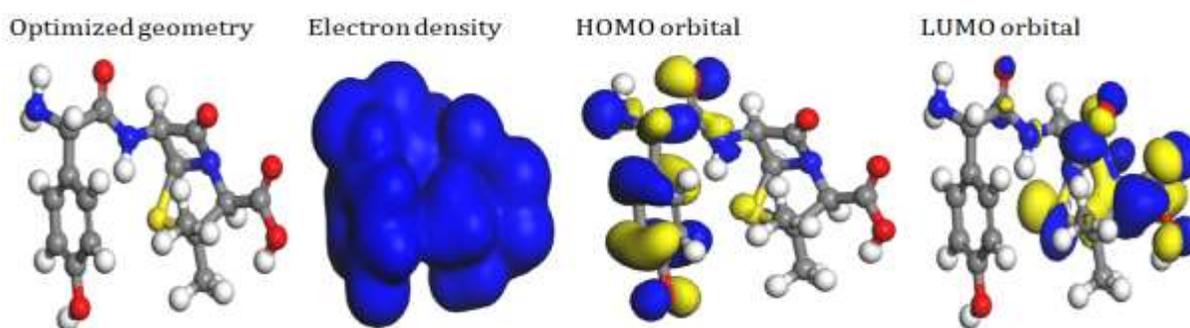

Figure 1: Optimization geometry, Electron density, Homo, and LUMO orbitals of amoxicillin

Table 1: Frontier energies of the molecule amoxicillin

Energy parameters	Energy (eV)	Energy parameters	Energy (eV)
E_{HOMO} (eV)	-5.608	σ $(eV)^{-1}$	0.535
E_{LUMO} (eV)	-1.873	ΔN_{Fe}	3.044
ΔE (eV)	3.774	ΔN_{Al}	1.736
IE (eV)	5.608	ΔN_{Cu}	0.662
AE (eV)	1.873	ω (eV)	3.746
χ (eV)	3.741	ΔE_{b-d} (eV)	-0.467
η (eV)	1.868	ε $(eV)^{-1}$	0.267

The energy needed to remove an electron from the highest occupied orbital is known as the ionization potential, or HOMO energy [33,34]. In this way, the initiation of ionization processes is frequently linked to the HOMO energy threshold. Electrons in a molecule or substance can be easily stimulated or extracted when the energy of the HOMO is exceeded by an external energy source [12]. The chemical reactivity of molecules is influenced by the HOMO energy. A molecule is more reactive as a reducing agent or in nucleophilic processes when its HOMO energy is lower, which indicates a higher probability of electron donation [34]. On the other hand, lower reactivity in these areas is indicated by a larger HOMO energy. The value of EHOMO in Table 1 for this study was -5.608eV, indicating that amoxicillin might react and lessen the effect of corrosion on the metals under investigation's surface. In addition, the simulation process's binding energies on the surfaces attest to the molecule's capacity to minimize surface corrosion. This is in line with the findings of Abdulfatai *et al.* [10] for a few organic materials. High HOMO energy molecules or materials typically have shorter bandgaps, which improve conductivity. Determining the electrical characteristics of semiconductors and organic electronics requires knowledge of the HOMO energy threshold [12].

LUMO energy and AE

The lowest unoccupied orbital energy level in an element or molecule is represented by the LUMO energy [12]. The LUMO energy is the amount of energy required to transfer an electron from the

HOMO to this orbital. A low LUMO energy means that the orbital is closer to the HOMO in energy, which makes it easier for the molecule to absorb an electron from the metal surface [35]. The molecule Amoxicillin in Table 1 had an ELUMO of 1.873 eV based on the results of the EHOMO and ELUMO measurements. The molecule can have an adsorption or bon connection between its surface and itself to create an environment that prevents corrosion in the metals under study. AE is the energy shift that occurs when an electron is added to a neutral atom or molecule to form a negative ion [36]. Higher AE, on the other hand, suggests a stronger attraction for an additional electron, whereas lower AE indicates a weaker attraction [10–13]. A lower LUMO energy is often correlated with a greater AE in the context of the link between LUMO energy and AE [37]. The reason for this is that a lower LUMO energy indicates that the orbital is more energetically advantageous for the molecule or material to take an extra electron since it is closer to the vacuum level or the energy of an incoming electron [15].

ΔE_g

The difference in energy between the HOMO and LUMO, known as the HOMO-LUMO gap, can be utilized to predict the strength and stability of a transition metal complex. A larger HOMO-LUMO gap in a compound indicates greater stability. Based on Table 1, it is evident that the ΔE_g of amoxicillin was 3.774 eV lower than that of Kumar, Shallangwa *et al.* (2013). This indicate that, the molecule Amoxicillin is flexible in terms

of transfer of electrons from its molecule to the metal surface with ease.

χ

Through its impact on the adsorption of inhibitor molecules onto the metal surface, their electrical interactions with the metal, and the stability of the inhibitor in the corrosive environment, χ influences corrosion inhibition. Stronger interactions between molecules and metal surfaces are the outcome of higher χ molecules' ability to attract electrons, which improves corrosion inhibition. The electron χ value in Table 1 indicates a significant potential for amoxicillin to interact with the surfaces, which is further confirmed by this greater interaction increasing the inhibitor's adsorption into the metal surface. Effective corrosion inhibitors are molecules with increased χ because they often show better adsorption, improved electronic effects, and greater stability [12].

η and σ

η is a measure of the resistance of a molecule to charge transfer [13]. It represents the energy required to remove or add an electron to the molecule [36]. Molecules with high η are relatively resistant to electron transfer and tend to have stable electronic structures [37]. In the context of corrosion inhibition, inhibitors with higher η values do form more stable interactions with the metal surface, leading to better protection against corrosion [7-8]. As indicated in the Table 1, the stable interaction can involve the formation of coordinate bonds between the inhibitor molecule and the metal surface, which can prevent the access of corrosive species to the metal surface. σ is the inverse of η and represents the ease with which a molecule can accept or donate electrons [12]. Molecules with high σ values have low resistance to charge transfer and may exhibit more reactivity [38]. According to Afandiyeva *et al.* [39], inhibitors with higher σ values are more likely to interact chemically with corrosive species in the context of corrosion inhibition. This results in the formation of stable products on the metal surface, which effectively prevents corrosion. On

the other hand, over-reactivity may also cause the inhibitor to gradually decrease its proficiency. A molecule's overall softness and hardness determine how effective it interacts with metal surface, which in turn affects how effective the molecule is as a corrosion inhibitor [40]. Molecules with higher η values tend to form more stable interactions with the metal surface, while those with higher σ values may exhibit greater reactivity towards corrosive species. Both properties play important roles in determining the corrosion inhibition efficiency of a molecule [41].

ω, ε, and 1/ω

ω denotes a molecule's capacity to receive electrons. ε, which is the inverse of 1/ω, refers to a molecule's propensity to donate or exchange electrons ω and ε provide quantitative measures of electron-accepting and electron-donating abilities, respectively, which are crucial for understanding and predicting reactivity in organic chemistry. In Table 1 of the studied molecule amoxicillin, the values of the parameters are in good relationship with each other [16,35].

Fraction of electrons transferred (ΔN)

The ΔN is a crucial parameter in understanding the mechanism of corrosion inhibition by organic molecules on metals. It quantifies the degree of charge transfer between the inhibitor molecule and the metal surface during the inhibition process. When an organic inhibitor molecule adsorbs onto the metal surface, it can donate or accept electrons from the metal atoms, depending on the electronic structure of the inhibitor and the metal [39-43]. The ΔN quantifies this electron transfer process [12]. The extent of ΔN affects the charge density on the metal surface and the inhibitor molecule. A higher ΔN value indicates a greater transfer of charge from the metal to the inhibitor or vice versa [15-24]. This charge redistribution can lead to changes in the electronic structure of the metal surface, making it less susceptible to corrosion by inhibiting the initiation of corrosion processes such as metal dissolution or oxygen reduction [44]. In Table 1, ΔN was in the

order of ΔNFe> ΔNAl> ΔNCu with the values: 3.044> 1.736> 0.662 respectively it is demonstrated graphically in Figure 2. This shows that the transfer or charge exchange between the molecule amoxicillin will be massive between Fe-amoxicillin more than Al-amoxicillin and Cu-amoxicillin. According to Ayuba *et al.*, Singh *et al.*, Lukovitt *et al.*, Belghiti *et al.*, Nyijime *et al.* [13-16], if the value of *ΔN* is less than 3.6, and then the inhibition efficiency of the inhibitor molecules increases with electron releasing ability on metal surface.

ΔE_{b-d}

ΔE_{b-d} refers to the transfer of electrons from the metal surface back to the inhibitor molecule in a corrosion inhibition process [12]. This phenomenon is particularly relevant in the context of coordination complexes formed between metal surfaces and inhibitor molecules. When an inhibitor molecule adsorbs onto a metal surface, it can form coordination bonds with metal atoms [17]. In some cases, electrons from the metal surface can be donated back to the inhibitor molecule, leading to a modification of its electronic structure [16]. This *ΔE_{b-d}* affects the stability and reactivity of the inhibitor molecule on the metal surface. While *ΔE_{b-d}* may stabilize the inhibitor molecule on the metal surface, excessive electron transfer back to the inhibitor may weaken its adsorption and decrease its effectiveness as a corrosion inhibitor [13,23,25]. Coordination complexes formed between the metal and inhibitor molecules through *ΔE_{b-d}* may contribute to the formation of a stable and uniform film, providing effective corrosion protection by preventing the access of corrosive species to the metal surface [12,13]. Its impact on corrosion inhibition depends on the balance between stabilizing the inhibitor molecule and maintaining its reactivity towards corrosive species.

Table 2: Fukui result of the amoxicillin molecule

Atom	F(+)	F(-)	f(2)	Atom	F(+)	F(-)	f(2)
O(1)	0.001	0.121	-0.12	N(14)	0.063	0.005	0.058
C(2)	0.005	0.124	-0.119	C(15)	0.037	-0.007	0.044
C(3)	-0.002	-0.024	0.022	C(16)	0.034	-0.002	0.036
C(4)	-0.008	-0.034	0.026	C(17)	0.032	0.007	0.025
C(5)	-0.005	-0.007	0.002	C(18)	0.037	-0.002	0.039
C(6)	-0.008	-0.007	-0.001	O(19)	0.102	0.003	0.099
S(7)	0.026	0.121	-0.095	C(20)	0.059	0.003	0.056
C(8)	-0.002	0.014	-0.016	C(21)	0.032	0.008	0.024
C(9)	0.002	0.037	-0.035	O(22)	0.111	0.026	0.085
C(10)	-0.006	0.005	-0.011	N(23)	0.001	0.027	-0.026
N(11)	0.015	-0.007	0.022	C(24)	0.003	0.075	-0.072
C(12)	0.036	0.03	0.006	O(25)	0.017	0.073	-0.056
C(13)	-0.008	-0.003	-0.005	O(26)	0.004	0.061	-0.057

Fukui function, often used to identify the reactivity sites in molecules, can also provide insights into the corrosion inhibition of organic molecules on metals [13,45]. Fukui functions, such as the Fukui ω and the Fukui ε index, are derived from conceptual DFT and are used to predict the regions of a molecule that are most susceptible to electrophilic or nucleophilic attack [46]. Fukui functions can identify the most reactive or susceptible sites in an organic molecule towards electrophilic or nucleophilic attack [47,48]. In the context of corrosion

inhibition, these active sites can correspond to regions of the inhibitor molecule that are likely to interact with the metal surface or corrosive species. Active sites identified by Fukui functions exhibit stronger interactions with the metal surface due to their reactivity [49]. Molecules containing these active sites according to Ayubal *et al.* [13] adsorb strongly onto the metal surface forming a protective barrier that inhibits corrosion processes. Based on Table 2, the molecule amoxicillin has its highest Fukui ε index on C2 and Fukui ω on O22 which shows that these sights on the molecule are more reactive and more prompt to donate and accept electron from the metal surfaces (Table 3) [50]. Figure 3 presents the Fukui second function and the Fukui positive and negative index where O22 and C2 indicate a higher active sight on the molecule.
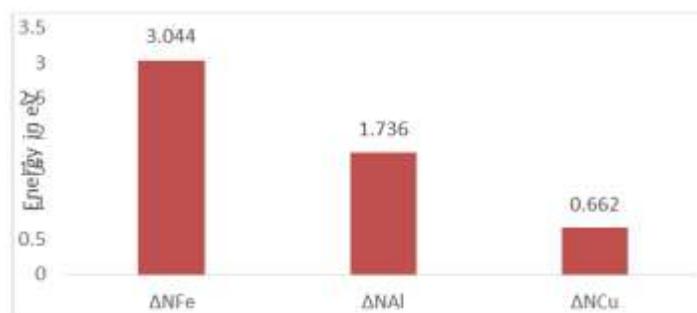

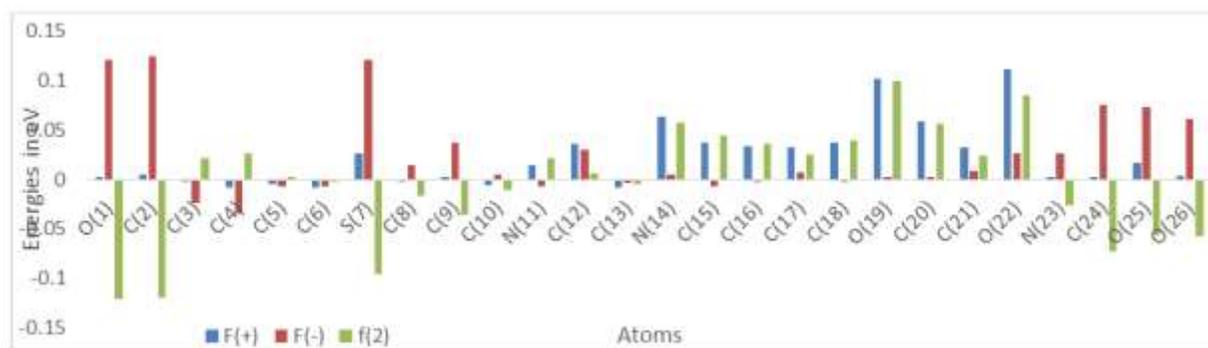**Figure 2:** The ΔN of Fe, Al, and Cu

Figure 3: Graphical representation of Fukui values and Fukui second function

Table 3: Adsorption energy of the molecule when simulated on the Fe-surface, Al-surface, and Cu-surface

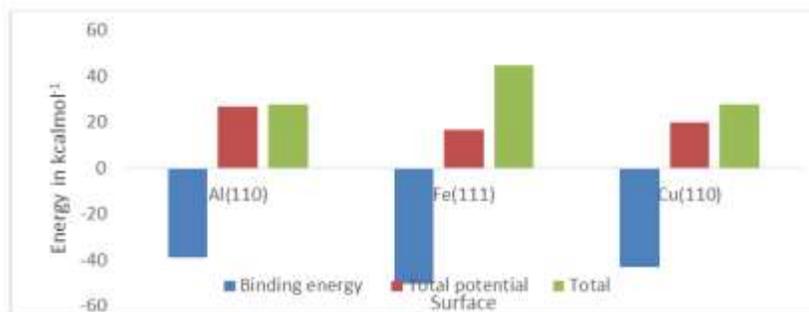| Surface	Binding energy (kcalmol^{-1})	Total energy of molecule (kcalmol^{-1})	Total potential energy of molecule (kcalmol^{-1})	Total kinetic energy (kcalmol^{-1})
Al(110)	-38.97 ± 0.0135	0.00 ± 0.00	26.93 ± 0.0027	27.85 ± 10.49
Fe(111)	-50.65 ± 2.65	0.00 ± 0.00	-16.63 ± 2.07	44.88 ± 3.32
Cu(110)	-43.24 ± 0.016	0.00 ± 0.00	20.18 ± 0.0026	27.96 ± 10.06

Figure 4: Binding energy, total potential energy of molecule, and total energy of amoxicillin on the surface of metal (Fe, Al, and Cu)
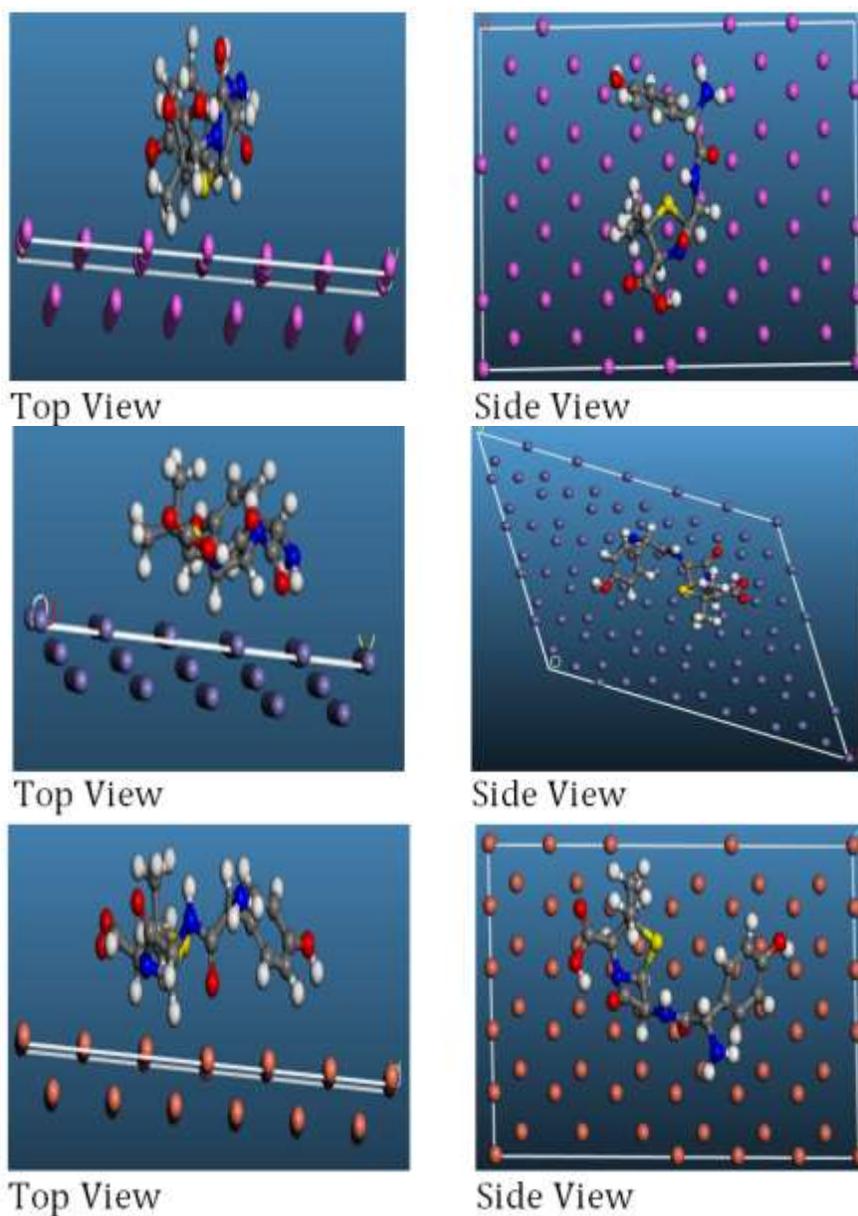

Figure 5: Amoxicillin molecule on the surface of metals (Fe, Al, and Cu) top view and side view

MD simulation is a computational technique used to model the behavior of atoms and molecules over time [51]. In corrosion inhibition studies, MD simulations are employed to investigate the adsorption behavior of inhibitor molecules on metal surfaces and assess their effectiveness in preventing corrosion. MD simulation in this research was performed using Forcite tool packages. The metal surfaces were modeled as a periodic array of atoms in a simulation cell, while the inhibitor molecule was introduced into the system. The result obtained showed that, The binding energies obtained for the inhibitor molecules on Fe(111), Cu(110), and Al(110) surfaces are -50.65, -43.24, and -38.97 (kcalmol^{-1}), respectively as also demonstrated in Figure 4. The highest binding energy is observed for Fe(111), indicating that the inhibitor molecule has the strongest affinity for iron surfaces. The lowest binding energy is observed for Al(110), suggesting that the inhibitor molecule has the weakest interaction with aluminum surfaces. The binding energy on Cu(110) falls between that of Fe(111) and Al(110), indicating intermediate affinity for copper surfaces. The binding energies obtained by the molecules during simulation on the surfaces (-50.65 kcalmol^{-1} on Fe(111), -43.24 (kcalmol^{-1}) on Cu(110), and -38.97 (kcalmol^{-1}) on Al(110) serve as indicators of the intensity of interaction between amoxicillin molecule and the specific metal surfaces. A diminished binding energy implies a less robust interaction, potentially indicating reduced efficacy in corrosion inhibition [1]. Findings involve looking at similar studies where MD simulations were employed to investigate the corrosion inhibition properties of amoxicillin on metal surfaces (Figure 5). Researchers may have used different simulation parameters, force fields, or metal surfaces, which can influence the binding energies and overall conclusions. Boyuan *et al.* and Ayaub *et al.* [1,13] in their separate research in an experimental study obtained a moderate corrosion inhibition of expired amoxicillin in HCl concentration observed a moderate inhibition efficiency between the molecule and the mild steel surface.

Conclusion

In this study, we employed DFT and simulation methods to investigate the corrosion inhibition properties of amoxicillin on Fe(111), Al(110), and Cu(110) surfaces. The results reveal insightful findings regarding the reactivity and adsorption behavior of amoxicillin on these metal surfaces. The results indicate that Fukui Nucleophilic sites C2 and S7, as well as Electrophilic site O22, are the most effective active sites for electron transfer between the molecule and the surfaces. This demonstrates the effective role of heteroatoms in the corrosion inhibition of amoxicillin. Binding energy -50.65 (kcalmol^{-1}), -38.97 (kcalmol^{-1}), and -43.24 (kcalmol^{-1}) for Fe(111), Al(110), and Cu(110) surfaces, respectively, and HOMO energy of -5.608 (kcalmol^{-1}) and LUMO energy of -1.873 (kcalmol^{-1}). Due to the binding energy effect, the surface interactions experienced by the molecule Amoxicillin are moderate overall. Among these interactions, Fe(111)-amoxicillin exhibited the most pronounced effect, followed by Al(110)-amoxicillin. On the other hand, Cu(110) showed the lowest binding energy, suggesting a weaker interaction with the molecule. The molecule interaction with the metal surface was physisorption hence the binding energy of the interaction was less than 100(kcalmol^{-1}). In conclusion, the molecule Amoxicillin had a mild inhibition on both surfaces Fe(111), Al(110), Cu(110).

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