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Research article

Anticorrosion activities of Cysteine on Iron, Aluminium and Copper using Density Functional theory (DFT)

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ABSTRACT

This research employs Density Functional Theory (DFT) to explore the corrosion inhibition properties of the molecule Cysteine (Cy) on Fe(110), Al(110), and Cu(110) surfaces. Through an analysis of the interactions between Cysteine (Cy) and each metal surface, pivotal binding sites and corresponding binding energies were identified. Our investigation highlights the significance of the Fukui Nucleophilic site O5 and Electrophilic site S6 in the inhibition process. The negative binding energy observed reflects system stability, indicative of energy release and a transition to a lower-energy state, commonly seen in atomic and molecular systems. Notably, variations in binding energies across different metal surfaces were observed, with Fe(110) exhibiting the highest binding energy (-52.75), followed by Al(110) (-30.58), and Cu(110) (-26.24). These findings deepen our understanding of corrosion inhibition mechanisms, offering valuable insights for the development of efficient corrosion inhibitors like Cysteine.

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1. Introduction

When a treated metal naturally changes into a more stable state, its oxide, hydroxide, or sulfide, the process is called corrosion. The material eventually deteriorates as a result of this corrosion process. Due to many uses of metals like copper, iron, and aluminum, corrosion is a major problem in many different industries [1]. Degradation of structures, loss of materials, and financial consequences are some of the negative outcomes of corrosion. Frequently used as an economical and effective remedy, inhibitors are used to lessen corrosion [2-5]. Because of their distinct chemical makeup and ability for interaction with metal surfaces, cysteine molecules have become one of the most promising sets of inhibitors for the control of corrosion [6]. Cysteine (Cy) is an amino acid, a building block of proteins, with the chemical formula C3H7NO2S. It contains a thiol (-SH) functional group, which makes it unique among the amino acids. This thiol group is responsible for cysteine's ability to form disulfide bonds with other cysteine residues, contributing to the structure and stability of proteins [7]. Hence Cysteine (Cy) is a powerful antioxidant that helps protect cells from damage caused by reactive oxygen species and its residues most at times active sites of enzymes, which participate in catalysis [8]. It is possible that cysteine can also be essential in the prevention of metals such as Aluminium, Iron and Copper in essential.

Despite extensive research in corrosion inhibition, there remain gaps in understanding the precise mechanisms by which inhibitors such as cysteine function on metal surfaces. Additionally, while cysteine has shown promise as a corrosion inhibitor, its effectiveness on different metals, particularly aluminium, iron, and copper, is not thoroughly elucidated using computational methods like Fukui function and frontier energies at atomic level. Moreover, the optimization of inhibitor concentrations and environmental conditions for maximum efficacy presents a challenge. These gaps and limitations underscore the need for further investigation into the corrosion inhibition mechanisms of cysteine on aluminium, iron, and copper surfaces [9-12].

In addressing the aforementioned gaps and limitations, the hypothesis of utilizing Density Functional Theory (DFT) and simulation techniques emerges as a promising approach. DFT, a computational quantum mechanical modeling method, offers insights into the electronic structure and properties of molecules and materials at the atomic level. By employing DFT simulations, we hope to explore the adsorption behavior of cysteine molecules on aluminium, iron, and copper surfaces taking consideration of the binding energy of the molecule cysteine on the various surfaces Fe(111)-CTN, Al(110)-CTN and

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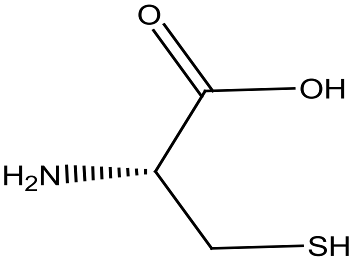
Cu(110)-CTN, thereby elucidating the mechanisms of corrosion inhibition.

The hypothesis posits that cysteine molecules interact with metal surfaces through coordination bonds, forming a protective barrier that impedes the corrosion process. DFT calculations can provide valuable information regarding the adsorption energy, charge transfer, and electronic structure of the cysteine-metal interface, facilitating a comprehensive understanding of the inhibition mechanism. Furthermore, molecular dynamics simulations can complement DFT calculations by simulating the dynamic behavior of cysteine molecules in corrosive environments. These simulations can elucidate the diffusion kinetics of cysteine on metal surfaces, as well as its interactions with corrosive species, thereby providing insights into the long-term effectiveness of cysteine as a corrosion inhibitor.

Scheme 1. Structure of Cysteine (Cy).



The proposed utilization of Density Functional Theory and simulation techniques offers a systematic approach to investigate the corrosion inhibition of aluminium, iron, and copper using cysteine molecules. By elucidating the underlying mechanisms and optimizing inhibitor-metal interactions, this research can contribute to the development of more efficient corrosion mitigation strategies in various industrial applications.

2. Materials and Methods

2.1 *Density Functional Method*

Quantum chemical calculations were conducted using the DMol3 module within the BIOVIA Material Studio 8.0 program (Accelrys, Inc.), employing the underlying principles of Density Functional Theory (DFT). The B3LYP function was applied to compute the parameters, utilizing a basis set of "double-numeric polarization" (DNP) in the gas phase model [11-16]. The calculation encompassed determining the Frontier energies of the molecule SO2 with equation 1-11 in accordance with the extended Koopman's theorem. These equations elucidate the initial electron distribution in the molecule and the computation of local reactivity, specifically the Fukui function f(r), through ab-initio quantum chemistry methods [17-19]. Before establishing their stable geometry, the molecules were drawn using ChemDraw Ultra 7.0.3 by Cambridge Software [20].

IE: Ionization energy (eV)	$IE = -E_{HOMO}$	(1)
AE: Electron affinity (eV)	$AE = -E_{LUMO}$	(2)
ΔE_g: Energy gap (eV)	$\Delta E_g = E_{LUMO} - E_{HOMO}$	(3)
χ: absolute electronegativity (eV)	$\chi = \frac{IE+AE}{2} = -\frac{(E_{HOMO} + E_{LUMO})}{2}$	(4)
η: global hardness (eV)	$\eta = \frac{IE-AE}{2} = \frac{(E_{LUMO} - E_{HOMO})}{2}$	(5)
σ: global softness $(eV)^{-1}$	$\sigma = \frac{1}{\eta} = -\frac{2}{E_{HOMO} - E_{LUMO}}$	(6)
ω: global electrophilicity index (eV)	$\omega = \frac{\mu^2}{2\eta} = \frac{\chi^2}{2\eta}$	(7)
μ: chemical potential (Debye)	$\mu \approx -\frac{1}{2}(IE + AE) = \frac{1}{2}(E_{LUMO} + E_{HOMO})$	(8)
ε: nucleophilicity$(eV)^{-1}$	$\varepsilon = \frac{1}{\omega}$	(9)
ΔE_{b-d}: Energy of back donation	$\Delta E_{b-d} = -\frac{\eta}{4} = \frac{1}{8}(E_{HOMO} - E_{LUMO})$	(10)
ΔN: Fraction of electron(s) transfer	$\Delta N = \frac{\chi Me - \chi Inh.}{2(\eta Me + \eta Inh)}$	(11)

The inhibitor molecule's absolute hardness, denoted as ηinh, and absolute electronegativity, represented by χinh, are comparable to those of Fe, Al, and Cu. In theory, the global hardness of iron, Aluminium and Copper surfaces are all equals 0 eV, and the electronegativity of bulk iron is χFe = 7.0 eV, χAl =5.6eV and χCu= 4.5ev assuming a higher density for metallic bulk compared to neutral metallic atoms [21–23]. The distinction between nucleophilic and electrophilic local Fukui functions lie in the definition of the Fukui second function (f2), also referred to as the dual descriptor Δf(k). These functions, based on the Fukui behavior of atoms, determine the electrophilicity or nucleophilicity of molecules [25]. If f2(r) > 0, site k favors a nucleophilic attack, whereas if f2(r) < 0, site k favors an electrophilic attack. Thus, f2(r) serves as a selectivity index for determining whether attacks are electrophilic or nucleophilic.

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

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

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

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

In this context, N represents the total number of electrons in the molecule, while N+1 denotes an anion formed by adding an electron to the Lowest Unoccupied Molecular Orbital (LUMO) of the neutral molecule, and N-1 signifies a cation formed by removing an electron from the Highest Occupied Molecular Orbital (HOMO) of the neutral molecule. The variable qk represents the net charge of atom k within the molecule, reflecting the electron density at a specific point r in space surrounding the molecule. The initial ground state geometry was utilized as the reference point for all subsequent calculations. Employing an atomic charge partitioning method, such as

Mulliken population analysis outlined in Equations, these functions were concentrated on the nuclei of the atoms [24-25].

2.2 Molecular Dynamic Simulations

To mimic the behavior of the SO2 molecule on closely packed surfaces of Fe (111), Fe(110), and Fe(100) atoms, a quench adsorption method known for its high stability was employed. This simulation was conducted using the FORCITE tool package integrated into the BIOVIA Materials Studio 8.0 software (Accelrys, Inc.). The simulation employed the COMPASS force field tool and the Smart algorithm approach within a simulation box measuring 17Å x 12Å x 28Å, aiming to model a representative surface area [28]. The Fe crystals were cleaved along the (111), (110), and (100) planes at a fractional depth of 3.0 Å, and the form of the bottom layers was fixed before surface optimization to mitigate edge effects stemming from molecular sizes. A 3x3 supercell was then generated by extending the surfaces. By maintaining a temperature of 350K, a balance was struck between excessive kinetic energy causing molecule desorption and insufficient kinetic energy hindering molecule movement across the surface [13,23]. The simulation, conducted over 5 ps with a time step of 1 fs, employed the NVT (microcanonical) ensemble to control temperature. The quenching process occurred every 250 steps for a total of 5000 cycles to ensure statistical accuracy of energy values on the Fe crystal surfaces examine. Utilizing FORCITE, the lowest energy interactions between molecules and Fe (111) surfaces were determined through geometry optimization [24-27].

Equations (16-17) were utilized to calculate the adsorption and binding energies of the SO2- Fe- surface.

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

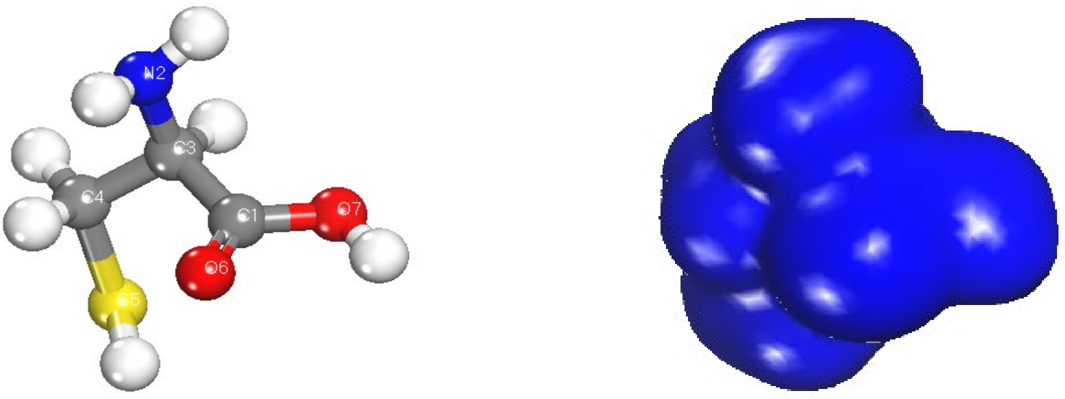
$$E_B = - E_A \quad (17)$$

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 [23-28].

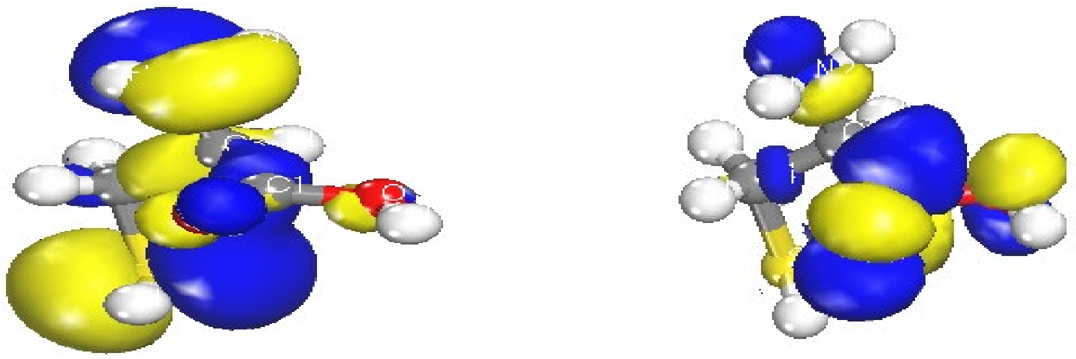
3. Results and Discussion

3.1 Frontier Energy

In DFT studies of corrosion inhibition, optimizing the molecular structure, understanding the electron density distribution, and tuning the energy levels of the HOMO and LUMO orbitals are essential for predicting and enhancing the effectiveness of inhibitor molecules [27-30].


Optimized molecule

Density of the molecule


HOMO Orbitals

LUMO orbitals

Figure 1: *Optimized, Density, HOMO and LUMO orbitals of the molecule*

In the context of corrosion inhibition, the energy levels of the HOMO and LUMO orbitals influence the ability of the inhibitor molecule to donate or accept electrons during the adsorption process onto the metal surface [37]. A lower energy HOMO indicates a better ability to donate electrons, facilitating adsorption onto the metal surface, while a higher energy LUMO suggests a greater ability to accept electrons, which can stabilize the adsorbed molecule. In Table 2 of the study, it can be seen that, the EHOMO value and the ELUMO values are in line with the study obtained by Zarrouk et al, Eddy and Ebenso, Abdulfatai et al [3, 9 and 10].

HOMO-LUMO gap, is an important parameter in determining the corrosion inhibition efficiency of a molecule in the following ways: energy gap between these orbitals is indicative of the molecule's ability to donate or accept electrons, which is crucial for its corrosion inhibition effectiveness. In the context of corrosion inhibition, an inhibitor with a narrow energy gap tends to have enhanced donor-acceptor properties, allowing it to readily interact with metal surfaces and adsorb onto them, thereby forming a protective barrier against corrosion [38-39]. A smaller energy gap often correlates with stronger adsorption due to increased electronic interactions between the inhibitor and the metal surface [39]. This strong adsorption helps stabilize the inhibitor layer on the metal surface, enhancing its corrosion inhibition efficiency. These can help with creating novel corrosion inhibitors with improved properties. In the study, the energy gap obtained by Cy is less than the energy gap obtained by Belghiti [16] on the simulation and statistical analysis on the relationship between corrosion inhibition efficiency and molecular structure of some hydrazine derivatives in phosphoric acid on mild steel surface.

Inhibitors with higher ionization energies tend to be more stable as they are less likely to undergo electron loss and subsequent degradation when interacting with metal surfaces. DFT calculations can predict the ionization energies of inhibitor molecules and correlate them with their ability to donate electrons, thereby influencing their corrosion inhibition efficiency [40-42]. On the other hand, inhibitors with higher electron affinities have a greater tendency to accept electrons from the metal surface, forming a stable protective layer [42]. While Inhibitors with higher electron affinities are more likely to form strong interactions with metal atoms, leading to enhanced adsorption and corrosion inhibition [43]. In the study as presented in Table 2, the values of I.E and A.E are in the limit of inhibitors that can form strong adsorption on the surface of metal. According to Mohammed and Rubba, Mammeri et al [22,23] incorporating ionization energy and electron affinity analyses through DFT into corrosion studies provides valuable insights into the electronic properties of inhibitor molecules and their interactions with metal surfaces. This knowledge can be leveraged to design and optimize corrosion inhibitors with enhanced effectiveness and stability.

According to Basma and Hadi [18], a hard molecule has low basicity and low electron-donating potential, while a soft molecule has high basicity and high electron-donating potential. The result of the study is in line with the study obtained by the Basma and Hadi. Also the result show that, 3.6065 eV of $\boldsymbol{\chi}$ shows a large number of electron transfers while 1.9195 eV of η is small., indicating that Incorporating hardness and softness analyses through DFT into corrosion inhibition studies offers a comprehensive understanding of the electronic structure and reactivity of inhibitor molecules. The electrophilicity index (ω) represents a molecule's ability to accept electrons, while nucleophilicity (ε), the reciprocal of electrophilicity ($1/\omega$), indicates a molecule's inclination to donate or exchange electrons. These indices offer quantitative assessments of electron-accepting and donating capabilities, respectively, playing a vital role in comprehending and foreseeing reactivity in organic chemistry. The values of these parameters for Cy in Table 2 exhibit a strong correlation, as noted in in research carried out by Kadhim et al. [32].

The effect of the fraction of electrons transferred (**ΔN**) on the corrosion inhibition can be seen in the values of fraction of electrons transferred (**ΔN**) in Table 2 of the Cy molecule on different surfaces using bulk. The higher the value of (**ΔN**), the greater the impact on the cell potential. In Table 2 Aluminum (Al) was recorded n = 0.9967 eV, iron (Fe) **ΔN** = 0.8839eV and copper (Cu) **ΔN** = 0.2327eV. The effect of corrosion inhibition will be greatest for aluminum, followed by iron, and then copper. This is because higher values of (**ΔN**) correspond to a greater change in cell potential, thus indicating a stronger impact on the inhibition of corrosion [44].

Table 2: Frontier energy parameters of the molecule Cysteine

Energy parameters	**eV**
E_{HOMO} (eV)	-5.526
E_{LUMO} (eV)	-1.687
ΔE (eV)	3.839
IE (eV)	5.526
AE (eV)	1.687
χ (eV)	3.6065
η (eV)	1.9195
σ (eV)$^{-1}$	0.52097
ΔNFe	0.8839
ΔNAl	0.9967
ΔNCu	0.2327
ω (eV)	1.694
$\Delta E_{b\text{-}d}$ (eV)	-0.4799
ε (eV)$^{-1}$	0.59032

3.2 Fukui

Fukui parameters, derived from conceptual density functional theory (DFT), provide insights into the reactivity of molecules by predicting how they may undergo nucleophilic or electrophilic attacks. These parameters are particularly useful in understanding the sites on a molecule that are most susceptible to chemical reactions. In the context of corrosion inhibition, Fukui parameters can help identify which parts of a molecule are likely to interact most strongly with the metal surface, thereby influencing its inhibition efficiency [31-32].

In this research, oxygen (O) has the highest positive Fukui parameter value (Fukui (+)), while sulfur (S) has the highest negative Fukui parameter value (Fukui(-)). A high positive Fukui parameter value for oxygen suggests that it is highly susceptible to nucleophilic attacks. In the context of corrosion inhibition, this could imply that oxygen atoms in the inhibitor molecule are likely to donate electrons to the metal surface, forming a protective layer that inhibits corrosion. Oxygen-containing functional groups, such as hydroxyl (-OH) or carbonyl (C=O) groups, are commonly found in corrosion inhibitor molecules due to their ability to interact with metal surfaces through coordination or hydrogen bonding [33]. The high positive Fukui parameter for oxygen supports the notion that these functional groups can play a crucial role in corrosion inhibition for cysteine.

Also, a high negative Fukui parameter value for sulfur suggests that it is highly susceptible to electrophilic attacks. In the context of corrosion inhibition, this imply that sulfur atoms in the inhibitor molecule are likely to accept electrons from the metal surface or other species present in the corrosive environment [34-35]. Sulfur-containing functional groups, such as thiol (-SH) or thione (C=S) groups, are also commonly found in corrosion inhibitor molecules due to their ability to form coordination bonds with metal ions or adsorb onto metal surfaces through sulfur-metal interactions [36]. The high negative Fukui parameter for sulfur supports the importance of these functional groups in corrosion inhibition. The second Fukui function indicated that, the molecule Cy is a nucleophile molecule which donate electron to the metal surfaces [37] this is graphically represented in Figure 2.

Table 1: The Fukui parameters of the molecule.

	(Fukui(+))		*(Fukui(-))*			
atom	Mulliken	Hirshfeld	Mulliken	Hirshfeld	f^2(Mulliken)	f^2(Hirshfeld)
C (1)	0.156	0.229	0.035	0.021	0.121	0.208
N (2)	0.082	0.04	0.178	0.231	-0.096	-0.191
C (3)	-0.047	0.018	-0.012	0.044	-0.035	-0.026
C (4)	0.016	0.017	-0.062	0.026	0.078	-0.009
S (5)	0.032	0.068	**0.356**	**0.306**	-0.324	-0.238
O (6)	**0.315**	**0.273**	0.029	0.032	0.286	0.241
O (7)	0.166	0.152	0.019	0.03	0.147	0.122

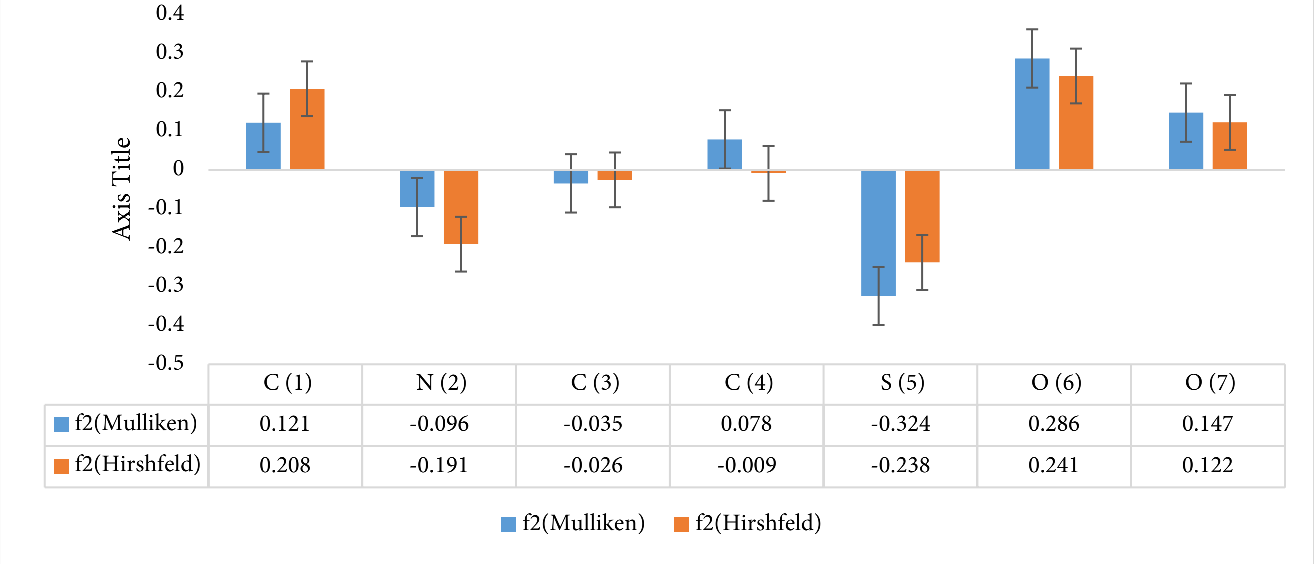


Figure 2: The graphical representation of the Second function (f^2) parameter of the molecule.

3.3 *Simulation*

Simulation is crucial in corrosion studies, offering essential insights and forecasts regarding corrosion processes and the efficacy of corrosion inhibition tactics. Through modeling material interactions with electrolytes and environmental elements, simulations clarify the mechanisms governing corrosion initiation, propagation, and mitigation [45-48]. Furthermore, by integrating kinetic and thermodynamic principles, simulations offer numerical estimates of corrosion rates, aiding in the evaluation of material degradation over time. Moreover, simulations contribute to cost-effectiveness by diminishing the necessity for extensive laboratory experiments [49-50]. This expedites research and minimizes resource expenditure while yielding valuable insights into corrosion phenomena.

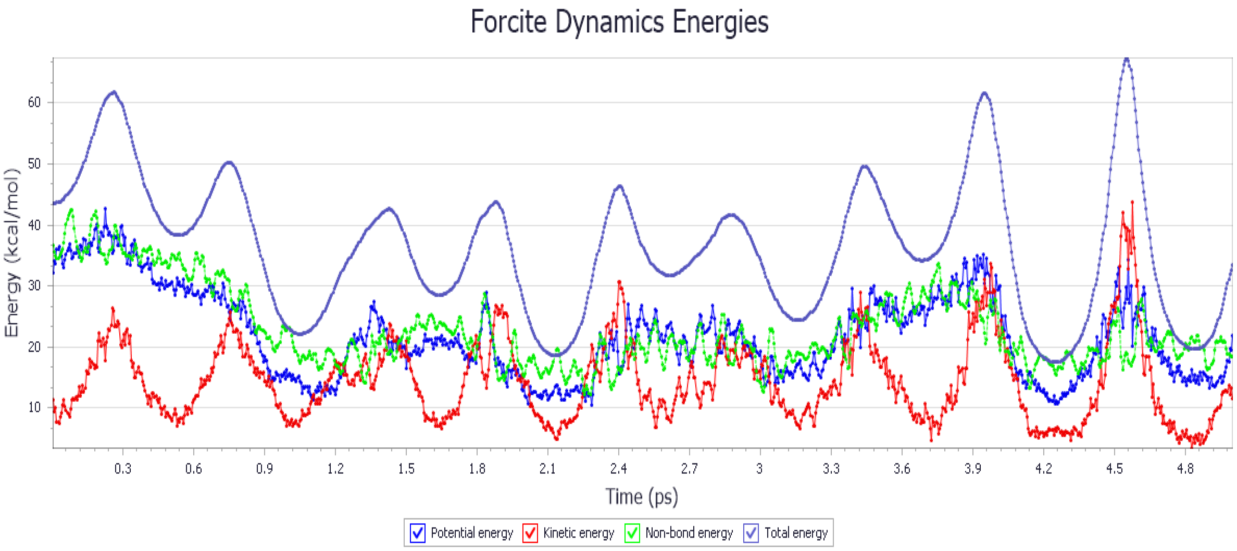
For the reasons mentioned, the binding energy of the molecule Cy was tested on the following metals to understand the corrosion inhibition behavior of the molecule. From the result in Table 3, the binding energies shows that energies is released when bonds are formed [51]. The binding energy of the system between *Fe(110)-Cy* was higher followed by *Al(110)-Cy* and then *Cu(110)-Cy*. The negative value of the binding energy is commonly seen in systems where atoms forming molecules or nucleons binding together in atomic nuclei. In these cases, the negative binding energy reflects the stability of the system, as energy is released and the system moves to a lower-energy state [52]

Table 3. Energies of the Simulation

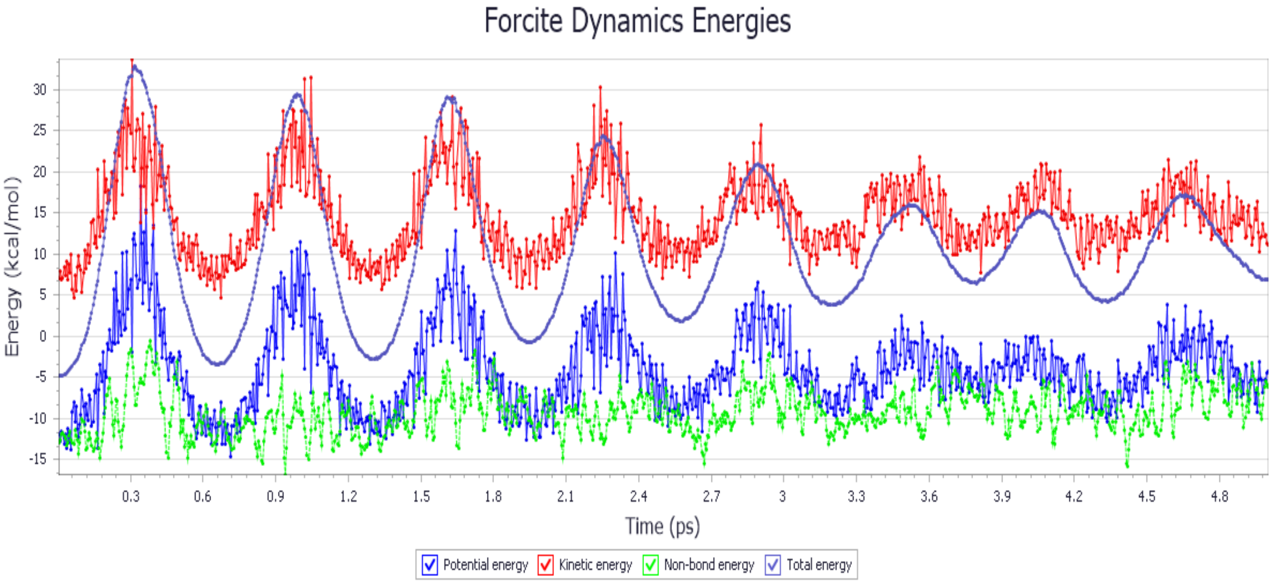
Surface	Binding energy	Total energy of molecule	Adsorption Energy
Al(110)	-30.58 ±0.00	0.00 ± 0.00	30.58 ±0.00
Fe(110)	-52.75 ± 0.15	0.00 ± 0.00	52.75 ± 0.15
Cu(110)	-26.24 ± 0.16	0.00 ± 0.00	26.24 ± 0.16

To assess the accuracy of a model or simulation in predicting the extent of corrosion inhibition between the metals and the Molecule Cy, Root Mean Square Deviation (RMSD) typically refers to a measure of the differences between values predicted by a model or simulation and the corresponding observed values is presented in the graphical form as shown in Figure 3a-c

A. Al-Cy



B. Fe-Cy



C. Cu-Cy

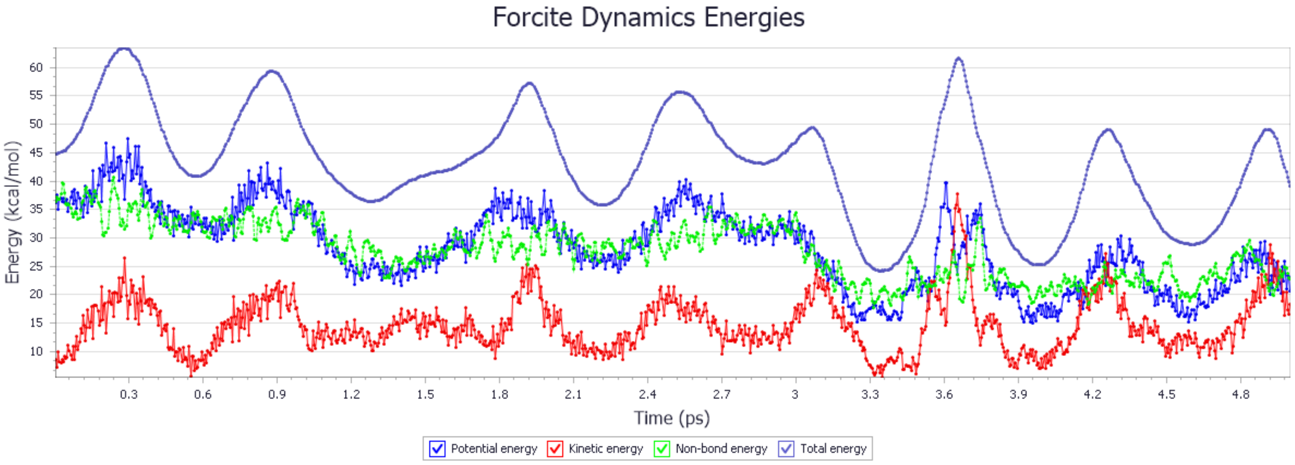
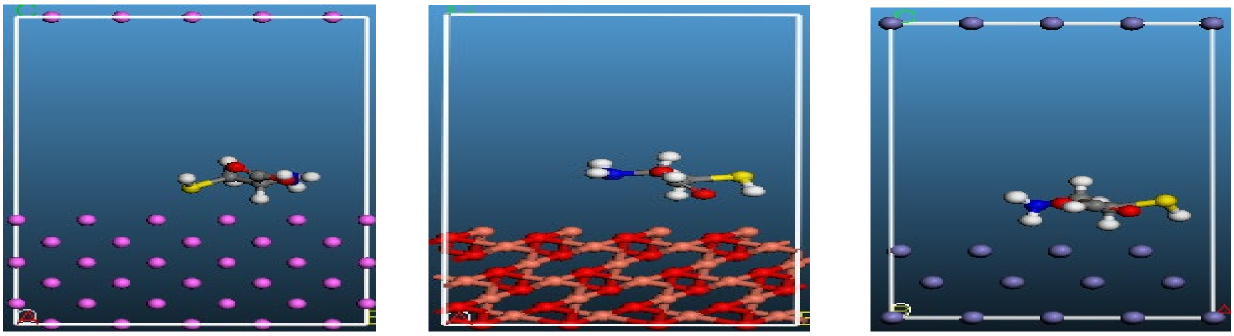


Figure 3A-C: The Root Mean *Square* Deviation (RMSD)

The molecule interaction and the surfaces *Fe(110)-Cy*, *Al(110)-Cy* and *Cu(110)-Cy* is presented in figure 4.



Al-Cy side View **Cu-Cy Side view** **Fe-Cy Side View**

Figure 4: The screen short of the molecule interaction with the surfaces of Fe*(110)-Cy* , *Al(110)-Cy* and *Cu(110)-Cy*.

4. Conclusion

In conclusion this research employed Density Functional Theory (DFT) to investigate the corrosion inhibition properties of the molecule Cy on Fe(110), Al(110), and Cu(110) surfaces. By analyzing the interactions between Cy and each metal surface, we identified key binding sites and evaluated the corresponding binding energies. Our findings highlight the significance of the Fukui Nucleophilic site O5 and Electrophilic site S6 as pivotal in the inhibition process. The negative value of the binding energy is commonly seen in systems where atoms forming molecules or nucleons binding together in atomic nuclei. In these cases, the negative binding energy reflects the stability of the system, as energy is released and the system moves to a lower-energy state. Moreover, we observed distinct variations in binding energies across the different metal surfaces, with Fe(110) exhibiting the highest binding energy (-52.75), followed by Al(110) (-30.58), and Cu(110) (-26.24). These insights contribute to a deeper understanding of the corrosion inhibition mechanisms and provide valuable guidance for future research in the development of efficient corrosion inhibitors like Cysteine.

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