



## Original Article

# Adsorptive properties of 4-Hexyl-tertrahydro-thiopyran-1,1-diode on Al(110) and Fe(111) surface using DFT method

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### ABSTRACT

Aluminum and iron are highly significant industrial commodities that are used to make anything from tools and concrete construction to roofing sheets and other roofing-related products. Even though they generate a protective oxygen barrier that prevents corrosion, they are nevertheless susceptible to corrosion in extreme conditions. In order to achieve the stable shape of the molecule HTTD, a theoretical investigation on the corrosion inhibition of metals like Aluminum and iron was conducted utilizing local density function B3LYP under limited spin polarization DNP foundation. The values of local/global reactivity parameters, including the ( $\omega+$ ) electroaccepting power and ( $\omega-$ ) electrodonating power between the inhibitor molecule and the metal surfaces, were demonstrated. These parameters included EHOMO, ELUMO, energy gap ( $\Delta E_g$ ), electronegativity ( $\chi$ ), global hardness ( $\eta$ ), global electrophilicity index ( $\omega$ ), and fraction of electron transfer ( $\Delta N$ ). Physisorption mode was defined as the mode of interaction of HTTD on Aluminium and Chemical Adsorption on Iron surface based on the simulation modeling output. The outcome of Fukui functions revealed that the focus point for the selectivity of electron donation and acceptance between the metal and the moiety is a hetero-atom present in the molecule such as oxygen, sulfur and the methylene (-CH<sub>2</sub>-) functional group.

## 1. Introduction

Iron in form of mild steel, and Aluminium are often utilized in construction, such as machine components and concrete construction [1]. It is essential to several industries. Regrettably, iron rusting causes significant environmental problems [2-4]. It is well recognized that organic compounds, whether in the form of well-known molecules or plant extracts, can be used as inhibitors in industrial settings to delay the corrosive process of these metals [5]. Iron and Aluminium are protected from corroding in acidic environments by the use of heterocyclic compounds with lone pairs of electrons in their heteroatoms, such as sulfur, nitrogen, and oxygen, and

delocalized electrons in their molecules [6-8]. In an effort to decrease this influence on society, more ecologically friendly materials are being used. These biological molecules are thought to have an adsorptive ability because they stop metallic materials from gaining an electron on the d-orbitals and forming oxide which is known as rust and resulting to corrosion [9]. Due to the presence of a lone pair of electrons on such an orbit, the various functional groups, heteroatoms, or polar atoms found in those biochemical molecules, such as sulfur, nitrogen, oxygen, phosphorus, etc., create both HOMO and LUMO centers

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for electron donation and acceptance between the surfaces [10].

In as much as the inhibition process must be explained via experimental approaches; however, these procedures are sometimes expensive and time-consuming. The potential for the successful use of theoretical chemistry in corrosion inhibition has been made possible by the continual advancements in hardware and software. Density functional theory (DFT) is one of the computational theories used in chemistry for the modeling and simulation of biological molecules to address common problems affecting the effective delivery of chemical processes globally [1-6]. Using density functional theory, the research on corrosion inhibition is currently gaining the most urgent attention. Examples include studying the helical structure of proteins, finding catalysts suitable for certain chemical reactions, and inhibiting [11].

The goal of the current investigation is to determine if 4-Hexyl-tetrahydro-thiopyran-1,1-dioxide (HTTD) can stop the corrosion of iron and Aluminium metal surfaces. This task is computationally completed by computing and modeling the parameters of quantum chemistry utilizing molecular dynamics. The researched compounds' structure is shown in Figure 1

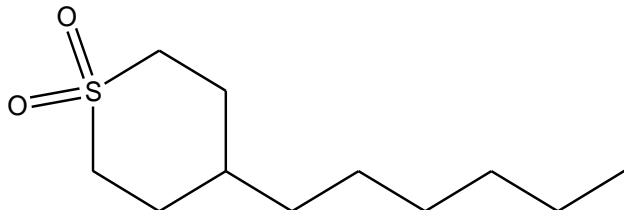


Fig 1. 4-Hexyl-tetrahydro-thiopyran-1,1-dioxide structure

## 2. Computational Methods

### 2.1. Sketching and Geometric Optimization of the molecules

ChemDraw Ultra 7.0.3 CambridgeSoft was used to create sketches of the investigated compounds. Each molecular structure needs to be optimized once it has been constructed to bring it to a stable configuration. The atoms' coordinates are changed iteratively during this process to bring the structure's energy to a stationary point or where the forces acting on the atoms are zero. During the energy reduction, a relative minimum on the energy hyper surface was sought after. It is anticipated that the geometry corresponding to this structure will closely resemble the system's real physical structure when it is in equilibrium [6-8]. The molecules' torsional and conformational

energies were reduced using DMol3 optimization, a feature of BIOVIA Materials Studio 8.0. (Accelrys, Inc.). From ChemDraw, the chemicals were imported into Materials Studio. The following parameters were used to do the optimization: limited spin polarization DNP+ basis for DFT-D. B3LYP was chosen as the local density functional in the water solvent [1-3].

### 2.2. Quantum Chemical Parameters Calculations

Calculations involving quantum chemistry were performed using the Dmol3 modules included in the Material studio 8.0 (from Accelrys Inc.) program. Dmol3 is software that computes the electronic characteristics of molecule clusters, surfaces, and crystalline solid materials from the first principle using the density functional theory (DFT) and a numerical radial function basis set. [12]. The double numeric with polarization (DNP) basis set and the functional methods B3LYP from the name Becke for the exchange portion and Lee, Yang, and Parr for the correlation component were used to do the density functional theory (DFT) computations. Because it is the best set available in Dmol3, this base set was chosen. [13]. According to Koopman's theory, the energy of the border molecular orbital, the energy of the highest occupied molecular orbital (EHOMO), and the energy of the lowest unoccupied molecular orbital (ELUMO) are connected in equation (2) and (3), respectively (3) [14-17].

$$IE = -EHOMO \quad (1)$$

$$EA = -ELUMO \quad (2)$$

The value of global hardness ( $\eta$ ), according to Pearson, is roughly described as given in equation (3). The global softness ( $S$ ) of the system, as shown in Equation 4, is the opposite of the global hardness.

$$\eta = \frac{IE-EA}{2} \quad (3)$$

$$S = \frac{1}{\eta} \quad (4)$$

The energy gap of the molecules is calculated using the relation given in equation 5. The energy gap is a parameter that, determine in the

$$\Delta Eg = ELUMO - EHOMO \quad (5)$$

The fraction of electrons transferred from the inhibitor to Fe-surface,  $\Delta N$ , this is calculated by using equation 6. The half electron transfer of the molecules is a parameter that demonstrate

$$\Delta N = \frac{\chi^{Fe} - \chi^{Inh}}{2(\eta^{Fe} + \eta^{Inh})} \quad (6)$$

According to the simple charge transfer model for donation and back donation of charges, when a molecule receives a certain amount of charge,  $\Delta N^+$ , then:  $\Delta E^+ = \mu^+ \Delta N^+ + \frac{1}{2} \eta (\Delta N^+)^2$  and when a molecule back-donates a certain

amount of charge,  $\Delta N^+$ , then:  $\Delta E^- = \mu^- \Delta N^+ + \frac{1}{2} \eta (\Delta N^+)^2$   
 Assuming the amount of charge back-donation is equal to the amount of charge received, the total energy change will be approximately be the sum of the contributions [15-18].

$$\begin{aligned} \Delta E_t &= \Delta E^+ + \Delta E^- & (7) \\ &= (\mu^+ - \mu^-) \Delta N^+ + \frac{1}{2} \eta (\Delta N^+)^2 + \frac{1}{2} \eta (\Delta N^-)^2 \\ &= (\mu^+ - \mu^-) \Delta N^+ + \eta (\Delta N^+)^2 \end{aligned}$$

But the most favourable condition corresponds to the case when the total energy change ( $\Delta E$  back-donation) becomes minimum with respect to  $\Delta N^+$ , which implies that:

$$\begin{aligned} \Delta N^+ &= -(\mu^+ + \mu^-) / 2 \eta \\ \Delta E_{bd} &= (\mu^+ - \mu^-)^2 / 4 \eta = - \frac{-\eta}{4} \end{aligned} \quad (8)$$

The electron donating ( $\omega^-$ ) and electron accepting ( $\omega^+$ ) powers of the molecules has been defined as shown in the equations 9 and 10 [19]

$$\omega^- \approx \frac{(3I+A)^2}{16(I-A)} \quad (9)$$

$$\omega^+ \approx \frac{(I+3A)^2}{16(I-A)} \quad (10)$$

$$\begin{aligned} \chi &= \text{Absolute electronegativity (eV)} \chi = \frac{I+A}{2} = \\ &= \frac{-1}{2} (E_{HOMO} - E_{LUMO}) \end{aligned} \quad (11)$$

The second order Fukui function ( $f^2$ ) the dual descriptor  $\Delta f(k)$ , was used in describing the donating and acceptability of the molecule and the metal which has theoretical electronegativity value ( $\chi_{Fe}=7.0\text{eV}$ , ( $\chi_{Al}=5.6\text{eV}$ ) and a global hardness of Aluminum and iron are  $0\text{eV}$  [2-5]. The second Fukui function has been defined as the difference between nucleophilic and electrophilic Fukui functions as in Equation. 11. If  $f^2(r) > 0$ , then site  $k$  prefers nucleophilic attack, whereas if  $f^2(r) < 0$ ; then site  $k$  prefers an electrophilic attack. This indicates that  $f^2(r)$  serves as an index of selectivity towards nucleophilic or electrophilic attacks [14, 19-20]

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

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

$$f(r) = f^+ - f^- = f^2 \quad (\text{Fukui function}) \quad (14)$$

### 2.3 Molecular Dynamics Simulation

To simulate a realistic portion of the surface, calculations were performed using the COMPASS FORCEFIELD and

Smart ALGORITHM in a simulation box of  $17 \times 12 \times 28$  with a periodic boundary condition. The fractional depth of 3.0 was used to split the Fe crystals along the (1 1 1) Plane and Al along (110). Prior to optimizing the iron surface, the lower layers' shape was limited. In order to minimize edge effects, the iron surface was then increased into a  $10 \times 10$  supercell. [1-4].

A tradeoff between a system with too much kinetic energy, where the molecule desorbs from the surface, and a system with insufficient kinetic energy, where the molecule cannot move across the surface, was made by fixing the temperature at 350 K to quench the molecules on the surface. [1-2,21].

The NVE (microcanonical) ensemble was used to set the temperature, with a time step of 1 fs and simulation duration of 5 ps. For the purpose of obtaining the statistical values of the energies on the surface of Fe, the system was programmed to quench every 250 steps. Different interactions were produced using forcite tailored molecular and surface architectures. Using the relationship in equation, the binding energy between the inhibitors and the Fe (111) surface was estimated by equation 14. [22]

$$\text{Binding Energy} = E_{\text{total}} - (E_{\text{inhibitor}} + E_{\text{Fe surface}}) \quad (14)$$

## 3. Results and Discussion

### 3.1 Frontier energies

The molecule of HTTD with the greatest occupied molecular orbital (HOMO), lowest vacant molecular orbital, and best structure is depicted in figure 2. (LUMO). Quantum chemical calculations are one method used in corrosion research that provides essential information on the selective reactivity of the inhibitor chemicals [22]. This illustrates the molecule's potential to interact with the metal surface (mild steel). How reactive inhibitor compounds are is dependent on the electronic properties of the atoms, including electron density and partial charges.

The HOMO dense region, which also acts as the active core, is the focus of electrophiles [3,9,11]. Figure 2 shows the ideal structure, HOMO and LUMO orbitals, and total electron density of the molecules under examination. The LUMO orbitals show the areas where molecules can take electrons from the iron's d-orbital present in mild steel [14-15]. The image shows the electron density of the whole molecule, demonstrating its power to boost the adsorption capacity on metal (mild steel) surfaces.

The HOMO and LUMO orbital regions amply show that the HOMO and LUMO behaviour of the molecules may be related to their capacity to adsorb [1]. The HOMO and LUMO orbitals are also filled by the hetero-atoms that are

present in ring structure of molecule.

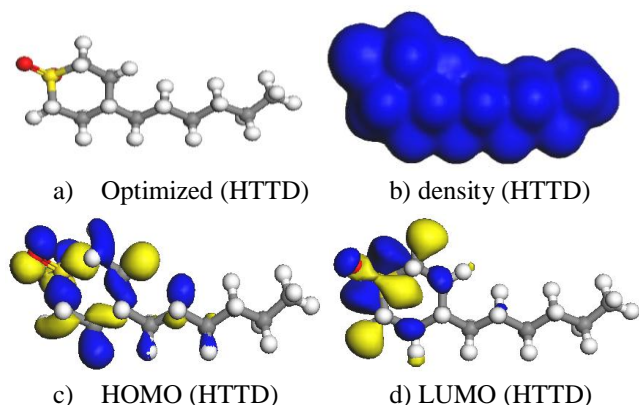


Fig 2. Present the HOMO, LUMO, Density and Optimized structures of HTTD

The HOMO is the region of the molecule that has the greatest ability to donate electrons, while the absence of electrons in a particular area of the molecule is indicated by the LUMO orbital. The region of the molecule that was previously studied contains both the HOMO and LUMO orbitals [1-6]. This may be the result of the hetero-atom being located near functional groups like withdrawing and donating groups in the molecule. [11]. Hence, the presence of both HOMO and LUMO regions is a certain sign that the molecule will be successful at preventing metal from corroding in a corrosive environment [5].

Table 1: The Frontier Energies of the Molecules

Parameters studied	HTTD
HOMO (orbital number)	60.000
LUMO (orbital number)	61.000
$E_{\text{HOMO}}$ (eV)	-6.910
$E_{\text{LUMO}}$ (eV)	0.332
IP (eV)	6.910
EA (eV)	-0.332
$\Delta E$ (eV)	7.242
electronegativity( $\chi$ )	3.289
Global hardness( $\eta$ )	3.621
Half-electron transfer( $\Delta N$ ) Fe	0.512
Half-electron transfer( $\Delta N$ ) Al	0.319
( $\omega^-$ )	3.591
( $\omega^+$ )	0.302

It is crucial to concentrate on factors that directly affect how electronically an inhibitor molecule interacts with a metal surface when building a composite index of an inhibitor molecule [1-2]. They include electron affinity (EA), energy gap ( $\Delta E_g$ ), electronegativity ( $\chi$ ), half of electron transfer ( $\Delta N$ ), and the molecular powers of electron donating ( $\omega^-$ ) and receiving ( $\omega^+$ ) [23]. To determine the compounds' overall reactivity, these energies were computed. The possible stability of the molecules during reaction was explained by global reactivity. The

level of electron transfer from molecules to the empty orbitals of the mild steel (iron) surface is indicated by the greatest value of  $E_{\text{HOMO}}$ . In the HDDT molecule under study,  $E_{\text{HOMO}}$  and  $E_{\text{LUMO}}$  values were in agreement, just as they were with the values established by other corrosion research [9]. However, the lowest value of  $E_{\text{LUMO}}$  is a sign that the molecule is more receptive to receiving electrons from the metal surface than the molecule with the highest  $E_{\text{LUMO}}$ . Ionization potential (I.E) and  $E_{\text{HOMO}}$  values are closely related since the  $-I$  always equals the  $E_{\text{HOMO}}$  values of the molecules and the electron affinity always equals the  $E_{\text{LUMO}}$ . As a result, the number of the electron transfer is within the range of the molecule being examined on both the Al and Fe surfaces. This shows that improving the capacity of inhibitor, electrons will be donated on both surfaces (metal and Inhibitor) as such, the best inhibitor is related with the largest proportion of electrons transmitted. Fe surface is more effective compare to Al surface on the investigated surfaces. [10-14].

A bigger  $\omega^+$  value translates into a stronger capacity to receive charge, whereas a lower  $\omega^-$  value of a system makes it a better electron donor, according to the power of electron donator and acceptor estimated from the molecules obtained from the computation was high, indicating that the molecule has a greater capacity for donation on both sides. [18].

The energy gap is another critical element. The difference between a molecule's LUMO and HOMO energies is known as the energy gap [10–15]. The possibility of a sluggish transfer of electrons between molecule's atoms is indicated by an increase in the LUMO-HOMO differential [9–13]. The reduced energy gap of the investigated compounds demonstrates their enormous potential. The size of the molecule HTTD indicates a delayed electron transfer from the molecule to the surface during the inhibition process.

### 3.2 Fukui Function

The local reactivity of the inhibitor compounds was examined using Fukui of different functions. The Fukui functions, electrophilic, and nucleophilic sites of attack on the molecules under consideration were the main points of attention. The orbital regions and selectivity are tested by electrophilic and nucleophilic (f - and f +) reactions. They demonstrate the significance of examining the mechanisms behind the inhibitors' interactions with surfaces [10-11]. The atom in the molecule which has the greatest Hirshfield or Milliken value, indicates the region where reaction is likely to occur in the molecule, is where these nucleophilic and electrophilic assaults are detected [12]. In Table 2, Hirshfield and Milliken are denoted by the letters H and M,

respectively.

Table 2: Fukui functions of the molecule

Atom	$f_k^+(M)$	$f_k^+(H)$	$f_k^-(M)$	$f_k^-(H)$	$f^2(M)$	$f^2(H)$
S ( 1 )	0.205	0.169	0.037	0.073	0.168	0.096
C ( 2 )	-0.089	0.043	-0.010	0.047	-0.079	-0.004
C ( 3 )	-0.017	0.022	0.022	0.034	-0.039	-0.012
C ( 4 )	-0.019	0.005	0.014	0.013	-0.033	-0.008
C ( 5 )	0.001	0.021	-0.032	0.029	0.033	-0.008
C ( 6 )	-0.069	0.041	-0.000	0.047	-0.069	-0.006
C ( 7 )	0.037	0.007	-0.057	0.010	0.094	-0.003
C ( 8 )	-0.045	0.006	0.047	0.018	-0.092	-0.012
C ( 9 )	-0.011	0.002	0.008	0.010	-0.019	-0.008
C ( 10 )	0.032	0.002	-0.039	0.003	0.071	-0.001
C ( 11 )	-0.095	0.001	0.092	0.002	-0.187	-0.001
C ( 12 )	-0.102	0.003	0.101	-0.000	-0.203	0.003
O ( 13 )	0.144	0.135	0.169	0.138	-0.025	-0.003
O ( 14 )	0.119	0.111	0.138	0.133	-0.019	-0.022

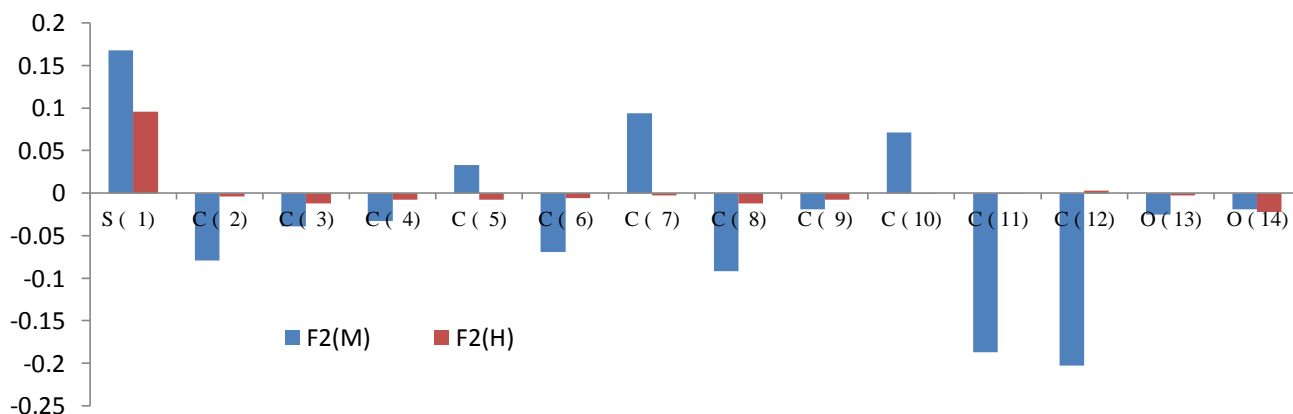


Fig 3. Graphical representation of second-order Fukui function of HTTD moiety

The reaction molecule's nucleophilicity and electrophilicity are defined by the Fukui second function, which makes use of the atoms in the molecule to determine both properties. Electrophilicity was 71% and nucleophilicity was 29% for Milliken in the molecule HTTD under study [1-4]. The outcome demonstrates that throughout the inhibition process, the molecule will receive electrons from the metal surface more frequently than it would donate to the metal surface.

### 3.3 Dynamic Simulation of Molecules

To evaluate the inhibitor's adsorption on the metal surface at the molecular level, molecular dynamic modeling was used. The low-energy of the molecule was determined using the forcite quench, which sampled a wide range of low-energy configurations. The inhibitor molecules' apparent adsorption on mild steel might be seen by

The Fukui functions shown in Table 2 indicate that the oxygen heteroatoms O(13) and O(14) will be in charge of the electron transport between the surfaces [13]. The fact that the oxygen atom will experience an electron transfer is the cause of the high oxygen values that Moiety found for both nucleophilic and electrophilic reactions [19].

simulating the interactions between the inhibitor and the surface of the Fe (111) and Al(110) crystal.

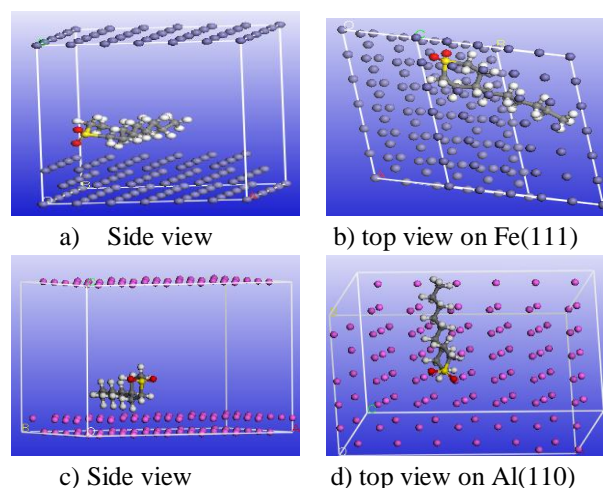


Fig 4. The snapshot of HTTD on Fe (111) and Al (110)

Table 3: Present adsorption energy obtained from the computational simulation of the molecules

Properties (kJ.mol <sup>-1</sup> ) HTTD	Fe	Al
Total Potential Energy	-171.432±0.0	-43.183±0.0
Energy of the Molecule	-64.239±0.0	-140.254±0.0
Energy of Fe (110)	0.000 ±0.0	0.000 ±0.0
Adsorption energy	-108.564±0.0	-43.183±0.0
Binding energy	108.564±0.0	43.183±0.0

### 3.4 Mechanism of inhibition.

The fact that both surfaces' adsorption energy values are negative demonstrates how possible and spontaneous the interaction of molecules with metal surfaces is. [9-12]. The molecule's binding energy was higher on the surface of iron and lower on surfaces of Aluminum. This suggests that the binding between the Aluminum surface and the molecule HTTD is less strong than it is with the iron surface, which is above 100 Kcal/mol. Surface adsorption reactions are referred to as physisorption when the amount of adsorption energy is larger than -100 Kcal/mol, and as chemisorption when it is less. [1-9]. The values of the Adsorption energies between the surfaces in the simulated reaction results of the inhibitor molecule on both the Al (110) and Fe (111) investigated were -43.1830.0 Kcal/mol for Al and -108.5640.0 Kcal/mol for Fe. For an adsorption energy value to be more than -100 Kcal/mol (the threshold value), Belghi et al. and Nyijime et al. conclude in their respective studies that such an interaction between the molecule and the surface of the metal during corrosion inhibition is known as physisorption [6,9]. In this experiment, the Aluminum surface had a greater contact with the molecule than the iron metal surface. [12,21-23]. According to the data, the physically attached HTTD

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molecule only slightly inhibited the Aluminum surface while iron inhibition efficiency underwent chemical adsorption, as shown by the Fukui energy parameters.

## 4. Conclusion

Based on the investigation, the DFT quantum chemical method was used to explore the molecule HTTD in order to determine how well it may inhibit Fe (111) and Al (110) surfaces. According to the obtained Binding and Adsorption energies of the inhibition process, Fe surfaces' inhibition process was more chemisorption-based, and Al surfaces' inhibition process was a physical mechanism. The inhibition process was driven by the transfer of electrons between the metal crystal surface and the molecule, as shown by the number of electron transfer ( $\Delta N$ ) values for Iron and Aluminium. The Fukui value of the molecule indicates that its adsorptive power on surfaces was through hetero-atoms of the functional groups based on the Fukui values, which shows significant potential. The molecule will be more welcoming, according to the second Fukui function, which aids in understanding. It receives electrons before donating its own to the crystal surfaces based on the larger per cent of the negative graph shown in figure 2.

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## Conflict of Interest

The authors declare that they have no conflict of interest

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