# Computational study of 4-cyclohexylimidazolidin-2-one as a potential corrosion inhibitor for Sn (111) surface

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# Computational study of 4-cyclohexylimidazolidin-2-one as a potential corrosion inhibitor for Sn (111) surface

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***Abstract***— Tin is a metal that is extensively used in various human endeavors. Therefore, its deterioration is not surprising. Researchers from all over the world have been working to halt this unwanted corrosive process. This study looked at the effects of density functional theory (DFT) on the corrosion inhibitor's molecular ability, including energy gap, energy of highest occupied molecular orbital, and energy of lowest unoccupied molecular orbital. It also looked at chemical reactions, including total hardness, softness, electronegativity, and the electron fraction transition from the anti-corrosion molecule to the tin atom. It looked at how 4-cyclohexylimidazolidin-2-one might help stop corrosion on the Sn (111) surface. We calculated surface interactions between the inhibitor molecules and the tin surface using Monte Carlo simulation. The outcome demonstrated the inhibitor's robust interactions with the Sn (111) surface. These results provide a foundation for the development of environmentally friendly corrosion inhibitors for the tin surface.

**Keywords—** Electronegativity, Tin, Suppression, Differential Adsorption, Anti-Corrosion.

## I. INTRODUCTION

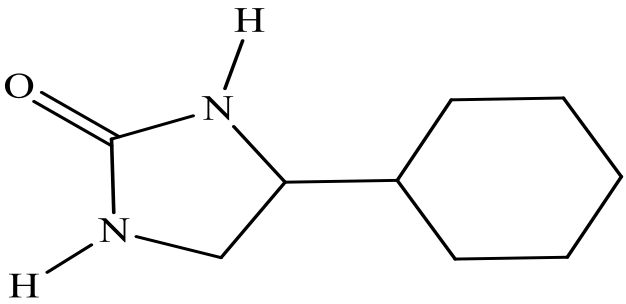
The lightweight, strength, electrical and thermal conductivity, heat and light reflection, and non-toxic and sanitary properties of tin and its alloys make them valuable for a wide range of engineering applications. When exposed to moisture, tin becomes nonreactive because a stable oxide deposit forms on its surface, despite being a reactive metal according to the electrochemical series (Eo = −0.14 V). Aqueous acids dissolve tin and release hydrogen gas throughout the process; pure water does not destroy tin [1]. Acid solutions typically accompany pickling tin alloys for electrochemical and chemical etching processes, which often result in substantial dissolution. Acid solutions are. Most industries use acid solutions to remove unwanted and undesired scaling. Industries use solutions of sulphuric and hydrochloric acids for general cleaning procedures [2] [3] inhibitors control the dissolution of metals and the absorption of acids [4]. We can employ inorganic or organic compounds that adsorb on a metallic surface and isolate it from its surroundings to inhibit corrosion [5]. Conjugated double bonds with distinct aromatic systems and heterocyclic compounds containing polar functional groups (N, S, O, and P) are among the organic molecules used as corrosion inhibitors in acidic conditions. The compounds in question are classified as adsorbateWe classify these compounds as adsorbates, active both chemically and physically [6][7]. We need to address this significant issue for safety, environmental, and financial reasons in a variety of chemical, mechanical, metallurgical, biochemical, and medical engineering applications [8][9][10]. als, and fluid combinations for production are among the strategies that can prevent corrosion attacks [11]. The most effective strategy for preventing the catastrophic degradation of metals and alloys in corrosive conditions among these techniques is to adopt corrosion inhibition. Corrosion inhibitor is one of the most practical and affordable ways to manage corrosive attacks on metals [12]. When introduced to an environment in modest quantities, corrosion inhibitors (synthetic or natural) decrease the pace at which the environment attacks metals. A lot of researchers have looked at tin corrosion in acidic so many researchers have examined the corrosion of tin in acidic solutions [13][14][15][16] hods are increasingly being used in corrosion inhibition research due to their potential to aid in the design of novel compounds with superior corrosion inhibition characteristics. Synthesise those by testing several compounds and synthesizing those that show great promise for corrosion inhibition, Researchers are increasingly using density functional theory (DFT) and Monte Carlo (MC) techniques to predict the inhibitory potential of compounds for corrosion on geometrical, electrical, and binding property bases on metal surfaces.

A growing number of corrosion studies have included extensive Monte Carlo simulations and quantum chemical calculations [17][18][19]. These computations typically investigate the relationship between the characteristics of the inhibitor molecules and their corrosion inhibition efficiency. [20] highlighted in their comprehensive review the application of quantum chemistry techniques to corrosion inhibitor investigations of several organic compounds. [21] investigated novel supramolecular (SCPs) compounds such as {[Ni (EIN)4(NCS)2]} SCP1 and {[Co (EIN)4(NCS)2]} SCP2 as corrosion inhibitors for stainless steel in a chloride environment using the B3LYP/6-31G DFT. The calculated values of quantum chemical parameters, such as EHOMO, ELUMO, energy gap (ΔE), dipole moment, electronegativity (χ), electron affinity (A), global hardness (n), softness (σ), ionisation potential (IP), fraction of ionizationd electrons (ΔN), global electrophilicity (w), and energy total (Etot), were correlated with their experimental results. [22] presented two different Using the 6-31GDFT method, [22] studied two

different isomeric forms of tetrazole molecules and their derivatives, including 1H and 2H tautomers, as corrosion inhibitors in two configurations: parallel and perpendicular to the Cu (1 1 1) surface. hardness (η), electronegativity (χ), and electron fraction transitions from the anti-corrosion molecule to the copper atom (ΔN) were calculated, and the IE was associated with. We calculated the Mulliken partial charges, EHOMO, EHOMO, ΔE, total hardness (·), electronegativity (χ), and electron fraction transitions from the anti-corrosion molecule to the copper atom [23] used the B3LYP/6-311G basis set to look into how well the old drugs 6-mercaptopurine (MP) and 6-thioguanine (TG) could stop corrosion on the surface of aluminium (Al) (111). ted for each of the expired drugs, both in the liquid and gas phases, of which results show no significant difference in the structures of the expired drugs. [24] theoretically explored the interactions Using the B3LYP/6-311G (d, p) method, [24 ] looked into how certain thiosemicarbazide derivatives interact with surfaces of Al (111) and Cu (111). [25] considered the electrostatic potential (ESP) surface analysis to identify the reactive areas and determined Fukui indices for N+1 and N-1 electron species at the geometry of the selected thiosemic. Their results showed that the ΔE, ELUMO, χ, η, EHOMO, σ, and ΔN localization and the condensed Fukui function (f- and f+) analysis in the reactive region were instrumental in characterizing organic adsorbates.

[26] conducted a study using MC simulations to investigate the adsorption behavior of an amino acid-based corrosion inhibitor on a steel surface. The simulations' insights into the coverage, orientation, and interactions of the inhibitor molecules aided in understanding the inhibition mechanism. [27] investigated whether the Monte Carlo simulation could replicate the real environment conditions of corrosion inhibition in the solution phase. The corrosion inhibition efficiency of phthalimide derivatives was PP-$OCH_3$ > PP-$CH_3$ > PP-H > PP-Cl > PP-$NO_2$. The theoretical study was consistent with previously reported experimental results.

[18] used molecular dynamics simulations and Monte Carlo (MC) simulations to investigate the surface interactions between the inhibitor molecules and the metal surface. As a result, they discovered that the inhibitor pyrazolylnucleosides strongly interacts with the Cu (111) surface, making it very good at stopping copper corrosion. Quantum chemical simulations were used in this study to look at how the structure of 4-cyclohexylimidazolidin-2-one affects its ability to stop corrosion. We then used Monte Carlo (MC) techniques to simulate the compound's adsorption process on the Sn (111) surface.




4-cyclohexylimidazolidin-2-one

Fig. 1. Chemical structure of
4-cyclohexylimidazolidin-2-one utilized as inhibitor

## II. METHODOLOGY/COMPUTATIONAL DETAILS

### *A. Quantum Chemical Calculations*

There was full equilibrium in the molecular structures of the 4-cyclohexylimidazolidin-2-one compound in water with the help of the hybrid function of B3LYP (Becke three-parameters Lee, Yang, and Parr) and basis sets 6-311G+ (d.p.) as triple basis functions in Gaussian 09W software. To begin with, the study looks at the theoretical parameters of electronic inhibitors, including their energy band gap (ΔE), fraction of electron transfer (ΔN), electron affinity (A), ionisation potential (I), electronegativity (χ), hardness (η), and softness (π). This analysis also includes the frontier molecular orbitals (ELUMO and EHOMO). By applying the relations listed below [28] [29] [30] one can determine the computational parameters based on the values of EHOMO and ELUMO.

$$\text{Electron affinity (A)} = E_{LUMO} \quad (1)$$

$$\text{Ionization Potential (I)} = E_{HOMO} \quad (2)$$

$$\text{Energy gap } (\Delta E) = E_{LUMO} - E_{HOMO} \quad (3)$$

$$\text{Chemical hardness } (\eta) = \left(\frac{\delta^2 E}{\delta N^2}\right)_v = \left(\frac{\delta \mu}{\delta N}\right)_v = \frac{E_{LUMO} - E_{HOMO}}{2} \quad (4)$$

$$\text{Global softness } (\sigma) = 2\left(\frac{\delta N}{\delta \mu}\right)_{v(r)} = \frac{1}{\eta} = \frac{2}{\Delta E E_{LUMO} - E_{HOMO}} \quad (5)$$

$$\text{Global electronegativity } (\chi) = \frac{-(E_{HOMO} + E_{LUMO})}{2} \quad (6)$$

$$\text{Fractions of electrons transferred } (\Delta N) = \frac{(\chi_{Sn} - \chi_{inh})}{2 \times (\eta_{Sn} - \eta_{inh})} \quad (7)$$

Where, $\chi_{Sn}$ = 4.42 eV and $\chi_{inh}$ = absolute electronegativities of the tin and inhibitor respectively. $\eta_{Sn}$ = 0 eV and $\eta_{inh}$ = absolute hardness of the tin and inhibitor respectively.

*B. Monte-Carlo (MC) Simulations*

The BIOVIA material Studio 2020 program was used to determine the best location for the 4-cyclohexylimidazolidin-2-one inhibitor on the surface of Sn (111). The literature suggests that the Sn (111) crystal surface used in this simulation is at its most stable [24]. Initially, the geometrical optimization of the inhibitor molecule and water was done using the estimating module. Force field and compass stimulation were applied to 4-cyclohexylimidazolidin-2-one on an optimal Sn (111) surface. The Monte-Carlo technique was used to search the substrate-adsorbate system configuration space to find low-energy adsorption sites [31].

## III. Results & Discussion

*A. Quantum Chemical Calculations*

The EHOMO and ELUMO orbitals are two descriptors that help explain corrosion inhibition efficiency. DFT is one of the most helpful techniques for analyzing inhibitor/surface interactions. The effectiveness of inhibitors to stop corrosion grows as the energy gap between the LUMO and HOMO orbitals narrows [32]. Table 1 result the 4-cyclohexylimidazolidin-2-one inhibitor has a low ELUMO (-0.0312 eV) and a high EHOMO (-0.259 eV) as shown in Table 1. This means that it can bind to a metal surface by giving and taking electrons [33][27] says the 4-cyclohexylimidazolidin-2-one inhibitor, which exhibits modest energy gaps. These low energy gaps explain the efficiency of corrosion prevention between the inhibitor and the tin metal, as well as the ability of electron-hole transit [21]. The corrosion inhibition interactions could also be discussed using electronic indices like χ, η, N, σ, and ω. The tin surface. According to [34] [24] [22] and others, the surface of tin is very reactive with inhibitors that are strong at attracting electrons, nucleophile Table 1 shows that the 4-cyclohexylimidazolidin-2-one inhibitor has a higher electronegativity (0.145) and a higher global softness (8.814), which suggests that it might be able to stop tin from corroding. The inhibitor resists charge transfer with high global hardness and electrophilicity values. The results of ESP demonstrated the inhibitor's S and N atoms' strong nucleophilicity [35].

Table 1. Quantum parameters for the studied 4-cyclohexylimidazolidin-2-one compound

| Parameter | $E_{LUMO}$ | $E_{HOMO}$ | $M$ | $\Delta E$ | $\eta$ | $\sigma$ | $\chi$ | $\Delta N_{Sn}$ |
|---|---|---|---|---|---|---|---|---|
| 4-cyclohexylimidazolidin-2-one | -0.0312 | -0.259 | 4.589 | 0.227 | 0.114 | 8.814 | 0.145 | -18.82 |

*B. Monte-Carlo (MC) Simulations*

The most reliable adsorption configurations of a 4-cyclohexylimidazolidin-2-one can be calculated effectively using MC modeling. Figure 3 displays the simulation results for the 4-cyclohexylimidazolidin-2-one under examination, while Table 2 provides further details. Figure 3 displays the most advantageous configuration of the adsorbed molecule on the tin (111) metal surface. Additionally, the motive, which is abundant in electrons from inhibitory molecules, adsorbed the specified molecules onto the energy ratios (dEads/dNi) of the inhibitors show the interactions between the occupied orbitals of 4-cyclohexylimidazolidin-2-one and the vacant orbitals of tin (111). These are equal to the energies of substrate–adsorbate configurations where one of the adsorbate components (−2.823 kcal mol−1 of water) has been taken away [36] Table 2 compiles these values. Adsorption energy values that are more negative indicate a stronger and more stable bond between the adsorbed molecules and the metal. When two materials combine during the adsorption process, they bond a molecule, ion, or electron (referred to as the adsorbent) to the solid surface; this process is known as decreasing energy [13] [37] [38]. The higher adsorption energy of 4-cyclohexylimidazolidin-2-one on the hardened Sn surface, shown in Table 2, means that the 4-cyclohexylimidazolidin-2-one molecule sticks strongly to the surface, creating a layer that keeps the tin from breaking down. rom degradation. The results demonstrate how effective 4-cyclohexylimidazolidin-2-one was as a tin inhibitor.

Table 2. Results and descriptors measured by the Monte Carlo simulation for adsorption 4-cyclohexylimidazolidin-2-one molecules Sn (111) in kcal $mol^{-1}$

| Compound | dEad/dNi | Adsorption energy | Rigid adsorption energy | Deformation energy | Total energy |
|---|---|---|---|---|---|
| 4-cyclohexylimidazolidin-2-one | -47.816 | -34.163 | -53.789 | -40.136 | -87.952 |
| Water | -2.823 | -3.523 | -2.421 | -1.103 | -2.420 |

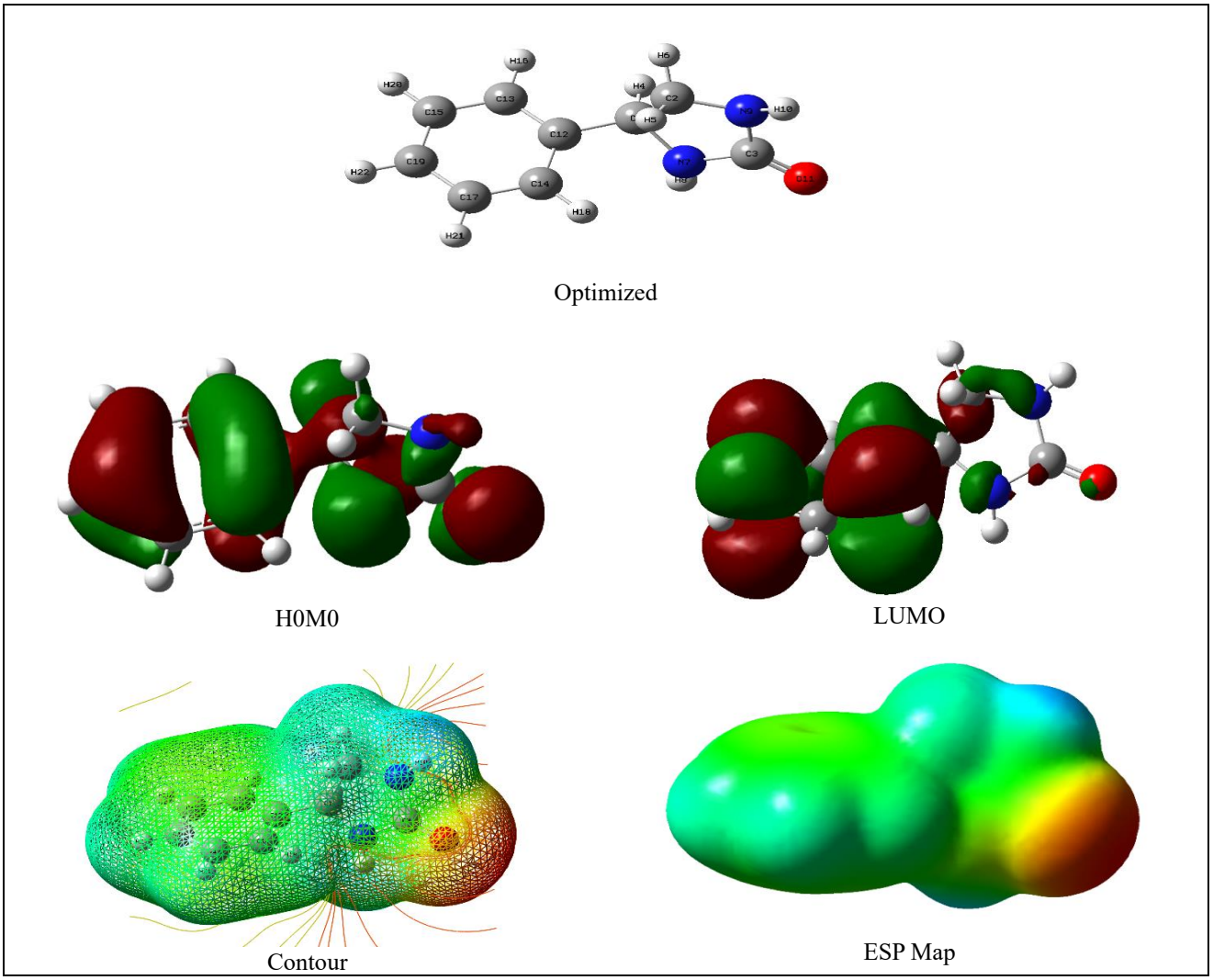



Fig. 2. The frontier molecular orbital density distribution for the investigated 4-cyclohexylimidazolidin-2-one (HOMO, LUMO, Contour, and ESP Map)

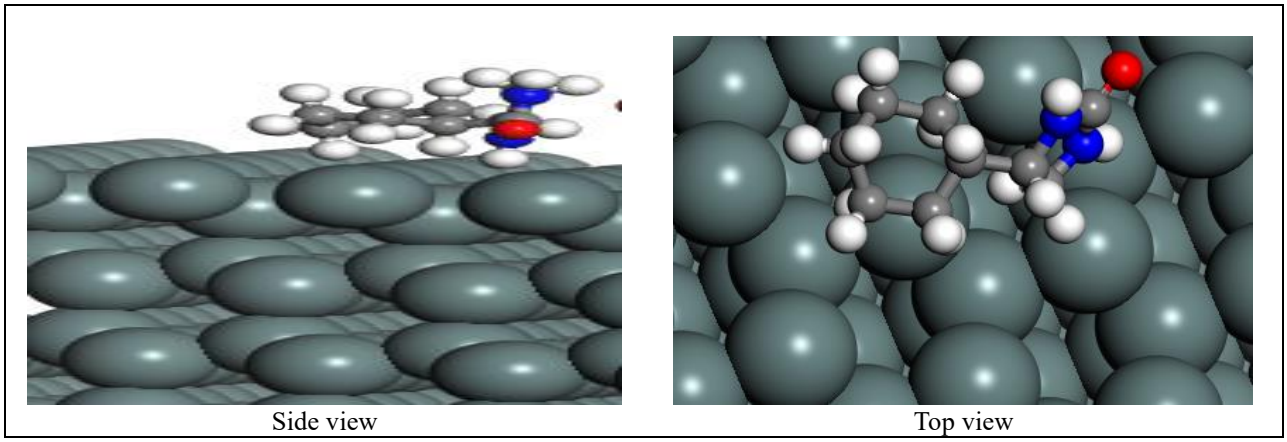



Fig. 3. The most appropriate conformation for adsorption of the 4-cyclohexylimidazolidin-2-one molecules on Sn (111)

## IV. Conclusion

At B3LYP, we assessed the corrosion inhibition activity of 4-cyclohexylimidazolidin-2-one at the molecular level using Monte Carlo simulation and density functional theory with various basis sets. The research project yielded the following findings. The frontier molecular orbital results revealed higher EHOMO values (i.e., less negative); 4-cyclohexylimidazolidin-2-one's electronegativity value is low, and it is more likely to react while acting as an electron donor. The ESP result demonstrated the compound's O and N atoms' strong nucleophilicity. According to MC simulations, the inhibitors flat-adsorb onto the metal surface with rather large adsorption energies. However, many organic compounds and their derivatives, as corrosion inhibitors, exhibited high activity between them and metal surfaces theoretically. Regrettably, there is a deficiency in experimental studies for certain promising corrosion inhibitors. We should expand the production of the 4-cyclohexylimidazolidin-2-one compound, which is based on corrosion inhibition on tin surfaces, to provide more experimental options for inhibition.

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