Computational Analysis of Aluminum Corrosion Inhibition Potentials Using SelectedThiosemicarbazide Derivatives

ABSTRACT

Aluminum, a metal with a rich cultural history, remains vital in numerous industrial applications. However, its susceptibility to corrosion in harsh environments poses significant challenges. Traditional corrosion inhibitors have been developed to counteract this issue, but they often come with drawbacks such as high costs and harmful environmental and health impacts.This study employed density functional theory (DFT) to evaluate the potential of two compounds—2-(4-methylbenzylidene)hydrazinecarbothioamide (MBHC) and N-phenylhydrazinecarbothioamide (PHC)—as corrosion inhibitors for aluminum surfaces. Electrostatic potential (ESP) analysis revealed that the sulphur and nitrogen atoms in these compounds exhibit nucleophilic behaviour, making them effective for corrosion inhibition.The research highlighted MBHC's superior performance over PHC in corrosion prevention. Molecular orbital theory and Monte Carlo simulations demonstrated that MBHC formed stronger and more stable complexes with the aluminum surface, as reflected in its higher adsorption energy of −461.73 eV compared to PHC's −163.43 eV.These findings pave the way for developing environmentally friendly inhibitors to protect aluminum surfaces, combining efficiency with sustainability.

Keywords:adsorption energy; DFT; Potentials; Aluminum; inhibitor; Simulation

1. INTRODUCTION

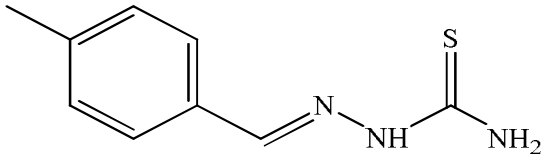
In the crust of the globe, aluminum is the third most frequent metal overall and the fourth most prevalent in the crust specifically. After iron, aluminum is typically regarded as the second most significant metal. It has unique mechanical characteristics because of its low density (2.7 g cm^{-3}), which is just about one-third that of mild steel. As a result, aluminum and its alloys offer a high strength-to-weight ratio. In addition, a wide range of metal machining processes can be readily applied to them, and they exhibit good electrical and thermal conductivity. Furthermore, aluminum and its alloys have been fully recycled and reused, meaning that the items made from recycled metal are similar to those that were made before recycling in terms of quality and attributes (Olufumilayo& Olakunle, 2021) Because of its excellent strength-to-weight ratio and affordable price, aluminum and its alloys are widely used in aerospace, automotive, electrical parts, building, packaging, and chemical industries (Rouniya& Shandilya, 2019; Becker, 2019; Emadi et al., 2019).. In non-aggressive conditions, an Al_2O_3 coating naturally forms on the alloy surface to preserve aluminum (Arrousse et al., 2022). Because of its numerous flaws and pores, the oxide layer is rapidly dissolved by corrosive OH^- or Cl^- ions. However, because key alloy components like copper and magnesium are present, aluminum and its alloys are highly susceptible to localized corrosion in harsh conditions. This alloy's microstructure is rather complicated, and several phases with different compositions have been found (Liu et al., 2017). Since an

oxide layer forms on aluminum and prevents the metal from oxidizing further, aluminum has a high level of corrosion resistance in both aqueous solutions and the environment. However, in some conditions, such as acidic media, aluminum becomes extremely prone to corrosion. There are already several efficient protection techniques available, including surface coatings, organic inhibitor addition, anodic oxidation protection, and plasma electrolytic oxidation protection (Gummanar et al., 2023; Markus, 2019; Yang et al., 2017). Inhibitors, which prevent corrosion on metal surfaces by forming a protective coating on them, are the most widely used and least expensive of them across a variety of industries. Products with an organic base are frequently used to prevent corrosion. Organic compounds with heteroatoms (N, S, and O) in a conjugated system exhibit excellent efficacy in preventing metal corrosion (Verma et al., 2016; Iroha &Akaranta, 2020; Nkem et al., 2021). The effectiveness of corrosion inhibition has been precisely established by experimental research, however, the precise mechanism by which inhibitors contribute most to corrosion inhibition has not been thoroughly addressed. Costs and time for research are significant. These issues are bridged by the theoretical study, which is now backed by sufficient hardware and software. The electron density of the molecule determines the corrosion inhibition efficiency, and theoretical research can determine this density with high accuracy. When evaluating corrosion inhibition in a molecule, theoretical research is just as important as actual research. Questions concerning experimental results based on the interactions of organic inhibitors with metal surfaces can be addressed using quantum chemical computations (Ebenso et al., 2021). Verma et al. (Verma et al., 2021) underlined in their thorough review the application of quantum chemistry techniques to corrosion inhibitor investigations of several organic compounds. Uzah, (2024)theoretically explored the interactions between selected thiosemicarbazide derivatives on Al (111) and Cu (111) surfaces by using the B3LYP/6-311G (d, p) method. The Electrostatic potential (ESP) surface analysis used to identify the reactive areas., was considered, and Fukui indices were determined for N+1 and N-1 electron species, at the geometry of the selected thiosemicarbazide derivatives reference N-electron. Their results showed that the ΔE, E_{LUMO}, χ, η, E_{HOMO}, σ, and ΔN localization and the condensed Fukui functions (f- and f+) analysis in the reactive region were instrumental in characterizing organic adsorbates.

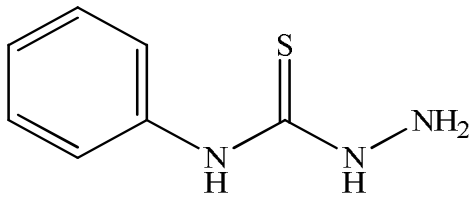
Ibrahim et al. (2023) investigated the potentiality of the 6-mercaptopurine (MP) and 6-thioguanine (TG) expired drugs toward the corrosion inhibition of the aluminum (Al) (111) surface, using the B3LYP/6-311G basis set. ΔE, E_{HOMO}, E_{LUMO}, μ, and η parameters were all calculated for each of the expired drugs, both in the liquid and gas phases, of which results show no significant difference in the structures of the expired drugs. Khabazi and Chermahini, (2023) presented Two different isomeric forms of tetrazole molecules and their derivatives, including 1H and 2H tautomers, as corrosion inhibitors were studied in two configurations, parallel and perpendicular to the Cu (1 1 1) surface, using the 6-31GDFT method. The Mulliken partial charges, E_{HOMO}, E_{HOMO}, ΔE, total 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 ΔE and the frontier orbital electron density. It wasobserved that tetrazole molecules were physically adsorbed onto the copper surface.

The performance of each inhibitor concerning its structure and orientation, as well as the mechanism by which an inhibitor clings to metal surfaces, may be fully explained by the use of the methods of density functional theory and Monte Carlo simulation (Sulaiman et al., 2019). Hadisaputra et al., (2022) investigated the real environment conditions of corrosion inhibition in the solution phase can be replicated by the Monte Carlo simulation. The corrosion inhibition efficiency of phthalimide derivatives was PP-OCH3 > PP-CH3 > PP-H > PP-Cl > PP-NO2. The theoretical study was consistent with previously reported experimental results.The surface interactions between the inhibitor molecules and the metal surface wereinvestigated by Oukhrib et al., (2021) using molecular dynamics simulations and Monte Carlo (MC) simulations. As a result, they found that the inhibitor pyrazolylnucleosides have

strong interactions with Cu (111) surface, and therefore have excellent predictive inhibition power against copper corrosion.Derivatives of thiosemicarbazide are widely used in medical chemistry to create medications that combat germs, fungi, viruses, depression, etc. Its primary biological functions are DNA doping transporter, anticancer, and DNA retaining capacity. No computational study has been published on the corrosion prevention of MBHC and PHC derivatives of Thiosemicarbazide on Aluminium Surfaces. However, some of these derivatives are said to be effective deterioration inhibitors for Aluminium in acidic media.The corrosion inhibition of MBHC and PHC (Fig.1): on Al (111) surfaces are studied in this work, along with the impacts of quantum parameters and the molecule's adsorption process.



(*E*)-2-(4-methylbenzylidene)hydrazinecarbothioamide (MBHC)



N-phenylhydrazinecarbothioamide (PHC)

Fig.1. The chemical structures of MBHC and PHC

2. COMPUTATIONAL DETAILS

2.1 DFT Study

Studies on corrosion inhibition commonly employ the density functional theory (DFT). When it comes to organic compounds' ability to suppress corrosion, the DFT approach provides an accurate description. Predicting the chemical properties of chemical species, such as the maximum occupied molecular orbital–lowest unoccupied molecular orbital (HOMO–LUMO), electron affinity (A), ionization potential (I), energy gap (ΔE), hardness (η), fraction of electrons transferred (ΔN), softness (σ), and electronegativity (χ), is the main goal of research on inhibitors. The following paper used theoretical calculations to anticipate the effectiveness of the Thiosemicarbazide derivatives E)-2-(4-methylbenzylidene)hydrazinecarbothioamide (MBHC) and N-phenylhydeazinecarbothioamide (PHC) (Fig.1). Employing the Gaussian 09W programming suite, the B3LYP technique coupled to 6-311G+ (d,p) basis sets were utilized to optimize all compounds geometrically. This approach is widely used in the research of organic corrosion inhibitors. Then, several relevant global and local variables of the molecule's electronic configuration were computed. The I, A, ΔE, ΔN, η, σ, χ, $E_{LUMO,}$ and E_{HOMO} as well as maps of electrostatic potential were also computed (Verma et al., 2021; Khabazi&Chermahini,2023).

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

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

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

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

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

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

$$\Delta N = \frac{(\chi_{Al} - \chi_{inh})}{2 \times (\eta_{Al} - \eta_{inh})} \quad (7)$$

Where, χ_{Al} = 4.26 eV and χ_{inh}= absolute electronegativities of the aluminum and inhibitor respectively.η_{Al} = 0 eVand η_{inh} = absolute hardness of the aluminum and inhibitor respectively.

2.2 Monte Carlo simulation.

The interactions between the chemical compounds and metal surface were theoretically studied by the Monte Carlo simulation The simulation was conducted in Material Studio 2020 (Biovia, USA) using COMPASS force-field (condensed phase), on the Al (111) surface (three dimensions to the slab model) under periodic boundary conditions. The energies and chemical adsorption mechanisms components were calculated using the Ewald and atom-based summations, or responsibly to the Adsorption Locator module, built-in Materials Studio 2020 which used Monte Carlo simulations to pinpoint the most stable arrangement of the adsorbates on the Al (111) surface is the most stable of the many aluminum surfaces (Bourzi et al., 2020; Uzah, & Mbonu, 2023),

3. RESULTS AND DISCUSSION

3.1. DFT Results

Table 1 is a list of the calculated quantum chemical parameters. Given structures that are optimized HOMO and LUMO density distribution of PHC and MBHC, Fig.2 shows that PHC has fewer adsorption centers than MBHC, indicating that MBHC has a higher capacity for high-protective adsorption. As a result, the high E_{HOMO} energy increases the inhibition performance by reflecting a greater connection between the molecule and the metal surface through the donor-acceptor process. (Guo et al., 2017;Hadisaputra et al., 2022). MBHC can readily interchange electrons with the iron surface, as evidenced by its higher E_{HOMO} value of −0.218 eV compared to PHC's −0.210 eV. On the other hand, the fact that MBHC has a lower E_{LUMO} value indicates that it is an excellent inhibitor of electron acceptance and supports its superior performance (−0.018 eV) over PHC (−0.042 eV) (Khabazi&Chermahini,2023; Uzah& Mbonu, 2024). Better adsorption on aluminum surfaces is indicated by the narrower energy gap (ΔE) of MBHC (0.1493 eV) (Fouda et al., 2023). Further quantum chemical characteristics were derived, including ionization potential (I = $-E_{HOMO}$), electron affinity (A = $-E_{LUMO}$), global softness (σ), global hardness (η), electronegativity (χ), and number of electron transfer (ΔN). The literature claims that a molecule with a high (η) value is less reactive, whereas a high (χ) value indicates that the molecule may find it difficult to transfer its electrons to an acceptor (Kaya & Kaya, 2015; Uzah et al., 2023). The findings in Table 1 demonstrate that MBHC has lower (η) and (χ) values than PHC, indicating that it is more reactive and can transfer electrons through donor-acceptor interactions with metal molecules. (Uzah,2024). Within a group of inhibitors, the electron donation tendency is described by the charge transfer rate ΔN. According to Lukovits ((Jabri et al., 2022; Uzah et al., 2023), the efficiency of the inhibition increases as the electron donor capacity at the steel/electrolyte increases if ΔN < 3.6. Table 1 displayed ΔN values are all 3.6 lower than the original values. Therefore, the quantum chemical characteristics of MBHC performed better at its level of inhibition than the PHC inhibitor.

Inhibitor	MBHC	PHC

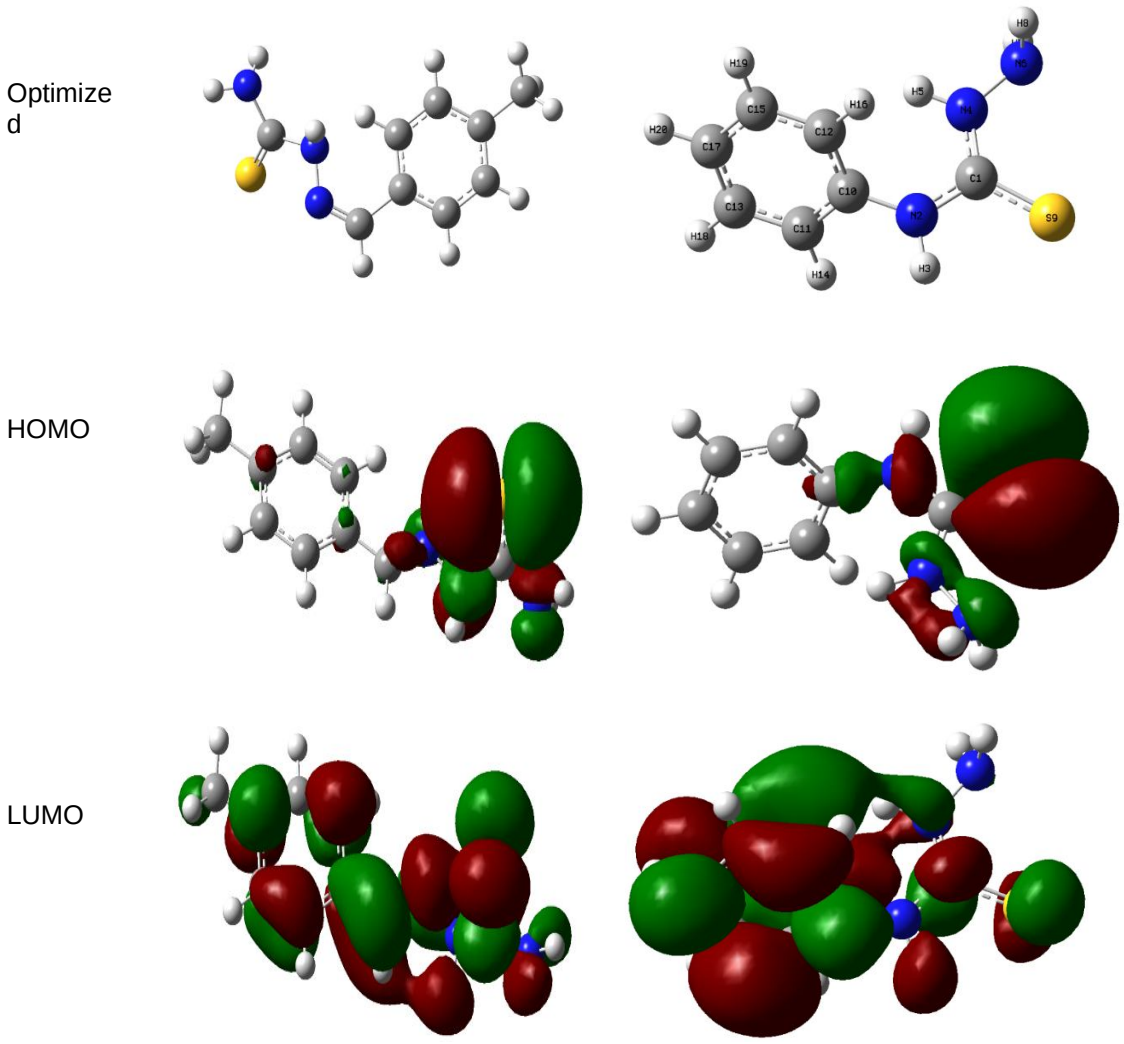


Fig.2. The frontier molecular orbital density distribution for MBHC and PHC investigated compounds (Optimized, HOMO, and LUMO).

Table 1. The quantum chemical variables for MBHC and PHC inhibitors using the B3LYP/6-31G+ (d, p) basis set.

C	E_{LUMO}	E_{HOMO}	ΔE	H	Σ	X	ΔN_{Al}
MBHC	-0.0180	-0.2178	0.1493	0.0747	13.40	0.143	-20.66
PHC	-0.0422	-0.2095	0.1673	0.0837	11.95	0.0948	-18.54

3.2 Electrostatic Potential (ESP) Map

ESP map displays the three-dimensional charge distribution of the molecule (Fig.3). This map aids in the visualization of the molecule's variable charge areas, which helps forecast electrophilic and nucleophilic molecule-attack scenarios (Thakur & Kumar, 2023). The

highest positive region vulnerable to nucleophile assault is shown as blue in the ESP plot. On the other hand, the negative region that is vulnerable to electrophilic attack is shown in red. The MBHC and PHC sulfur and nitrogen atoms are found to have the highest electron density. Consequently, it is expected that these atoms will actively participate in the adsorption process on the Aluminum surface.

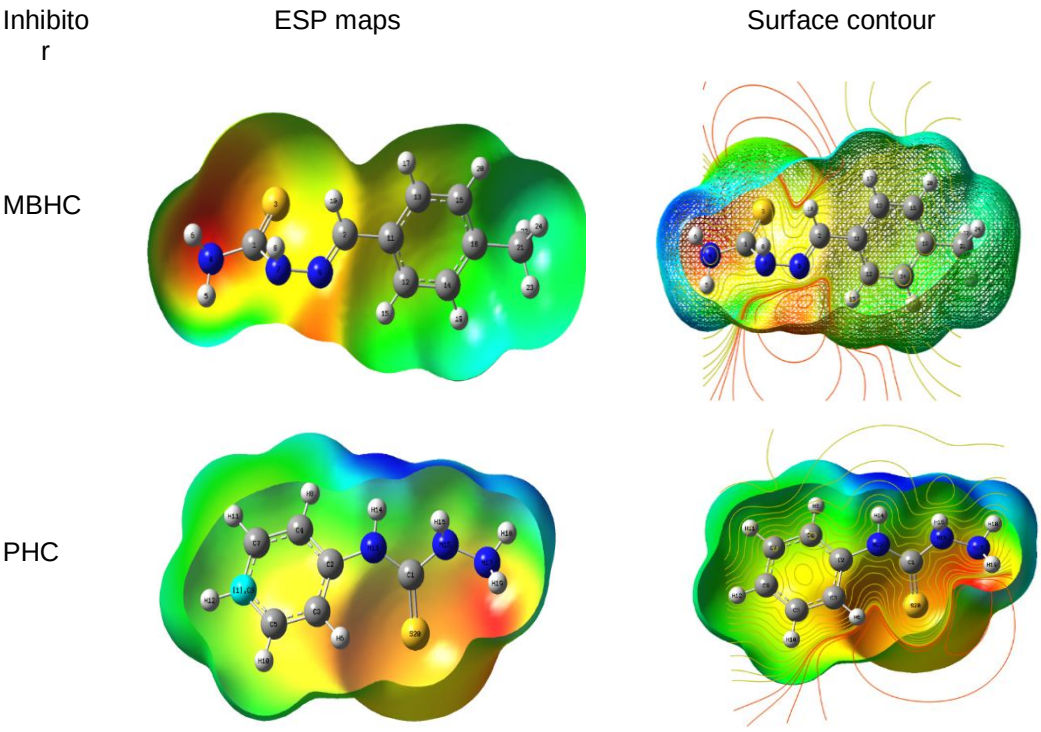


Fig.3. ESP maps and surface contours illustration of the MBHC and PHC investigated

3.3 Monte Carlo simulation.

To reduce the amount of contact area between the metal surface and corrosion-causing materials (such as water, acidic, or alkaline media), molecules need to align their structures as closely as possible in parallel to the metal surface. Adsorption is the term for this process. Therefore, Monte Carlo simulation was applied to determine and identify the inhibitors under evaluation and their ability to adsorb onto the surface of Al (111). Fig.4 shows the optimal MBHC and PHC adsorption mode on the aluminum surface under study.

Table 2 displays the molecule under investigation's adsorption characteristics, which include total energy, rigid adsorption energy, adsorption energy, and deformation energy. We have previously defined these parameters (Bourzi et al., 2020; Uzah, 2025). in our previous work. The total rigid adsorption energy before and after an adsorbate's surface relaxation is known as the "adsorption energy," and it is the most significant energy characteristic in adsorption. Table 2 indicates that the inhibitor attaches to the surface of Al (111) spontaneously based on the negative value of the adsorption energies (Uzah, & Mbonu, 2023). The differential

adsorption energy (dE_{ad}/dN_i), which is the energy needed or released to remove a portion of the adsorbate (i.e., desorption energy), is defined by assuming that the surface energy of Al is zero. The inhibitor's adsorption energy of -461.73 kcal mol^{-1} for MBHC and 163.43 kcal mol^{-1} for PHC and its desorption energy of --461.73 kcal mol^{-1} (MBHC) and –80.754 kcal mol^{-1} (PHC) indicate that the adsorption process is substantially preferred. The inhibitor preferentially adsorbs on the Al (111) surface with little to no competition because it adsorbs with significantly less energy, even in the presence of water (--4.28 kcal mol^{-1}) (Benzidia et al., 2022; Uzah, 2025).

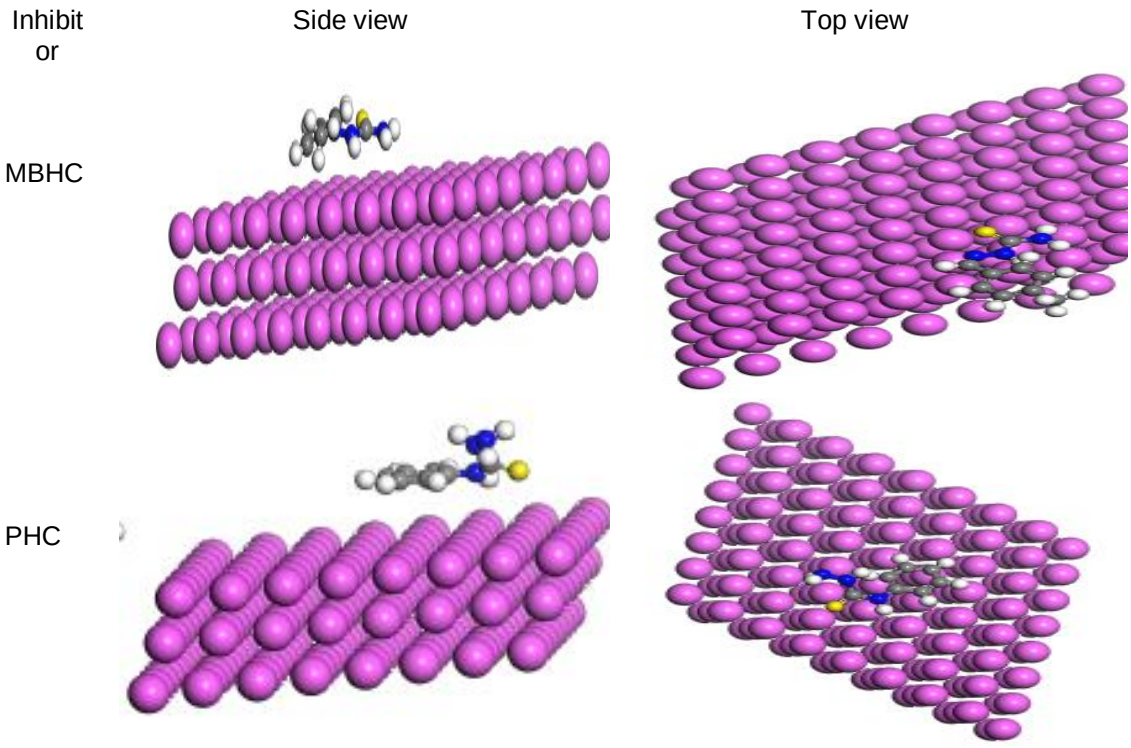


Fig.4.The most appropriate conformation for adsorption of the MBHC and PHC molecules on Al (111)

Table 2. Results and descriptors measured by the Monte Carlo simulation for adsorption of MBHC and PHC molecules on Al (111)

Compound	dEad/dNi	Adsorption energy	Rigid adsorption energy	Deformation energy	Total energy
MBHC	-461.73	-461.73	-30.707	-431.02	-3.272
PHC	-80.75	-163.43	-55.83	-107.61	-5.75
Water	-4.281	-8.297	-7.346	-0.950	-7.346

4. CONCLUSION

The corrosion inhibition potential of E)-2-(4-methylbenzylidene)hydrazinecarbothioamide (MBHC) and N-phenylhydeazinecarbothioamide (PHC) was analyzed and measured using density functional theory calculations employing the B3LYP/6-31G+ (d,p) basis set. This was done to determine whether these compounds had a potentially strong ability to inhibit corrosion in aluminum and its alloys. In contrast to PHC, MBHC has a lower electronegativity and ΔE, (0.1612 eV) values, which may be attributed to the presence of an aromatic ring and heteroatom in its structure, which demonstrated a stronger and mutual connection between the inhibitor and the metallic surface according to the results of the Density Functional Theory analysis: Furthermore, the results showed that MBHC had the largest ΔN value (0.258232 eV), indicating improved chemical stability and reactivity. In light of this, MBHC is more likely than PHC to react as an electron donor.de, which effectively inhibits the corrosion of alloys including aluminum. MBHC was predicted by Monte Carlo simulations to function as a more potent anti-corrosion agent than PHC, particularly in acidic environments.

DISCLAIMER (ARTIFICIAL INTELLIGENCE)

Authors hereby declare that NO generative AI technologies such as Large Language Models (ChatGPT, COPILOT, etc.) and text-to-image generators have been used during the writing or editing of this manuscript.

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COMPETING INTERESTS

Competing interests The authors declare no conflict of interest.

AUTHORS' CONTRIBUTIONS

The manuscript was written with contributions from all authors. All authors read andapproved the final manuscript

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