
COMPUTATIONAL INVESTIGATION OF ACTIVE PALM OIL COMPONENTS AS ECO-FRIENDLY CORROSION INHIBITORS FOR COPPER METAL

Usman Sani^{1,*}, Abdulazeez Abdulateefa², Amaram Jonah Adams², Toyese Oyegoke²

¹Kaduna Polytechnic

²Ahmadu Bello University Zaria

Email: usb934@gmail.com*, abdulazeezabdulateef001@gmail.com, jonahamaram@gmail.com,
Oyegoketoyese@gmail.com

*Corresponding author: Usman Sani

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ABSTRACT

This study investigates the corrosion inhibition potential of selected palm oil constituents using Spartan24 by PM6 Methods in a aqueous medium and a convergence criterion of $1E-5$ a.u. with SCFCYCLE of 99000. The constituents considered includes: myristic, linoleic, stearic, oleic, lauric, and palmitic acids on copper exposed to corrosive compound typically found in industrial environments. Quantum chemical parameters, including total electronic energy (E), highest occupied molecular orbital energy (E -HOMO), lowest unoccupied molecular orbital energy (E -LUMO), energy band gap (E_{gap}), and interaction energy gap (IEG), were evaluated to understand the reactivity and inhibition efficiency of these compounds and were compared with that of styrene an active corrosion protection component of paint. Among the analysed compounds, Linoleic acid demonstrates the highest inhibition capability for copper corrosion protection caused by aggressive species like H_2SO_4 , HCl , HNO_3 , and $NaCl$. Its superior electronic properties: high HOMO (9.66 eV), low E_{gap} (9.53eV), low IEG (6.41eV) values and molecular structure make it an excellent candidate for corrosion protection applications. These findings suggest that linoleic acid could serve as an efficient, eco-friendly inhibitor in copper corrosion prevention

Keywords: Corrosion; Inhibitors; HOMO-LUMO; E_{gap} ; Corrosion Inhibition

1. INTRODUCTION

Metal Corrosion is one major problem worldwide especially where corrosive environments are employed in practically every industry, Building, petroleum and gas processing, marine and steel processing industries. It is defined as the destructive and unintentional attack of metals caused by a chemical and/or electrochemical reaction with the environment, and it usually refers to the metal's electrochemical oxidation (Kadhim *et al.*, 2021).

Corrosion of metal can be slowed or prevented using a variety of techniques. Organic molecules, plastics, and polymers are often utilized as protective coatings on metals, as are cathodic and/or anodic protection using inhibitors, material modification, and environmental alteration. A number of limitations, on the other hand, restrict the potential uses of currently available methods (Faraj and Alamiery 2022). Over the years, a lot of corrosion inhibitors have been developed but the commercially viable and widely applied inhibitors are toxic to man and his environment. At present a lot of efforts are being geared towards sustainable ecofriendly (green) alternatives to these toxic chromate industrial inhibitors (Alexander *et al.*, 2024). About 2.5 trillion on a global scale is spent annually on corrosion and corrosion-related problems. This huge economic loss is estimated at 3.4 % of global GDP (Ogunleye *et al.*, 2021; Speight, 2014; Kobzar and Fatyeyeva, 2021; Verma *et al.*, 2019; Feng *et al.*, 2018).

Palm oil is an edible, abundant, and environmentally friendly natural product. It is also one of the most widely used and discovered natural oils in Asian countries such as Malaysia. Palm oil has distinct properties, such as a similar content of both saturated and unsaturated fatty acids (50:50) The unsaturated fatty acids are subjected to a variety of reactions with several compounds to produce a diverse variety of products (Wasmi *et al.*, 2015). Palmitic acid being the primary saturated fatty acid and oleic acid being the primary unsaturated fatty acid. The use of palm oil for purposes other

than food is of particular interest because it has the highest fossil energy balance and the lowest production cost when compared to other commodities. Because both oleic and palmitic acids contain carbonyl groups, palm oil has the potential to act as a corrosion inhibitor (Calderon et al., 2017). Palm oil can be used as an environmentally friendly corrosion inhibitor instead of conventional methods. Most of the palm oil derivatives had corrosion prevention efficiencies of 80–90% (Faraj and Alamiery 2022). The aim of this work is to investigate the active component in the palm oil and their potential for corrosion inhibition of copper metal in different corrosive environment Using computational approach.

2. COMPUTATIONAL METHODOLOGY

Figure 1 showed the workflow of this research, where the molecular structures of the copper cluster, corrosive, and fatty acids from palm oil were first constructed in the spartan modelling environment. The initial molecular structure was then adjusted to reduce its potential energy. The energy minimization step removes unrealistic atomic positions and provides a stable structure that can be used for subsequent calculations. In the molecular interaction step, molecular species were brought together to investigate their interactions. This involve placing the molecule on an expected active site on the copper cluster to study the adsorption and interaction behaviour. The atomic positions, bond lengths, and bond angles were systematically adjusted until the structure reaches a stable minimum-energy configuration in the geometrical interaction step. This provides the optimized geometry of the molecular system. Following geometry optimization, electronic properties are calculated to understand the chemical behaviour of the system. These include HOMO, LUMO energy gap, Interaction energy gap (IEG) and electrostatic potential. Detail of formula used to calculate these properties would be provided on request.

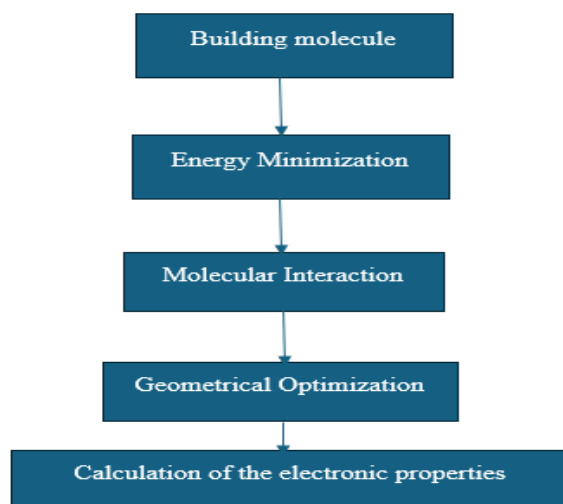


Figure 1: Block flow diagram of the computational study

2.1 Computational Tool and Software

SPARTAN24, a computer Software package for molecular simulation, designed and developed by Wavefunction Inc. USA, was used for the modelling, simulation and all the computational calculations were done on HP ProBook 650 G2, RAM 8G, 2.40GHz and i3-7100U CPU

All geometrical optimizations and energy calculation were conducted using PM6 method in an aqueous medium and a convergence criterion of 1E-5 a.u. with SCFCYCLE of 99000, GEOMETRYCYCLE of 99000 and SCFTOLERANCE of 5.

3. RESULT AND DISCUSSION

The selection of an appropriate metal cluster is fundamental in computational investigations because the electronic characteristics of the cluster strongly influence adsorption behaviour and the predicted corrosion inhibition performance. Previous computational studies have demonstrated that square-shaped copper clusters possess greater thermodynamic stability than pyramid-shaped clusters owing to their lower electronic energy and wider HOMO–LUMO energy gap (Oyegoke et al., 2023). Consequently, the square Cu_4 cluster was adopted in this study as the representative copper surface model and the cluster was as shown in figure 2.

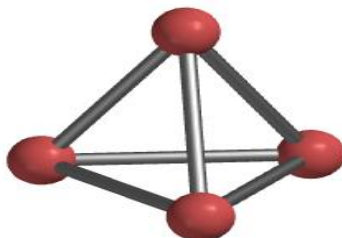


Figure 2: Most stable cluster model for the copper metal

An optimized molecular structure of potential palm oil corrosion inhibition constituents and that of styrene were shown in Figure 3.

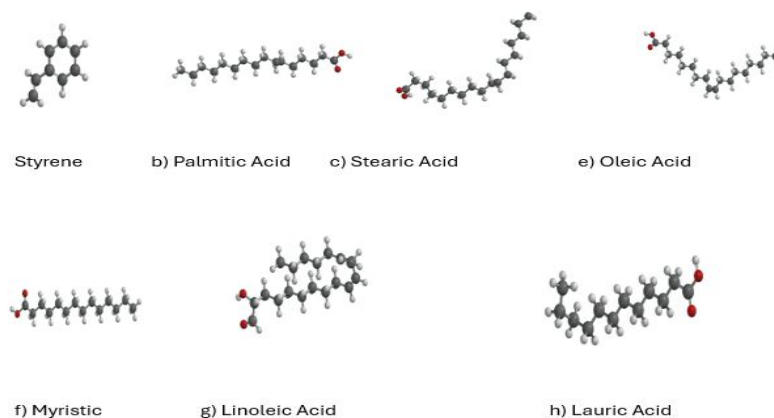


Figure 3: Optimized Molecular Structures of styrene and Palm oil constituent

Table 2 shows the list of the corrosive species for copper and their molecular descriptors. Similar properties were presented in Table 3 for the corrosion inhibitors.

Quantum chemical parameters such HOMO, LUMO, HOMO–LUMO energy gap (E_{gap}) and interaction energy gap (IEG) are widely recognized as reliable indicators for predicting molecular reactivity and adsorption characteristics during corrosion processes (Gece, 2008; Kaya et al., 2016).

The Cu_4 cluster exhibited a HOMO–LUMO energy gap of **9.28 eV**, confirming its electronic stability throughout the adsorption calculations. Among the aggressive media investigated, sulfuric acid and nitric acid exhibited the lowest interaction energy gaps ($\text{IEG} = 5.52$ and 5.29 eV, respectively), indicating stronger electronic interactions with the copper surface than water, hydrochloric acid and sodium chloride. These observations agree with established corrosion theory, where mineral acids readily destabilize the passive oxide film on copper through proton-assisted oxidation reactions, thereby accelerating metal dissolution (Bentiss et al., 2005).

The relatively large HOMO–LUMO gaps observed for water and hydrochloric acid indicate comparatively lower intrinsic electronic reactivity than sulfuric and nitric acid.

Table 2: Molecular properties of copper and the corrosive species

COMPOUND	Formula	E _{gap}	IEG
Copper Cluster	Cu ₄	9.28	9.28
Water	H ₂ O	15.98	10.61
Sulfuric acid	H ₂ O ₄ S	11.57	5.52
Sodium chloride	NaCl	9.77	6.84
Hydrogen chloride	HCl	13.68	8.63
Nitric acid	HNO ₃	11.30	5.29

The electronic descriptors of the selected palm oil constituents are presented in Table 3. Among all the investigated compounds, linoleic acid exhibited the smallest HOMO–LUMO energy gap (9.53 eV), indicating the highest molecular reactivity and the greatest tendency to participate in charge-transfer interactions with the copper surface. A lower energy gap generally facilitates electron excitation, enhances molecular polarizability and promotes stronger adsorption on metallic substrates (Gece, 2008). The slightly lower E_{gap} of linoleic acid (9.53 eV), compared with H₂O₄S (11.57eV), NaCl (9.77eV), HCl (13.68eV) and HNO₃ (11.30eV), indicates that its frontier molecular orbitals are separated by a smaller energy difference, suggesting that electron excitation or electron transfer may occur relatively more readily

Linoleic acid, also known as *cis*, *cis*-9,12-octadecadienoic acid, is a polyunsaturated fatty acid with the molecular formula C₁₈H₃₂O₂. The structure includes a long carbon chain of 18 carbon atoms, with two *cis* double bonds located at the 9th and 12th positions from the carboxylic acid end. Figure 4 shows the molecular structure of Linoleic acid.

The superior inhibition behaviour of linoleic acid can also be attributed to its molecular structure. Unlike myristic, palmitic and stearic acids, linoleic acid contains two carbon–carbon double bonds together with a polar carboxylic acid group.

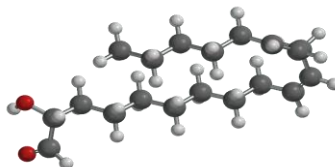


Figure 4: Molecular structure of Linoleic acid

Oleic acid, which contains only one double bond, exhibited a slightly larger energy gap (**10.15 eV**) than linoleic acid, suggesting lower electronic reactivity and comparatively weaker adsorption. Likewise, palmitic, stearic, myristic and lauric acids all possessed energy gaps exceeding **11 eV**, reflecting lower molecular softness and reduced adsorption tendencies. These saturated fatty acids therefore exhibit weaker inhibition potential because the absence of π -electron systems limits effective interaction with the copper surface. The interaction energy parameters further support these observations. Linoleic acid recorded one of the lowest interaction energy values among the investigated fatty acids, indicating a thermodynamically favourable interaction with the Cu₄ cluster. Lower interaction energies generally correspond to stronger adsorption and higher inhibition efficiency because less energy is required for inhibitor molecules to occupy active corrosion sites.

Table 3: Molecular and interacting properties of copper, palm oil constituents and the paint constituent

COMPOUND	Formula	Egap	IEG
copper Cluster	Cu ₄	9.28	9.28
Myristic Acid	C ₁₄ H ₂₈ O ₂	11.47	7.09
Linoleic	C ₁₈ H ₃₂ O ₂	9.53	6.41
Stearic acid	C ₁₈ H ₃₆ O ₂	11.61	7.21
Oleic	C ₁₈ H ₃₄ O ₂	10.15	7.09
Lauric acid	C ₁₂ H ₂₄ O ₂	11.42	7.15
Palmitic	C ₁₆ H ₃₂ O ₂	11.41	7.10
STYRENE	C ₈ H ₈	9.30	6.61

Styrene was included as a representative constituent commonly encountered in commercial coating formulations. Although styrene exhibited a relatively small HOMO–LUMO energy gap (9.30 eV), comparable to that of linoleic acid, its inhibition performance is expected to be inferior because its adsorption is governed primarily by π -electron interactions where it has no oxygen atom that is present in the other fatty acids which are strongly coordinating functional groups (Ashassi-Sorkhabi et al., 2006). In contrast, the carboxyl functional group present in all fatty acids provides oxygen atoms capable of forming stronger coordinate interactions with copper. Consequently, adsorption occurs through both electrostatic attraction and chemisorption, producing a more compact and durable protective film. This observation demonstrates that molecular functionality is equally as important as electronic reactivity when designing effective green corrosion inhibitors.

Overall, the computational results indicate that the corrosion inhibition efficiency of the investigated palm oil constituents follows the approximate order:

Linoleic acid has the highest inhibition efficiency with Egap/IEG of 9.53/6.41, Oleic acid with 10.15/7.09, followed by Palmitic acid, Lauric acid and Myristic acid with values of 11.41/7.10, 11.42/7.15 and 11.47/7.07 respectively, and lastly Stearic acid. The observed differences of the saturated acids are marginal and are probably because of the computational uncertainty. This trend agrees with previous computational investigations reporting that unsaturated fatty acids generally outperform saturated fatty acids because their greater electron density and enhanced molecular softness promote stronger adsorption on metallic surfaces (Faraj et al., 2022; Obot et al., 2019).

4. CONCLUSION

Among the investigated compounds, linoleic acid exhibited slightly lower HOMO–LUMO energy gap (9.53 eV), compared with H₂O₄S (11.57eV), NaCl (9.77eV), HCl (13.68eV) and HNO₃ (11.30eV), that suggests that linoleic acid possesses comparatively greater electronic reactivity and potential for electron interaction with the copper surface. This behaviour may favour adsorption of linoleic acid on copper and facilitate the formation of a protective organic film, thereby reducing the accessibility of corrosive species to the metal surface. Consequently, linoleic acid may have potential as a green organic corrosion inhibitor for copper. Future studies should focus on experimental approach to prove the findings of this research. Other electronic descriptors should also be calculated such as adsorption, electron density using density functional theory which give more precise computational results.

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