

Original Research Article: A Comparative Computational Stimulation Studies on Corrosion Inhibition and Adsorptive Qualities of Coumarin Derivative on Iron, Zinc, Copper and Aluminium

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ABSTRACT

Metals, such as Iron, zinc, aluminium, and copper are vital in various industries and construction. However, these metals are susceptible to corrosion upon exposure to corrosive elements. Metals used at homes and part of our car bodies under goes corrosion at a little contact of the corrosion factors. In this research, a coumarin derivative was theoretically studied using quantum parameters such as Electronegativity (χ), Global hardness (η), Electron donating power (ω^-), Electron accepting power (ω^+), Global softness (σ), Global hardness (η), and fraction of electron transfer (ΔN) couple with the simulation process to ascertain and compare the corrosion inhibition of metals such Zn, Al, Cu, and Fe. Based on the results, low magnitude of E_{LUMO} combined with the high magnitude of E_{HOMO} reveals that Coumarin-6-ol, 3,4-dihydro-4,4-dimethyl-7-nitro- (CML) molecule was reactive by serving as a donor, hence confirming the predicted inhibition of the simulated parameters. The electronegativity atoms have a significant effect on the corrosion inhibition efficiency of CML inhibitor molecule, and the atom with a negative charge depicts the potential of a HOMO center. The binding energy of the inhibitor (CML) on the metals were in order of CML-Fe (111) > CML-Cu (110) > CML-Al (110) > CML-Zn (110) for -90.768834 kcal/mol, -48.643544 kcal/mol, -45.734485 kcal/mol, and -26.909952 kcal/mol, respectively. According to the results, CML inhibitor molecule shows high significant corrosion protection properties and is shown to be highly effective on CML-Fe (111) compare to the other metals studied. All CML-metal contact in the study depicts a physical adsorption based on the values of binding and obtained adsorption energy.

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Introduction

When a refined metal is transformed by any chemical means into a more stable oxide, the process is known as corrosion. Corrosion is the slow decomposition of materials such as metals by chemical interactions with their surroundings; this refers to the electrochemical oxidation of metals in response to an oxidant, such oxygen, etc. [1-2].

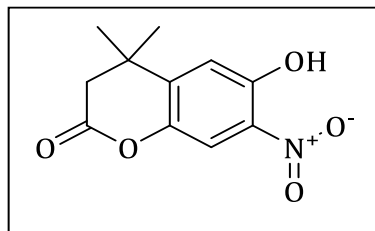
Though, there are several important metal alloys that are employed in various industrial products. Iron, in the form of steel, is used in building materials and automobile parts, titanium is used in technological gadgets, and aluminum is used in packaging [1-3]. These metals were chosen based on their longevity, strength, and resistance to the environment [2]. Copper is widely utilized in the fabrication of wire, sheets, and pipes as well as in the electronic and maritime industries, power plants, heat exchangers, and cooling towers due to its outstanding corrosion resistance and high electrical and thermal conductivity [3-6].

On the other hand, aluminum is a very light metal with a specific weight of 2.7 g/cm^3 , as well as stable in terms of its physical properties, chemical composition, and mechanical properties, and it conducts electricity [7]. Although aluminum has a layer of oxygen-based protection called Al_2O_3 , it is nevertheless prone to corrosion to some extent depending on environmental conditions including temperature, high levels of acidic anions like Cl^- and SO_4^{2-} , and other aggressive anions.

This corrosion ultimately reduces the effectiveness of industrial instruments, causing significant financial losses [4]. It also has a severe impact on the performance of systems built using these metals. Given the widespread use of metals like Zn, Al, Cu, and Fe in the manufacturing and construction industries, research has been conducted and is still being conducted in these fields to lessen or completely remove the corrosion effects. In the global advancement of technology, corrosion has grown to be a very difficult problem, though

many metals may have their corrosion rate reduced using corrosion inhibitors. Generally, inhibitors act to reduce the anodic or the cathodic reaction or both of them in the metal environment [7]. Inorganic and organic are the two basic divisions of corrosion inhibitors. But due to their strong corrosion inhibition efficacy, organic corrosion inhibitors and their derivatives are often utilized [8]. The chemical makeup, structure, electrical characteristics, nature of the metal, and environmental factors of corrosion inhibitors all affect how effective they are in preventing corrosion. The organic compounds serving as corrosion inhibitors are characterized with presence of heteroatoms such as O, P, S, and N and conjugated pi-bonds in their structure [10]. The use of inorganic inhibitors such as Molybdates MoO_4^{2-} and tetra borates $\text{B}_4\text{O}_7^{2-}$ were examples of inorganic inhibitors that provide weak corrosion inhibition efficiency also label as toxic inhibitors.

A number of researchers have investigated the usage of the experimental technique since time immemorial. Nevertheless, the process is time-consuming and rife with human error. To the best of our knowledge, neither the structure of coumarin nor its adsorption capabilities on metals like Zn, Al, Cu, and Fe have been theoretically compared. Hence, in this research, Coumarin-6-ol, 3,4-dihydro-4,4-dimethyl-7-nitro- was investigated using DFT principles and dynamic simulation on the copper (Cu), aluminum (Al), zinc (Zn), and iron (Fe) surfaces to compare the molecule effectiveness on the above surfaces will be done by calculating the adsorption energy of the molecule on the surface through quench dynamic simulation of the inhibitor and the surfaces. The result obtained will be used to analyze the inhibition quality of the molecule on both surfaces. Furthermore, quantum parameters such as, the highest occupied molecular orbital HOMO, the lowest unoccupied molecular orbital LUMO, ionization potential, activation energy, electronegativity (χ), electrophilicity (ω), global hardness (η), electron global softness (σ), back donation E_{b-d} , and numbers of electron transfer



Scheme 1 Coumarin-6-ol, 3,4-dihydro-4,4-dimethyl-7-nitro-

(ΔN) as well as energy gap of the molecule will be used to analyze the inhibition process. For the best of our knowledge, little was studied on the based molecule of coumarin. In this research, a specific coumarin molecule "Coumarin-6-ol, 3,4-dihydro-4,4-dimethyl-7-nitro-" was studied on the different surfaces of Al, Zn, Cu, and Fe to compare its adsorptive behaviors on the surfaces (Scheme 1).

Theoretical Methods

Quantum Chemical Calculations

Quantum chemical calculations were performed using a DMol³ module in the BIOVIA Material Studio 8.0 program (Accelrys, Inc.) with underlying fundamentals of Density Functional Theory (DFT). The B3LYP function was used to calculate the parameters with the basis set to "double-numeric plus polarization" (DNP) in the aqueous phase.

$$\chi: \text{absolute electronegativity (eV)} \quad \chi = \frac{IE+AE}{2} = -\frac{(E_{HOMO}+E_{LUMO})}{2} \quad (4)$$

$$\eta: \text{global hardness (eV)} \quad \eta = \frac{IE-AE}{2} = \frac{(E_{LUMO}-E_{HOMO})}{2} \quad (5)$$

$$\sigma: \text{global softness (eV)}^{-1} \quad \sigma = \frac{1}{\eta} = -\frac{2}{E_{HOMO}-E_{LUMO}} \quad (6)$$

$$\omega: \text{global electrophilicity index (eV)} \quad \omega = \frac{\mu^2}{2\eta} = \frac{\chi^2}{2\eta} \quad (7)$$

$$\varepsilon: \text{nucleophilicity (eV)}^{-1} \quad \varepsilon = \frac{1}{\omega} \quad (8)$$

Back donation was determined by equation (9). Backdonation calculatet the power of the molecule been able to received electron freely from the surface.

ΔE_{b-d} : Energy of back donation

Koopman's extended theorem, following Equations (1-9), calculated the energy quantum parameters which determine the initial electron distribution in the molecule and local reactivity calculation of the Fukui function $f(r)$ from ab-initio quantum chemistry:

$$IE: \text{Ionization energy (eV)} \quad IE = -E_{HOMO} \quad (1)$$

$$AE: \text{Electron affinity (eV)} \quad AE = -E_{LUMO} \quad (2)$$

Equations (1) and (2), respectively, relate 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).

The energy gap of the molecules was computed using Equation (3). The energy gap is a factor which determines both the stability and reactivity of an inhibitor molecular

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

The value of global hardness (η) is approximated as shown in equation (4). Equation (5) demonstrates that the global softness (S) of the system is the opposite of global hardness while Equations (7) and (8) were used to calculate the (ω) global electrophilicity index and nucleophilicity, respectively.

$$\Delta E_{b-d} = -\frac{\eta}{4} = \frac{1}{8}(E_{HOMO} - E_{LUMO}) \quad (9)$$

The difference in electronegativity drives the electron transfer, and the sum of the hardness parameters acts as a resistance. To calculate the

number of fraction of electrons transferred, a theoretical value for the electronegativity of bulk Al, Zn, Cu, and Fe were used $\chi_{Al} = 5.60$ eV, $\chi_{Zn} = 4.45$ eV, $\chi_{Cu} = 4.45$, and $\chi_{Fe} = 7.0$ eV based on the Pearson Bulk electronegativity value, and a global hardness of $\eta_{Metals} = 0$, by assuming that for a metallic bulk $I = A$ [13] because they are softer than the neutral metallic atoms [5-7].

$$\Delta N: \text{Fraction of electron(s) transfer } \Delta N = \frac{\chi_{Metal} - \chi_{Inh.}}{2(\eta_{Metal} + \eta_{Inh.})} \quad (10)$$

The electron donating (ω^-) and electron accepting (ω^+) powers, and also net

$$\omega^-: \text{electron donating power (eV)} \quad \omega^- = \frac{(3IE + AE)^2}{16(IE - AE)} \quad (11)$$

$$\omega^+: \text{electron accepting power (eV)} \quad \omega^+ = \frac{(IE + 3AE)^2}{16(IE - AE)} \quad (12)$$

Molecular Dynamic Simulations

Using a high stability quench adsorption approach on a surface of densely packed Fe (111), Zn(110), Cu(110), and Al(110) surfaces, the investigated Coumarin derivative was simulated. A FORCITE toolkit included in the BIOVIA Materials Studio 8.0 software package (Accelrys, Inc.) was employed during the simulation procedure. Condensed-phase optimized molecular potentials for atomistic simulation studies (COMPASS) force field tool computations were carried out in a simulation box with dimensions of 17 x 12 x 28 to replicate a realistic area of the surface. The crystal planes were cleaved across the Metal crystals at a fractional depth of 3.0. The bottom layers' form was constrained before the surfaces were optimized to avoid edge effects brought on by the molecules sizes. A 6 x 6 supercell was created by expanding the surfaces. By setting the temperature at 350K, a balance was reached between a system with too much kinetic energy, where the molecule desorbs from the surface, and a system with not enough kinetic energy, where the molecule cannot move over the surface. The temperature was set using the NVT (microcanonical) ensemble with a time step of 1 fs and simulation duration of 5 ps. to ascertain the statistical values of the energies on the metal crystal's surfaces. Every

Half-electron transfer (ΔN) in Equation (10) was computed which showed the proportion of electrons transported from the inhibitor to the surface of the metal as an indicator of the type of electron transfer between the inhibitor molecule and the metal surface.

electrophilicity of the molecules were defined in Equations (11-12), respectively:

250 steps throughout the course of 5000 cycles, the process was meant to be quenched. Using FORCITE geometry optimized geometries of the molecules and the Fe (111), Cu (110), Zn (110), and Al (110) surfaces, the lowest energy interactions between the molecules were discovered [3-4, 10,14]. The Coumarin derivative's adsorption and binding energies to the surfaces of Fe (111), Zn(110), Cu(110), and Al(110) were calculated from the simulation process using Equations (13,14).

$$E_A = E_T - (E_i + E_s) \quad (13)$$

$$E_B = - E_A \quad (14)$$

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 [3-4, 10,14].

Results and Discussion

Quantum Chemical Parameters

Global reactions describe the potential behavior of a molecule on the metal surfaces in line with Koopman's expanded theorem. This has to do with the molecule's HOMO and LUMO

energies. Electronegativity, global hardness, electron donating power, electron accepting power, global softness, global hardness, and proportion of electron transfer. Global reactions characterize molecule's reactivity in terms of distribution of electrons [13].

EHOMO and ELUMO

The E_{LUMO} Eigen value represents molecule's ability to accept electrons from the d or p-orbital of the metal. In addition, the value of the molecule's EHOMO pursues determines its capacity to contribute an electron to the metal's deficient orbital [14]. The negative E_{HOMO} in Table 1 indicates that the molecule CML may detect a suppression of physisorption on the metal surface [15-16].

Energy Gap

A metric used to determine how well a molecule is inhibited is the change in energy, often known as the energy gap. The molecule is able to reduce the excitation energy needed to remove an electron from the final occupied orbital on the molecule, as seen by the smaller value of the energy gap [17]. The value of the energy gap discovered for the molecule under investigation is consistent with the energy gaps discovered by Kumar *et al.* and Kubba *et al.* [18-20]. Both authors show in their independent investigations that the lower value of Energy gap may be used as a tool to block any chemical under study.

Half Electron Transfer

The number of electrons transferred by the molecule depicts how effective electrons are being transferred from the molecule to the surface. According to the literature, efficiency of inhibition of any inhibitor molecule increases when the number of electrons transferred (ΔN) is less than 3.6 [21-22]. The efficiency of the inhibition, however, declines when number of electrons transferred (ΔN) is larger [10]. Hence, efficiency of the inhibition process of inhibitor molecule on the metal surface cannot be channel to the size of molecule alone, but both

the transfer of electrons between the molecule and the metal surface [1-9].

In the molecule studied inhibition efficiency on the surface is in the order, $(\Delta N_{Fe}) > (\Delta N_{Al}) > (\Delta N_{Cu}) > (\Delta N_{Zn})$. The order of the examined molecule's surface inhibition effectiveness is $(N_{Fe}) > (N_{Al}) > (N_{Cu}) > (N_{Zn})$ which indicate the fact that (NCu) and (NZn) exhibited negative electron transfer values, their electronegativity values were lower than those of the inhibitor compound CML.

Back Donation

Back donation of the inhibitory process will be preferred when the global hardness value is positive and the energy of back donation (E_{b-d}) is negative [24,33]. When the molecules come into close contact with one another during this process, the charge is successfully transmitted to the metal surface [5]. However, a molecule's capacity to take electrons is indicated by the electrophilicity index (ω). The term nucleophilicity (ϵ), which denotes the opposite of electrophilicity ($\epsilon = 1/\omega$), refers to a molecule's capacity to provide or accept electrons. In contrast to molecules with high electrophilicity indices, compounds with high nucleophilicity efficiently suppress corrosion, according to the literature [1].

Power of Electron Donation and Acceptance

The ability of the molecule to accept charge is strengthened by a higher electron accepting power (ω^+) value obtained. The power of the electron donator (ω^-) and acceptor (ω^+) estimated from the molecule obtained from the computation was high, as presented in Table 1, indicating greater molecular capacity of the molecule to donate an electron to the metal surface.

Ionization Potential (I, E) and Electron Affinity (EA)

The amount of energy released by a molecule during the inhibitor-metal adsorption process as a result of electron lost and acquired is shown using ionization potential (IE) and

electron affinity (EA) [20]. There was good agreement between the CML under study's electron affinities and ionization potentials. The resistance of an atom to a transferred charge was quantified by the term "global hardness". The procedure of molecule adhering to any metal surface is made easier by how lower the value of the global hardness is. In the outcome, the hardness showed that molecule CML had a stable equilibrium configuration since a molecule's hardness value drops when it deviates from equilibrium. The tested molecule's outcome was consistent with that of Ogede *et al.* [36]. Global hardness and softness are inversely correlated. It also serves as a gauge for how well an atom or group of atoms can accept electrons. In addition to being more reactive than hard molecules, soft molecules are more susceptible to changes in electron density [11-15]. A soft molecule has a modest energy gap compared to a hard molecule's big energy gap. Therefore, particularly effective inhibitors are predicted to have a lower global hardness value and a higher softness value. Furthermore, the positive value for global hardness in Table 1 shows how easily the back donation on the molecule might take place.

Figure 1 displays the optimized screen short of the molecule. According to the molecule's electron density, the whole molecule can be

employed to stop a process on a metal surface [25-27]. The HOMO orbitals display the molecules' orbitals that can provide electrons to the vacant orbitals on the metal surface. On the other hand, LUMO orbitals show the molecule's inadequate orbital [28-30]. The rich d or p- orbitals of the metals can provide these orbitals with electrons.

Fukui Functions

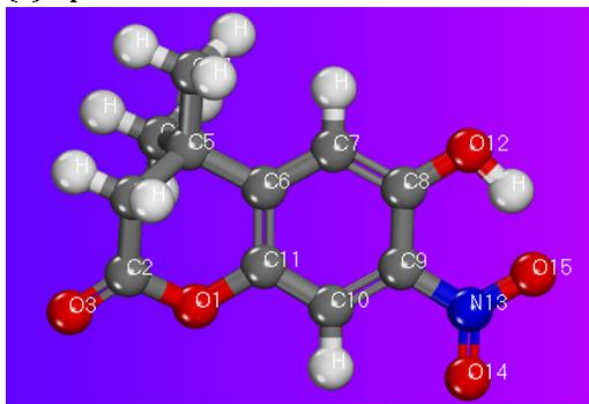
The Fukui orbitals of the CML molecule are demonstrated in Figure 2a. The Fukui functions show potential orbitals for electron transfer between molecules and potential vacant sites on surfaces, and vice versa [15,31]. O14 and O15 in the picture had the highest Fukui (+) values, 0.18 and 0.155, respectively. According to the results of the Fukui functions, O12 depicts the highest Fukui (-) of 0.144, clearly demonstrating that the molecule is capable of inhibition [32-38].

The molecule's nucleophilic or electrophilic characteristics on the surface are explained by its second Fukui function as presented in Figure 2b. According to the information provided, the molecule's nucleophilicity and electrophilicity on the surface were both equivalent. This indicates that a molecule's capacity for giving and accepting energy is equal [10-15].

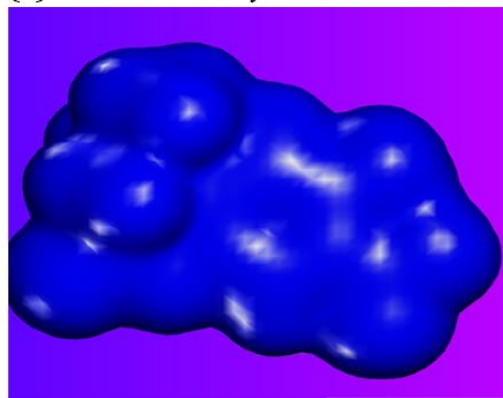
Table 1 Energy parameters of the molecule CML

Parameters (eV)	Aqueous	Gas
EHOMO	-6.164	-5.891
ELUMO	-3.943	-3.769
ΔE (eV)	2.221	2.122
(I) (eV)	6.164	5.891
(A) eV	3.943	3.769
(η)	1.111	1.061
(χ)	0.900	0.943
ω	5.054	4.830
ϵ	11.495	10.994
(ΔN_{Fe})	0.087	0.091
(ΔN_{Al})	1.946	2.170
(ΔN_{Cu})	0.546	0.770
(ΔN_{Zn})	-0.574	-0.350
(ω^-)	-0.604	-0.380
(ω^+)	14.164	13.541
ΔE_{b-d}	33.952	33.074
	0.278	0.265

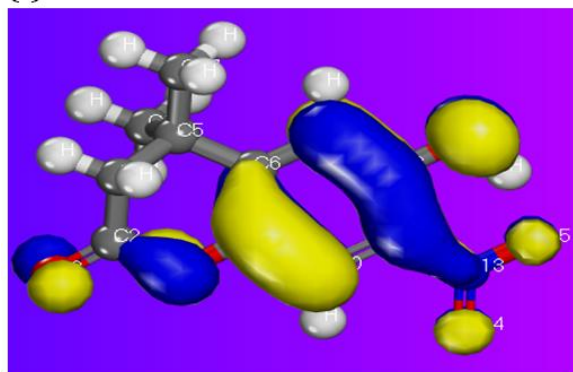
(a) Optimized Molecule



(b) Electron Density



(c) HOMO orbitals



(d) LUMO orbitals

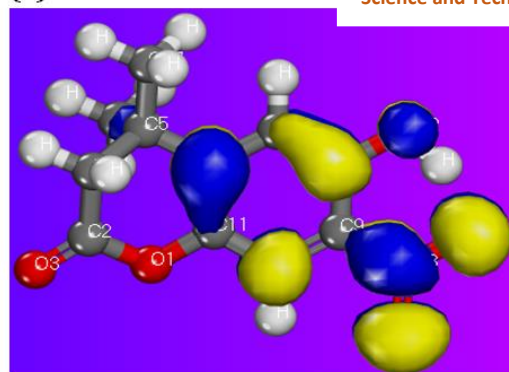
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Figure 1 (a) Optimized molecule (b) Electron density of the molecule (c) HOMO orbitals of the molecule (d) LUMO orbitals of the molecule

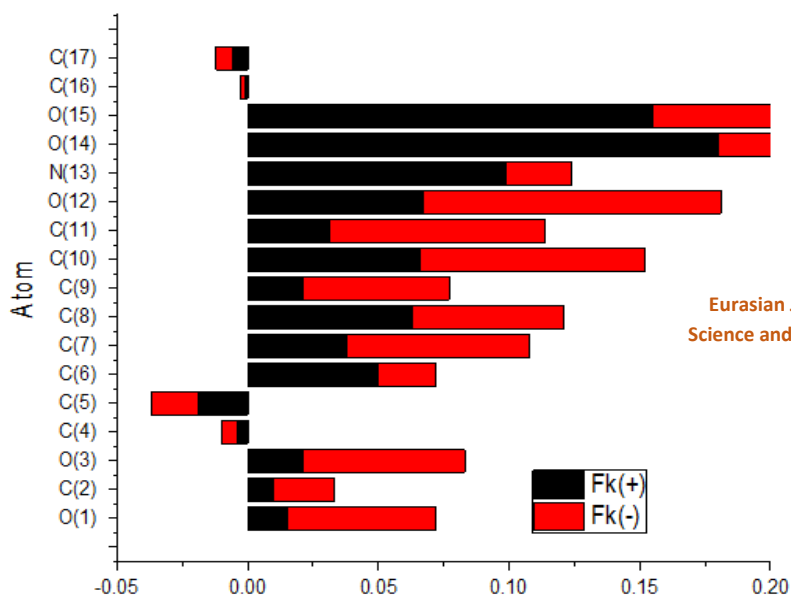
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Figure 2a Fukui function of the molecule CML

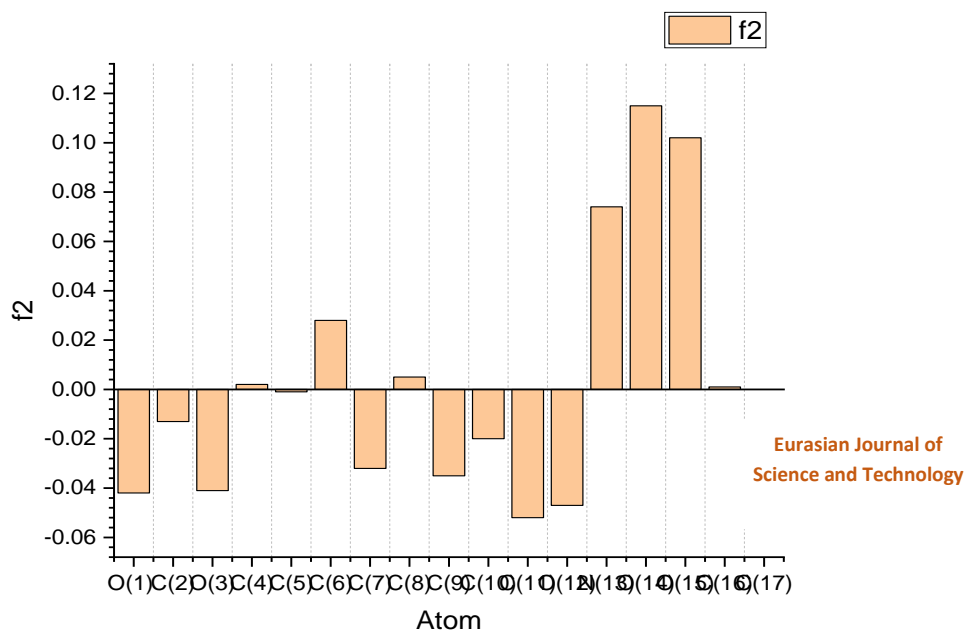


Figure 2b Fukui second function of the molecule CML

Molecular Simulation

Figure 3 a-d depict the inhibitor molecule CML on the metals surface used during simulation. The Al, Cu, and Zn, 110 surfaces were used hence their closed packed and high density of the surface. Surface 111 was used for Fe because the surface is denser and more closed packed [9-11].

The RMSD of the simulations is also shown, as illustrated in Figure 3a-d with various

simulation energies. During the simulation, the stability of a molecule was controlled using the Root Mean Square Deviation (RMSD) method. The RMSD trajectories of all the simulated energies during the molecule quenching on the metal surfaces are shown in Figure 3a-d.

Red denotes kinetic energies, blue, potential energies, green, non-bonding energies, and light blue, the total energy of the molecule with its final, minimal structure.

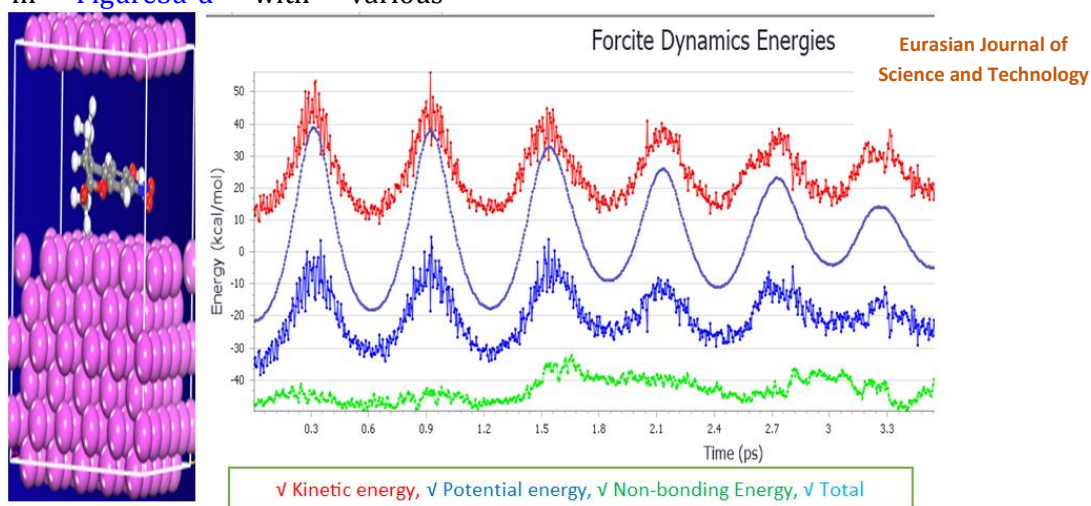


Figure 3a CML on the aluminum (110) surface

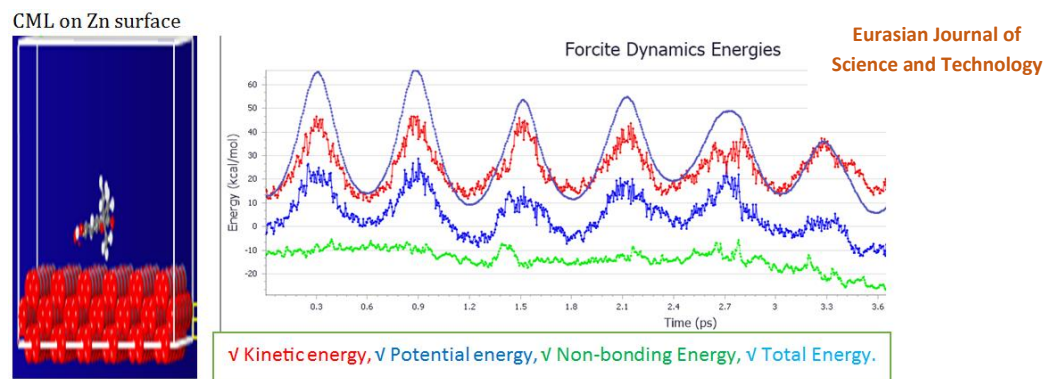


Figure 3b CML on zinc(110) surface

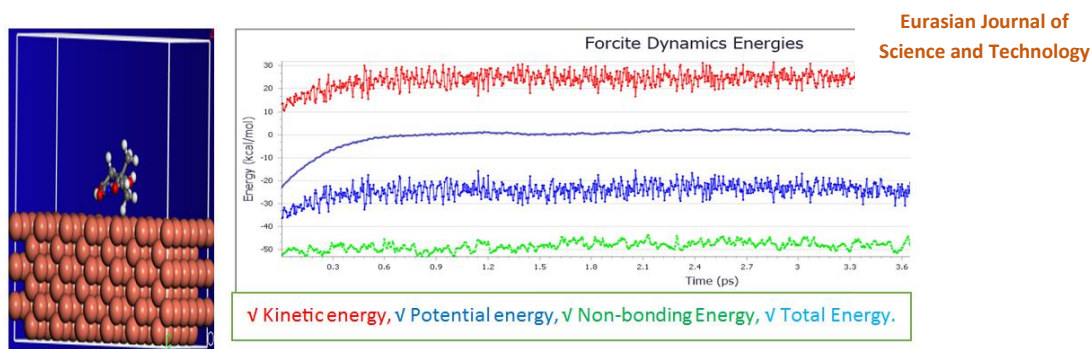


Figure 3c CML on copper (110) surface

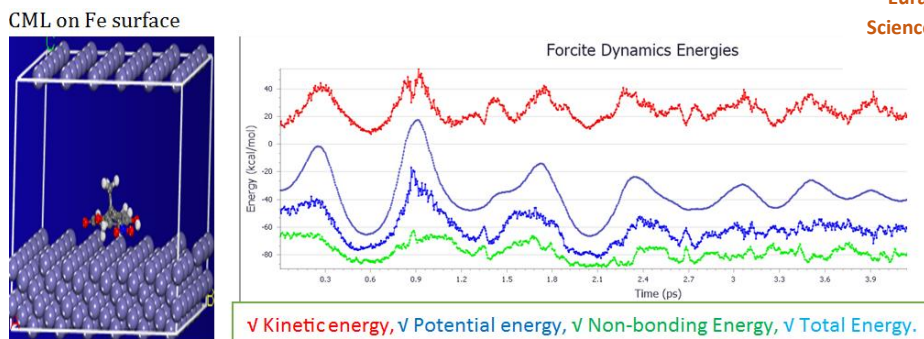


Figure 3d CML on iron (111) surface

Mechanism of Inhibition

Understanding how the protective inhibitor interacts with the metal surface is necessary for understanding the mechanism of inhibition. Since most metals have positive charges, the adsorption energy of the interactions between molecules and surfaces also plays a role in the mechanism of chemical inhibition [1,15]. To further understand the type and degree of interaction with the metals, four (4) metals, namely aluminum, zinc, copper, and iron, were

simulated in this study using a CML derivative. Through the sampling of several potential low energy configurations on the surfaces, quench molecular dynamics was utilized to determine the lowest energy of the inhibitor molecule capable of inhibition on the metals surfaces. The obtained results from simulation parameters in Table 2 showed that, with the exception of zinc, the predicted binding energies (E_{Bind}) from the interaction between CML and the metals were rather high, indicating

a strong and spontaneous adsorption on the metals surfaces [19]. It is crucial to know that, higher binding energies result in a more stable inhibitor-surface contact, which controls corrosion processes [1, 34-35]. The presence of beneficial electronic features, such as electron-rich centers and planar shape, among others, is blamed for the high value of binding energy obtained at Fe (111) with the molecule CML [35]. The CML inhibitor binding energy to the metals surfaces were: -90.768834kcal/mol, -48.643544kcal/mol, -45.734485kcal/mol, and -26.909952kcal/mol for CML-Fe (111), CML-Cu (110), CML-Al (110), CML-Zn (110), respectively in the order of CML-Fe (111)> CML-Cu (110)> CML-Al (110)> CML-Zn (110). The results showed a strong physisorption on

the metal surfaces like Fe, Cu, and Al with a mild energy recorded on the Zn surface [30]. This may be because the Zn metal's d-orbital is completely occupied. As a result, there may be a limit at which Zn received electrons from the inhibitor molecule hence inhibition efficiency of the molecule was demonstrated to depends also on the number of the electron transferred by the number of half electron transferred (ΔN). The presence of a conjugation system at the oxygen atoms of the molecule caused a dissociative adsorption that is advantageous to crack the intramolecular bond of the adsorbate on the metal crystal surfaces because electron rich centers in the molecule enhance electrostatic interaction with material surfaces [1,6,25].

Table 2 Calculated molecular simulation parameters for CML on AL, Cu, Al and ZN

Properties (Kcal/mol)	Fe	Zn	Cu	Al
Surface Energy	0.0000±0.0	0.0000±0.0	0.0000±0.0	0.0000±0.0
Adsorption Energy	-90.768834±0.1	-26.909952±0.8	-48.643544±0.0	-45.734485±0.7
Binding Energy	90.768834±0.1	26.909952±0.8	48.643544±0.0	45.734485±0.7

Conclusion

The study used simulation and the Density Function Theory (DFT) to compare the coumarin derivatives on the corrosion inhibition on the crystal surfaces of iron, zinc, copper, and aluminum. Based on the values of the Density Function Theory (DFT) and adsorption/binding energy obtained from molecule simulation on the surface, the following can be deduced from the CML inhibitor on the surfaces. (1) The low E_{LUMO} and high E_{HOMO} indicate that, CML molecules are reactive and can serve as a donor to the metal surface. (2) The corrosion inhibition effectiveness of the CML inhibitor molecule is significantly influenced by the electronegativity atoms, based on the high Fukui values recorded at Oxygen atoms. (3) The simulation's binding energy has a high value for Fe (111), indicating a significant inhibition with the surface and also indicating physical adsorption, whereas Zn (110), Cu (110), and Al (111) have low values, indicating a mild inhibition. The order of inhibition process on the metals was CML-Fe (111)> CML-Cu (110)> CML-Al (110)> CML-Zn (110).

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References

- [1] Stojanovic B., Bukvic M., Epler I., Application of aluminum and aluminum alloys in engineering, *Applied Engineering Letters*:

- Journal of Engineering and Applied Sciences*, 2018, [Crossref], [Google Scholar], [Publisher]
- [2] Teixeira A.P.C., Tristão J.C., Araujo M.H., Oliveira L.C., Moura F.C., Ardisson J.D., Amorim C.C., Lago R.M., Iron: a versatile element to produce materials for environmental applications, *Journal of the Brazilian Chemical Society*, 2012, **23**:1579 [Crossref], [Google Scholar], [Publisher]
- [3] Raskar R., Gaikwad A., The uses of copper and zinc aluminates to capture and convert carbon dioxide to syn-gas at higher temperature, *Bulletin of Chemical Reaction Engineering & Catalysis*, 2014, **9**:1 [Crossref], [Google Scholar], [Publisher]
- [4] Scully J. C. The Fundamentals of Corrosion, Third Edition (International Series on Materials Science and Technology) 3rd Edition 1975 [Google Scholar], [Publisher]
- [5] Sedik A., Athmani S., Saoudi A., Ferkous H., Ribouh N., Lerari D., Bachari K., Djellali S., Berredjem M., Solmaz R., Alam M., Experimental and theoretical insights into copper corrosion inhibition by protonated amino-acids. *RSC Advances*, 2022, **12**:23718 [Crossref], [Google Scholar], [Publisher]
- [6] Nyijime T.A., Chahul H.F., Ayuba A.M., Iorhuna F., Theoretical Study of Interaction Between Thiadiazole Derivatives on Fe (110) Surface, *Journal of Chemistry Letters*, 2023,**4**:86 [Crossref], [Google Scholar], [Publisher]
- [7] Al-Amiery A.A., Mohamad A.B., Kadhum A.A.H., Shaker L.M., Isahak W.N.R.W., Takriff M.S., Experimental and theoretical study on the corrosion inhibition of mild steel by nonanedioic acid derivative in hydrochloric acid solution, *Scientific Reports*, 2022, **12**:4705 [Crossref], [Google Scholar], [Publisher]
- [8] AlMashhadani H.A., Saleh K.A., Electrochemical Deposition of Hydroxyapatite Co-Substituted By Sr/Mg Coating on Ti-6Al-4V ELI Dental Alloy Post-MAO as Anti-Corrosion, *Iraqi Journal of Science*, 2020, 2751 [Crossref], [Google Scholar], [Publisher]
- [9] Afandiyeva L., Abbasov V., Aliyeva L., Ahmadbayova S., Azizbeyli E., El-Lateef Ahmed H.M., Investigation of organic complexes of imidazolines based on synthetic oxy-and petroleum acids as corrosion inhibitors, *Iranian Journal of Chemistry and Chemical Engineering*, 2018, **37**:73 [Crossref], [Google Scholar], [Publisher]
- [10] Jafari H., Mohsenifar F., Sayin K., Effect of alkyl chain length on adsorption behavior and corrosion inhibition of imidazoline inhibitors, *Iranian Journal of Chemistry and Chemical Engineering (IJCCE)*, 2018, **37**:85 [Crossref], [Google Scholar], [Publisher]
- [11] Ahmed A. A, Abu B. M., Abdul A. H. K., Lina M. S., Wan N. R. W.I & Mohd S. T., Experimental and theoretical study on the corrosion inhibition of mild steel by nonanedioic acid derivative in hydrochloric acid solution. *Scientific Reports*. 2022,**12**:4705 [Crossref], [Google Scholar], [Publisher]
- [12] Ayuba A., Uzairu A., Abba H., Shallangwa G.A., Theoretical study of aspartic and glutamic acids as corrosion inhibitors on aluminium metal surface, *Moroccan journal of chemistry*, 2018, **6**:6 [Crossref], [Google Scholar], [Publisher]
- [13] Iorhuna F., Ayuba A., Nyijime A., Hussain M., Ibrahim M., Comparative Study of Halogen Substituted Isocyanatophosphine as an Adsorptive Inhibitor on Al (110) Crystal Surface, using Density Functional Theory. *Progress in Chemical and Biochemical Research*, 2023, **6**:211 [Crossref], [Google Scholar], [Publisher]
- [14] Kubba R.M., Al-Joborry N.M., Theoretical study of a new oxazolidine-5-one derivative as a corrosion inhibitor for carbon steel surface, *Iraqi Journal of Science*, 2021, 1396 [Crossref], [Google Scholar], [Publisher]

- [15] Al-Rudaini K.A.K., Al-Saadie K.A.S., Milk Thistle Leaves Aqueous Extract as a New Corrosion Inhibitor for Aluminum Alloys in Alkaline Medium, *Iraqi Journal of Science*, 2021, 363 [Crossref], [Google Scholar], [Publisher]
- [16] Mohammed M.A., Kubba R.M., Experimental Evaluation for the Inhibition of Carbon Steel Corrosion in Salt and Acid Media by New Derivative of Quinolin-2-One, *Iraqi Journal of Science*, 2020, 1861 [Crossref], [Google Scholar], [Publisher]
- [17] Iorhuna F., Ayuba A.M., Nyijime T.A., Muhammedjamiu H., A DTF and Molecular thermodynamic Simulation on the Adsorption Inhibition of Cytarabine a Nucleotides as a Potential Inhibitor on the Aluminium Metal Surface, *Eurasian Journal of Science and Technology*, 2023, 3:217 [Crossref], [Google Scholar], [Publisher]
- [18] El Ibrahimy B., Jmiai A., El Mouaden K., Oukhrib R., Soumoue A., El Issami S., Bazzi L., Theoretical evaluation of some α -amino acids for corrosion inhibition of copper in acidic medium: DFT calculations, Monte Carlo simulations and QSPR studies. *Journal of King Saud University-Science*, 2020, 32:163 [Crossref], [Google Scholar], [Publisher]
- [19] Esan T., Oyenyin O., Olanipekun A., Ipinloju N., Corrosion inhibitive potentials of some amino acid derivatives of 1, 4-naphthoquinone-DFT calculations, *Advanced Journal of Chemistry Section A*, 2022, 5:263 [Crossref], [Google Scholar], [Publisher]
- [20] Kubba R.M., Al-Joborry N.M., Al-Lami N.J., Theoretical and experimental studies for inhibition potentials of imidazolidine 4-one and oxazolidine 5-one derivatives for the corrosion of carbon steel in Sea Water, *Iraqi Journal of Science*, 2020, 2776 [Crossref], [Google Scholar], [Publisher]
- [21] Yavari Z., Darijani M., Dehdab M., Comparative theoretical and experimental studies on corrosion inhibition of aluminum in acidic media by the antibiotics drugs, *Iranian Journal of Science and Technology, Transactions A: Science*, 2018, 42:1957 [Crossref], [Google Scholar], [Publisher]
- [22] Al-Joborry N.M., Kubba R.M., Theoretical and Experimental Study for Corrosion Inhibition of Carbon Steel in Salty and Acidic Media by A New Derivative of Imidazolidine 4-One, *Iraqi Journal of Science*, 2020, 1842 [Crossref], [Google Scholar], [Publisher]
- [23] John S., Joy J., Prajila M., Joseph A., Electrochemical, quantum chemical, and molecular dynamics studies on the interaction of 4-amino-4H, 3, 5-di (methoxy)-1, 2, 4-triazole (ATD), BATD, and DBATD on copper metal in 1N H₂SO₄, *Materials and corrosion*, 2011, 62:1031 [Crossref], [Google Scholar], [Publisher]
- [24] Belghiti M., Echihi S., Dafali A., Karzazi Y., Bakasse M., Elalaoui-Elabdallaoui H., Olasunkanmi L., Ebenso E., Tabyaoui M., Computational 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, *Applied Surface Science*, 2019, 491:707 [Crossref], [Google Scholar], [Publisher]
- [25] Kadhim M.M., Juber L.A.A., Al-Janabi A.S., Estimation of the Efficiency of Corrosion Inhibition by Zn-Dithiocarbamate Complexes: a Theoretical Study, *Iraqi Journal of Science*, 2021, 3323 [Crossref], [Google Scholar], [Publisher]
- [26] Glossman-Mitnik D., Computational study of the chemical reactivity properties of the Rhodamine B molecule, *Procedia Computer Science*, 2013, 18:816 [Crossref], [Google Scholar], [Publisher]
- [27] Nahlé A., Salim R., El Hajjaji F., Aouad M., Messali M., Ech-Chihbi E., Hammouti B., Taleb M., Novel triazole derivatives as ecological corrosion inhibitors for mild steel in 1.0 M HCl: experimental & theoretical approach, *RSC*

- advances*, 2021, **11**:4147 [Crossref], [Google Scholar], [Publisher]
- [28] Eddy N.O., Ameh P.O., Essien N.B., Experimental and computational chemistry studies on the inhibition of aluminium and mild steel in 0.1 M HCl by 3-nitrobenzoic acid, *Journal of Taibah University for Science*, 2018, **12**:545 [Crossref], [Google Scholar], [Publisher]
- [29] Guo L., Zhu M., Chang J., Thomas R., Zhang R., Wang P., Zheng X., Lin Y., Marzouki R., Corrosion Inhibition of N80 Steel by Newly Synthesized Imidazoline Based Ionic Liquid in 15% HCl Medium: Experimental and Theoretical Investigations, *International Journal of Electrochemical Science*, 2021, **16**:211139 [Crossref], [Google Scholar], [Publisher]
- [30] Lgaz H., Masroor S., Chafiq M., Damej M., Brahmia A., Salghi R., Benmessaoud M., Ali I.H., Alghamdi M.M., Chaouiki A., Evaluation of 2-mercaptobenzimidazole derivatives as corrosion inhibitors for mild steel in hydrochloric acid, *Metals*, 2020, **10**:357 [Crossref], [Google Scholar], [Publisher]
- [31] Iorhuna F., Thomas N.A., Lawal S.M., A Theoretical properties of Thiazepine and its derivatives on inhibition of Aluminium Al (110) surface, *Algerian Journal of Engineering and Technology*, 2023, **8**:43 [Crossref], [Google Scholar], [Publisher]
- [32] Kılınççeker G., Baş M., Zarifi F., Sayın K., Experimental and Computational Investigation for (E)-2-hydroxy-5-(2-benzylidene) Aminobenzoic Acid Schiff Base as a Corrosion Inhibitor for Copper in Acidic Media, *Iranian Journal of Science and Technology, Transactions A: Science*, 2021, **45**:515 [Crossref], [Google Scholar], [Publisher]
- [33] Nyijime T., Chahul H., Ayuba A., Iorhuna F., Theoretical investigations on thiadiazole derivatives as corrosion inhibitors on mild steel, *Advanced Journal of Chemistry-Section A*, 2023, **6**:141 [Crossref], [Google Scholar], [Publisher]
- [34] Emmanuel O.O., Samuel O.B., Kolawole O.F., Dada A.D., Oluwafisayo A.E., Chibuzo E.B., Nureni I., Experimental and Theoretical Study on the Corrosion Inhibitive Potentials of Schiff Base of Aniline and Salicylaldehyde on mild steel in 0.5M HCl, *Advanced Journal of Chemistry Section B*, 2020, **2**:197 [Crossref], [Google Scholar], [Publisher]
- [35] Chinthapally K., Blagg B.S., Ashfeld B.L., Syntheses of Symmetrical and Unsymmetrical Lyso-bisphosphatidic Acid Derivatives, *The Journal of organic chemistry*, 2022, **87**:10523 [Crossref], [Google Scholar], [Publisher]
- [36] Ogede R.O., Abdulrahman N.A., Apata D.A., DFT computational study of pyridazine derivatives as corrosion inhibitors for mild steel in acidic media, *GSC Advanced Research and Reviews*, 2022, **11**:106 [Crossref], [Google Scholar], [Publisher]
- [37] Yadav D.K., Maiti B., Quraishi M., Electrochemical and quantum chemical studies of 3, 4-dihydropyrimidin-2 (1H)-ones as corrosion inhibitors for mild steel in hydrochloric acid solution, *Corrosion Science*, 2010, **52**:3586 [Crossref], [Google Scholar], [Publisher]
- [38] Muthukrishnan P., Jeyaprabha B., Prakash P., Corrosion inhibition and adsorption behavior of *Setaria verticillata* leaf extract in 1M sulphuric acid, *Journal of materials engineering and performance*, 2013, **22**:3792 [Crossref], [Google Scholar], [Publisher]

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