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**Original Research Article**

# Density Functional Theory and Molecular Dynamics Simulation Studies on the Corrosion Inhibition of Phenolic Acid-Based Derivatives on Aluminum Metal

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## Abstract

Aluminum and its alloys are widely used in industries due to their favorable mechanical properties, low density, and natural passivation. However, they remain susceptible to corrosion in acidic environments, necessitating effective and environmentally friendly inhibition strategies. In this study, the corrosion inhibition behavior of two phenolic acid derivatives, vanillic acid (VA) and isovanillic acid (ISVA), on aluminum was investigated using a combined density functional theory (DFT) and molecular dynamics (MD) simulation approach. DFT calculations revealed that VA exhibits a higher HOMO energy, smaller energy gap, greater global softness, and larger fraction of electrons transferred compared to ISVA, indicating stronger electron-donating ability, higher chemical reactivity, and enhanced adsorption propensity. Fukui function analysis identified oxygen atoms in hydroxyl and carboxyl groups as primary reactive sites, with O (4), O (8), O (11), and O (12) in VA and O (11) in ISVA, highlighting the crucial role of oxygen-containing functional groups in adsorption. MD simulations confirmed strong adsorption of both inhibitors on the Al (111) surface, with adsorption energies of -0.692 eV (VA) and -0.706 eV (ISVA), and revealed favorable molecular orientation, surface coverage, and hydrogen bonding interactions stabilizing the protective layer. Integrating DFT and MD results, VA was identified as the more effective corrosion inhibitor due to its higher reactivity, multiple active adsorption sites, and stronger electron-donating capability. This study provides molecular-level insights into corrosion inhibition mechanisms and supports the rational design of environmentally friendly inhibitors for aluminum in acidic media.

**Keywords:** Aluminum corrosion, Phenolic acid inhibitors, Vanillic acid, Density functional theory, Molecular dynamics, Adsorption mechanism.

## 1. INTRODUCTION

Aluminum and its alloys are extensively used in aerospace, construction, packaging, and transportation due to their low density, excellent mechanical properties, high electrical conductivity, and natural formation of a passivating oxide layer. Despite this, aluminum remains susceptible to corrosion in aggressive acidic media, such as hydrochloric and sulfuric acid solutions, which are commonly employed in industrial pickling, acid cleaning, and surface treatment (Roberge, 2021; Abu Orabi *et al.,* 2024). Corrosion in such environments compromises material performance, shortens service life, and incurs significant economic losses, making effective corrosion protection strategies critical. Among the available methods, the use of corrosion inhibitors is particularly practical and cost-effective. Organic inhibitors function by adsorbing onto metal surfaces, forming protective layers that block active corrosion sites and suppress electrochemical reactions (Bentiss *et al.,* 2022; Obot *et al.,* 2020). However, many conventional inhibitors present drawbacks such as toxicity, poor biodegradability, and environmental persistence, motivating research into environmentally friendly alternatives.

Phenolic acid derivatives have recently emerged as promising green corrosion inhibitors due to their hydroxyl and carboxyl functional groups and conjugated π-electron systems, which facilitate strong adsorption and interaction with metal surfaces (El Faydy *et al.,* 2023; Song *et al.,* 2024). They are generally non-toxic, biodegradable, and readily available, making them

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ideal candidates for sustainable corrosion mitigation in acidic conditions. In this study, VA and ISVA were identified as major phenolic constituents experimentally extracted from *Dioscorea bulbifera* leaves, highlighting the plant as a sustainable natural source of corrosion-inhibiting compounds (Ghosh *et al.,* 2015). Despite encouraging experimental results, corrosion inhibition occurs at the molecular scale, where experimental methods alone cannot fully elucidate adsorption mechanisms, electronic interactions, and inhibitor reactivity. To address this, DFT has been widely employed to investigate molecular electronic properties- such as HOMO and LUMO energies, energy gap (ΔE), chemical potential (μ), electronegativity (χ), global hardness (η) and softness (σ), and the fraction of electrons transferred (ΔN) which are critical predictors of inhibitor-metal interactions and adsorption tendencies (Obot *et al.,* 2020). Moreover, complementary to DFT, MD simulations allow dynamic and thermodynamic modeling of inhibitor-metal interactions under realistic conditions, including explicit solvent effects, temperature, and molecular motion. Molecular dynamics simulations provide insights into adsorption configurations, energies, surface coverage, orientation, and interaction stability over time, yielding a more accurate atomic-level representation of corrosion inhibition (Kaya *et al.,* 2021; Peng Liu *et al.,* 2023). In this study, an integrated DFT and MD simulation approach was employed to investigate the corrosion inhibition behavior of VA and ISVA on aluminum surfaces. DFT calculations were used to evaluate the electronic properties of the inhibitors, including frontier molecular orbitals, energy gaps, global reactivity descriptors, and reactive sites identified via Fukui function analyses. These calculations provide insights into the potential adsorption centers and the chemical reactivity of VA and ISVA, indicating their likely contributions to the formation of protective layers on the aluminum surface.

Molecular dynamics simulations, performed on an explicit Al (111) surface slab under aqueous conditions, complemented the DFT analysis by assessing the adsorption behavior, surface interactions, and stability of the inhibitor-metal complexes. Binding energy calculations were employed to qualitatively evaluate the strength of inhibitor adsorption and coverage on the metal surface. The novelty of this study lies in the combined use of DFT and MD simulations to investigate VA and ISVA inhibitors on aluminum, providing a comprehensive molecular-level understanding of adsorption mechanisms and surface interactions. This integrated approach allows for the rational design of environmentally benign phenolic acid-based inhibitors, offering insights that extend beyond previous single-method or purely experimental studies.

**Fig. 1: Dioscorea Bulbifera Leaves**

## 2. GENERAL METHODOLOGY

The corrosion inhibition behavior of VA and ISVA on aluminum in acidic media was investigated using a combined DFT and MD simulation approach. All DFT calculations were performed using the Forcite and DMol³ modules in Materials Studio 17.0. The inhibitor molecules were fully optimized in the aqueous phase to simulate realistic acidic environments. The B3LYP hybrid functional, in conjunction with the double numerical plus polarization (DNP) basis set, was employed to ensure accurate electronic structure predictions while accounting for solvation effects (Obot, Kaya, and Rani, 2020). Key quantum chemical descriptors were computed to evaluate molecular reactivity and adsorption propensity on aluminum, as well as the Fukui function analyses were carried out using both Mulliken and Hirshfeld population schemes to identify the most reactive sites for electrophilic, nucleophilic, and radical attacks. These analyses revealed oxygen atoms in hydroxyl and carboxyl groups, along with specific aromatic carbons, as the primary centers for adsorption and coordination with the aluminum surface (Alaoui *et al.,* 2025; Ibrahim *et al.,* 2023; Azeez *et al.,* 2024).

$$E_{\text{bind}} = E_{\text{complex}} - (E_{\text{metal}} + E_{\text{inhibitor}}) \text{ .................. } (1)$$

Where:

$E_{\text{bind}}$= binding energy (eV or kJ/mol)
$E_{\text{complex}}$= total energy of the metal surface with the adsorbed inhibitor
$E_{\text{metal}}$= energy of the clean metal surface
$E_{\text{inhibitor}}$= energy of the isolated inhibitor molecule

The DFT studies, MD simulations were conducted using the Forcite modules in Materials Studio to capture dynamic adsorption behavior under explicit aqueous conditions. A periodic Al (111) surface slab was constructed, and the inhibitor molecules were positioned above the surface. The COMPASS force field was employed along with the smart optimization algorithm to model interatomic interactions and adsorption energetics accurately. Simulations were performed under the NVT ensemble at 298 K with a timestep of 0.1 fs over a total duration of 50 ps to ensure adequate sampling of molecular motions and adsorption configurations. Adsorption energies ($E_{ads}$) were calculated as the difference between the total system energy and the sum of the isolated inhibitor and surface energies, where more negative values indicate stronger adsorption and higher inhibition efficiency (Nyijime *et al.,* 2023). MD analyses provided detailed insights into total potential energy, molecular energy, binding energy, hydrogen bonding interactions, surface coverage, and molecular orientation, offering a comprehensive understanding of inhibitor-metal interactions at the atomistic level (Kaya *et al.,* 2021; Peng Liu *et al.,* 2023). Finally, computational results from DFT and MD simulations were correlated with available experimental data from potentiodynamic polarization (PDP) and electrochemical impedance spectroscopy (EIS) studies to validate predicted inhibition efficiency and mechanistic interpretations. This integrated methodology provides a strong basis for predicting adsorption behavior, evaluating inhibitor-metal interactions, and guiding the rational design of environmentally friendly phenolic acid-based corrosion inhibitors (Bentiss *et al.,* 2022; El Faydy *et al.,* 2023).

## 3. RESULT AND DISCUSSION

### 3.1.1 Fukui Function Analysis of Vanillic Acid (VA)

The Fukui function analysis identifies the main reactive sites of VA (Table 1) during interaction with an aluminum surface. Oxygen atoms (O4, O8, O11, and O12) exhibit the highest electrophilic ($f^-$) and radical ($f^0$) indices, indicating their strong ability to accept electrons and form stable adsorption interactions with aluminum. In contrast, carbon atoms C3, C6, and C9 show higher nucleophilic ($f^+$) values, suggesting limited electron-donating regions. Overall, the results indicate that VA adsorbs predominantly through the oxygen atoms of its hydroxyl and carboxyl groups, forming a protective layer on aluminum. This behavior is consistent with previous DFT studies and supports other quantum chemical descriptors, confirming the effectiveness of vanillic acid as a corrosion inhibitor in acidic media.

**Table 1: Fukui Indices for Vanillic Acid**

| | **Electrophilic Attack (-)** | | **Nucleophilic Attack (+)** | | **Radical (0)** | |
|---|---|---|---|---|---|---|
| **ATOMS** | **Mulliken** | **Hirshfield** | **Mulliken** | **Hirshfield** | **Mulliken** | **Hirshfield** |
| C (1) | 0.047 | 0.047 | 0.051 | 0.044 | 0.049 | 0.045 |
| C (2) | 0.037 | 0.053 | 0.039 | 0.056 | 0.038 | 0.054 |
| C (3) | 0.095 | 0.090 | 0.102 | 0.093 | 0.098 | 0.091 |
| O (4) | 0.110 | 0.103 | 0.118 | 0.110 | 0.114 | 0.106 |
| C (5) | 0.047 | 0.051 | 0.044 | 0.050 | 0.045 | 0.051 |
| C (6) | 0.101 | 0.097 | 0.104 | 0.098 | 0.102 | 0.097 |
| C (7) | 0.036 | 0.056 | 0.034 | 0.047 | 0.035 | 0.052 |
| O (8) | 0.114 | 0.105 | 0.090 | 0.097 | 0.102 | 0.101 |
| C (9) | 0.108 | 0.108 | 0.118 | 0.103 | 0.113 | 0.106 |
| C (10) | 0.092 | 0.086 | 0.104 | 0.098 | 0.098 | 0.092 |
| O (11) | 0.108 | 0.103 | 0.096 | 0.102 | 0.102 | 0.102 |
| O (12) | 0.105 | 0.102 | 0.098 | 0.102 | 0.102 | 0.102 |

### 3.1.2 Fukui Function Analysis of Isovanillic Acid (ISVA)

The Fukui function analysis shows that ISVA interacts with the aluminum surface mainly through its oxygen-containing functional groups. The carboxyl oxygen O (11) is identified as the primary active site, exhibiting the highest electrophilic, nucleophilic, and radical Fukui indices, indicating its strong ability to both donate and accept electrons during adsorption. Other oxygen atoms, such as O (5) and O (12), contribute moderately, while aromatic carbon atoms C (9) and C (10) provide secondary interaction via π-electron density as shown in Table 2. Hydrogen atoms play a negligible role in adsorption. Overall, ISVA adsorption is dominated by oxygen atoms of the hydroxyl and carboxyl groups, with minor contributions from the aromatic ring. Compared to vanillic acid, ISVA possesses fewer highly reactive sites and lower overall reactivity, consistent with its larger HOMO-LUMO gap and lower softness, explaining its relatively weaker corrosion inhibition efficiency.

**Table 2: Fukui Indices for Isovanillic Acid**

| | **Electrophilic Attack (-)** | | **Nucleophilic Attack (+)** | | **Radical (0)** | |
|---|---|---|---|---|---|---|
| **ATOMS** | **Mulliken** | **Hirshfield** | **Mulliken** | **Hirshfield** | **Mulliken** | **Hirshfield** |
| C (1) | 0.064 | 0.059 | 0.065 | 0.059 | 0.064 | 0.059 |
| C (2) | 0.029 | 0.053 | 0.028 | 0.052 | 0.029 | 0.052 |
| C (3) | 0.063 | 0.068 | 0.062 | 0.068 | 0.063 | 0.068 |
| C (4) | 0.048 | 0.055 | 0.047 | 0.054 | 0.047 | 0.054 |
| O (5) | 0.043 | 0.062 | 0.057 | 0.061 | 0.042 | 0.062 |
| C (6) | 0.057 | 0.055 | 0.042 | 0.055 | 0.057 | 0.055 |
| O (7) | 0.044 | 0.053 | -0.022 | 0.052 | 0.043 | 0.052 |
| C (8) | -0.021 | 0.030 | 0.043 | 0.030 | -0.022 | 0.030 |
| C (9) | 0.045 | 0.063 | 0.057 | 0.063 | 0.044 | 0.063 |
| C (10) | 0.058 | 0.070 | 0.057 | 0.070 | 0.058 | 0.070 |
| O (11) | 0.098 | 0.099 | 0.095 | 0.097 | 0.097 | 0.098 |
| O (12) | 0.034 | 0.056 | 0.032 | 0.055 | 0.033 | 0.056 |
| H (13) | 0.061 | 0.038 | 0.062 | 0.039 | 0.061 | 0.038 |
| H (14) | 0.063 | 0.043 | 0.067 | 0.045 | 0.065 | 0.044 |
| H (15) | 0.043 | 0.027 | 0.044 | 0.027 | 0.044 | 0.027 |
| H (16) | 0.044 | 0.027 | 0.045 | 0.027 | 0.045 | 0.027 |
| H (17) | 0.041 | 0.026 | 0.042 | 0.026 | 0.042 | 0.026 |
| H (18) | 0.059 | 0.036 | 0.060 | 0.037 | 0.060 | 0.036 |
| H (19) | 0.062 | 0.039 | 0.064 | 0.040 | 0.063 | 0.040 |
| H (20) | 0.064 | 0.043 | 0.067 | 0.045 | 0.066 | 0.044 |

### 3.1.3 Fukui Function Analysis of the Studied Inhibitors

The Fukui indices derived from DND calculations highlight the reactive sites of VA and ISVA for nucleophilic ($f^+$) and electrophilic ($f^-$) attacks. For VA, the highest nucleophilic site is C (9) ($f^+ = 0.118$ Mulliken), suggesting that this carbon atom can donate electrons effectively to the aluminum surface, while the most electrophilic sites are O (4) and O (8) ($f^- \approx 0.110$-$0.114$), indicating their potential to accept electrons from the metal. Similarly, for ISVA, O (11) shows the highest Fukui indices for both nucleophilic ($f^+ \approx 0.095$-$0.097$) and electrophilic ($f^- \approx 0.098$-$0.099$) attacks, suggesting that this oxygen atom is the primary reactive center for adsorption on aluminum. These results indicate that adsorption of both inhibitors is likely dominated by oxygen-containing functional groups, facilitating coordination with the metal surface and enhancing protective layer formation.

The trends observed here are consistent with previous DFT studies, which demonstrate that heteroatoms such as oxygen in phenolic acids serve as key active sites for metal interaction and corrosion inhibition (Alaoui *et al.,* 2025; Ibrahim *et al.,* 2023; Rani and Basu, 2023; Azeez *et al.,* 2024). Furthermore, these findings align with experimental and theoretical studies on flavonoid-based green inhibitors from *Adansonia digitata* leaf extract, where Fukui function analysis successfully identified reactive sites responsible for adsorption and inhibition efficiency on metal surfaces (Abdullahi *et al.,* 2025).

### 3.2 Active sites

Fukui function analysis (Table 3) was employed to identify the most reactive sites of VA and ISVA toward electrophilic and nucleophilic attacks. For VA, the highest nucleophilic site was found to be the carbon atom C (9) with a Mulliken index of 0.118, while oxygen atoms O (4) and O (8) exhibited the highest electrophilic indices (Mulliken values of 0.110 and 0.114, respectively), indicating that these sites are most likely to accept electrons from the aluminum surface. Similarly, for ISVA, the oxygen atom O (11) was identified as the dominant reactive center, showing the highest nucleophilic and electrophilic Fukui indices ($f^+ \approx 0.095$-$0.097$, $f^- \approx 0.098$-$0.099$), suggesting its critical role in adsorption and interaction with the metal. These results indicate that oxygen-containing functional groups serve as primary active sites for inhibitor-metal coordination, while specific carbon atoms within the aromatic ring contribute to electron donation during adsorption (Ayuba *et al.,* 2020; Nyijime *et al.,* 2023).

**Table 3: Calculated Fukui Indices from DND for the Studied Inhibitor Molecules**

| **Nucleophilic($F^+$)** | | | | | **Electrophilic($F^-$)** | | | |
|---|---|---|---|---|---|---|---|---|
| **Molecule** | **Mullikan** | | **Hirshfield** | | **Mullikan** | | **Hirshfield** | |
| | **Atom** | **Value** | **Atom** | **Value** | **Atom** | **Value** | **Atom** | **Value** |
| VA | C (9) | 0.118 | O (4) | 0.110 | O (8) | 0.114 | C (9) | 0.108 |
| ISVA | O (11) | 0.095 | O (11) | 0.097 | O (11) | 0.098 | O (11) | 0.099 |

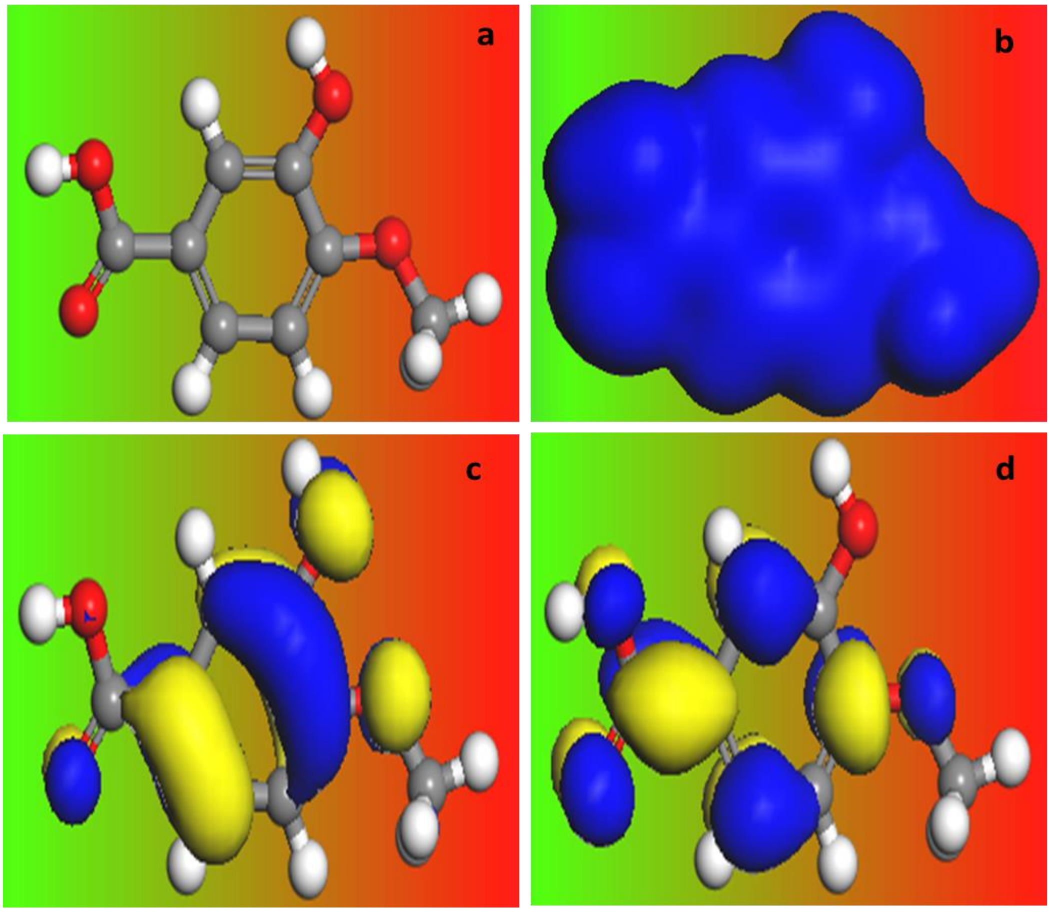

**Fig. 2: Electronic and Structural Properties of the Isovanillic Acid molecule: a) Geometry Optimized b) Total Electron Density c) Highest Occupied Molecular Orbital d) Lowest Unoccupied Molecular Orbital**

### 3.3 Quantum Chemical Parameters

The quantum chemical parameters of VA and ISVA provide insight into their corrosion inhibition potential on aluminum. VA exhibits a more negative E-HOMO of -7.727 eV than ISVA of -6.243 eV, indicating a stronger tendency to donate electrons to vacant orbitals of the aluminum surface, which facilitates chemisorption and protective film formation (Ibrahim *et al.,* 2023). Additionally, VA has a smaller energy gap ΔE = 1.691 eV compared to ISVA (ΔE = 4.347 eV), reflecting higher chemical reactivity and polarizability, which are favorable for adsorption (Azeez *et al.,* 2024). The global hardness and softness values further support this, with VA showing lower hardness (0.836 eV) and higher softness (1.198) relative to ISVA, implying stronger interaction with the metal surface (Alaoui *et al.,* 2025). The fraction of electrons transferred (ΔN) is also higher for VA (1.671 vs. 0.916 for ISVA), suggesting more effective electron donation to aluminum and the formation of a more stable protective layer (Table 4). Collectively, these descriptors indicate that VA is the superior inhibitor, consistent with literature reports linking low ΔE, high softness, and greater ΔN to enhanced inhibition efficiency in acidic media (Rani and Basu, 2023).

**Table 4: Computed Quantum Chemical Parameters of the Studied Inhibitor Molecules**

| Electronic/structural property | Vanillic Acid | Isovanillic Acid |
|---|---|---|
| $E_{HOMO}$ (eV) | -7.727 | -6.243 |
| $E_{LUMO}$ (eV) | -6.036 | -1.896 |
| ΔE(eV) | 1.691 | 4.347 |
| Molecular mass(g/mol) | 160.0 | 140.0 |
| Ionization potential (IP) (eV) | 7.727 | 6.243 |
| Electron affinity (EA) (eV) | 6,036 | 1.896 |
| Global Hardness(η) | 0.836 | 2.173 |
| Global softness Global Softness (σ) | 1.198 | 0.460 |
| Electronegativity (χ) | 6.892 | 4.069 |
| Fractions of Electrons Transferred (ΔN) | 1.671 | 0.916 |

### 3.4 Molecular Dynamics Simulations

The molecular dynamics simulation results as presented in Table 5, indicate that both VA and ISVA adsorb spontaneously and stably on the aluminum surface, as evidenced by their negative adsorption energies. ISVA exhibits a slightly more negative adsorption energy (-0.706 eV) and higher binding energy (0.706 eV) than VA (-0.692 Ev and 0.692 eV), suggesting marginally stronger adsorption under dynamic conditions. Similar trends have been reported for phenolic and oxygen-containing organic inhibitors interacting with metal surfaces, where negative adsorption energies are indicative of stable inhibitor-metal interactions (Kaya *et al.,* 2021; Peng Liu *et al.,* 2023). The higher total potential and molecular energies observed for ISVA arise from intrinsic structural differences and adsorption orientation rather than weaker surface interaction. Despite ISVA showing slightly stronger adsorption in MD simulations, VA is expected to exhibit superior inhibition efficiency when electronic reactivity is considered, as supported by its lower HOMO-LUMO energy gap, higher global softness, and greater electron transfer capability obtained from DFT calculations (Ibrahim *et al.,* 2023). Overall, the MD results complement the DFT findings and confirm that effective corrosion inhibition depends on both adsorption strength and molecular electronic properties (Bentiss *et al.,* 2022).

**Table 5: Calculated molecular dynamic simulation parameters for the studied Phenolic acids**

| Phenolic acids Energies (eV) | Vanillic Acid | Isovanillic Acid |
|---|---|---|
| Total Potential Energy | 0.573 | 0.644 |
| Energy of Molecule | 0.920 | 1.338 |
| Energy of Al (110) Surface | 0.0000 | 0.0000 |
| Adsorption Energy | -0.692 | -0.706 |
| Binding Energy | 0.692 | 0.706 |

### 3.5 Correlation between DFT and MD Results

The integrated DFT and MD simulations provide a multiscale understanding of the corrosion inhibition behavior of VA and ISVA on aluminum surfaces in acidic media. DFT calculations reveal that VA exhibits higher electron-donating ability, increased chemical softness, and multiple reactive centers primarily the oxygen atoms in hydroxyl and carboxyl groups, with additional stabilization from aromatic π-electrons allowing stronger and more distributed chemisorption on aluminum compared to ISVA, which displays fewer active sites (Obot *et al.,* 2020; Alaoui *et al.,* 2025). These electronic features suggest that VA can form a more stable and protective adsorbed layer. MD simulations validate these predictions by capturing the dynamic adsorption process in aqueous acidic conditions. Vanillic acid demonstrates superior surface coverage, favorable molecular orientation, and enhanced hydrogen-bonding interactions with the solvent, resulting in a compact and adherent protective film, while ISVA shows a more localized adsorption pattern (Kaya *et al.,* 2021; Bentiss *et al.,* 2022; Peng Liu *et al.,* 2023). The strong agreement between DFT predicted electronic reactivity and MD observed adsorption dynamics establishes a clear structure-activity relationship, linking molecular properties to inhibitor performance (Ibrahim *et al.,* 2023; Rani and Basu, 2023; Azeez *et al.,* 2024). This integrated DFT-MD framework provides a robust molecular-level explanation of aluminum corrosion inhibition and offers a rational strategy for the computational screening and design of environmentally benign corrosion inhibitors (El Faydy *et al.,* 2023).

## 4. CONCLUSION

This study employed a combined DFT and MD simulation approach to investigate the corrosion inhibition behavior of phenolic acid derivatives-vanillic and isovanillic acids on aluminum in acidic media. DFT calculations revealed that VA exhibits higher HOMO energy, smaller energy gap, greater global softness, and a larger fraction of electrons transferred compared to ISVA, indicating stronger electron-donating ability, higher chemical reactivity, and greater adsorption propensity on the aluminum surface. Fukui function analysis identified oxygen atoms in hydroxyl and carboxyl groups, particularly O (4), O (8), O (11), and O (12) in VA, as the most reactive sites for electrophilic, nucleophilic, and radical attacks, while O (11) was highlighted as the primary reactive site in ISVA. These results suggest that adsorption occurs predominantly via oxygen-containing functional groups, with additional contributions from aromatic π-electron density, facilitating stable inhibitor-metal interactions. MD simulations further confirmed strong adsorption of both inhibitors on the Al (111) surface in an aqueous environment, with adsorption energies of -0.692 eV for VA and -0.706 eV for ISVA, and revealed favorable molecular orientation, surface coverage, and hydrogen bonding interactions that stabilize the protective inhibitor layer. Generally, the computational results are consistent with experimental observations, demonstrating that VA provides superior corrosion inhibition compared to ISVA due to its higher reactivity, multiple active adsorption sites, and stronger electron-donating capability. This integrated DFT-MD study highlights the potential of phenolic acid-based derivatives as effective and environmentally friendly corrosion inhibitors for aluminum in acidic media and provides valuable molecular-level insights to guide the rational design of green inhibitors.

### Future Work

Future studies could extend this integrated approach to explore other naturally occurring phenolic compounds and their derivatives, investigate the effects of mixed inhibitor systems, and evaluate the influence of temperature, pH, and ionic strength on adsorption behavior. Additionally, coupling DFT-MD simulations with experimental electrochemical and surface characterization techniques could further validate the predictive capability of this computational framework and assist in the design of next-generation eco-friendly corrosion inhibitors.

### Conflicts of Interest

The authors declare that they have no conflicts of interest that could have influenced this work.

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