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DFT and Molecular Dynamics Simulation in the Discovery of Green Corrosion Inhibitors: Current Progress and Future Challenges

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Abstract: Growing environmental concerns associated with conventional corrosion inhibitors have intensified research into sustainable alternatives derived from plants, agricultural residues, and other renewable resources. Density functional theory (DFT) and molecular dynamics (MD) simulations have become valuable tools for investigating the molecular properties and adsorption mechanisms of green corrosion inhibitors. This review critically examines their complementary applications in inhibitor discovery, emphasizing phytochemical reactivity, inhibitor–metal interactions, adsorption energetics, and the relationship between computational predictions and experimental corrosion performance. DFT-based descriptors, including frontier molecular orbital energies, energy gaps, and charge distributions, are evaluated alongside MD-derived adsorption energies, molecular configurations, and interfacial properties. Particular attention is given to the influence of protonation, solvation, electrolyte composition, force-field selection, and metal-surface characteristics on computational reliability. The review also identifies persistent limitations, including the chemical variability of plant extracts, oversimplified surface models, inadequate sampling, and the overinterpretation of individual molecular descriptors. Emerging opportunities include integrating DFT and MD with electrochemical measurements, machine learning, and environmental assessment to improve candidate screening and mechanistic understanding. Future research should prioritize standardized computational protocols, uncertainty quantification, reproducibility, and validation under experimentally relevant conditions. Such integration could advance the transition from qualitative molecular interpretation towards more reliable prediction and rational design of effective, environmentally responsible corrosion inhibitors.

1. Introduction

Corrosion causes substantial economic losses and threatens the integrity of infrastructure in the oil and gas, chemical processing, marine, and construction industries (Alamri, 2020; Hamidah *et al*., 2021; Zakeri *et al*., 2022). Conventional corrosion inhibitors can provide effective protection, but environmental and health concerns associated with some formulations have encouraged the development of greener alternatives (Salleh *et al*., 2021; Zakeri *et al*., 2022). Plant extracts, agricultural residues, essential oils, amino acids, and other renewable materials have attracted considerable interest because they contain functional groups capable of interacting with metal surfaces (Aouarbi *et al*., 2021; Donkor *et al*., 2022; Zriouel *et al*., 2026).

Green inhibitors may contain phenolics, flavonoids, tannins, alkaloids, and other compounds containing oxygen, nitrogen, sulfur, or aromatic π-electron systems. These structural features can influence adsorption and the formation of protective interfacial films on metallic substrates (Donkor *et al*., 2022). Their performance depends on chemical composition, concentration, solubility, protonation, adsorption, and the surrounding corrosive environment. Consequently, natural origin alone does not guarantee effectiveness or environmental safety; systematic evaluation of inhibition performance and potential environmental impacts remains essential (Zakeri *et al*., 2022).

Experimental techniques such as weight-loss measurements, potentiodynamic polarization (PDP), electrochemical impedance spectroscopy (EIS), and surface characterization establish inhibition performance but may not fully explain the molecular mechanisms involved. Density functional theory (DFT) and molecular dynamics (MD) simulations complement these methods by investigating molecular electronic properties, adsorption behaviour, and inhibitor–metal interactions at the atomic scale (Zarrouk *et al*., 2013; Verma *et al*., 2018; Essien *et al*., 2023, 2024).

DFT characterizes electronic structure and molecular reactivity, whereas MD examines the dynamic behaviour and configurations of inhibitors near model metal surfaces. Their combined application can support candidate selection and mechanistic interpretation, particularly when computational predictions are compared with experimental measurements (Donkor *et al*., 2022; Zerrouk *et al*., 2025). However, calculated descriptors do not automatically predict experimental inhibition efficiency because solvent effects, surface conditions, inhibitor composition, and simulation assumptions can influence the results. This review evaluates the contributions, limitations, and future opportunities of DFT and MD in discovering sustainable corrosion inhibitors. Recent studies by Essien *et al*. (2023, 2024) and Ozoemena *et al*. (2024) illustrate the use of quantum-chemical calculations to interpret candidate inhibitor structures, while Boekom *et al*. (2020) provides a related pyridine adsorption and molecular-simulation case.

2. Green corrosion inhibitors and adsorption mechanisms

Green corrosion inhibitors are obtained from plant leaves, roots, bark, seeds, fruit peels, agricultural waste, and other renewable resources. Their potentially active constituents include phenolics, flavonoids, tannins, alkaloids, and other organic compounds containing hydroxyl, carbonyl, amino, sulfur-containing, and aromatic groups that can facilitate interactions with metallic surfaces (Donkor *et al*., 2022; Salleh *et al*., 2021). Corrosion protection can involve electrostatic attraction between charged inhibitor species and metal surfaces, donor–acceptor interactions, dispersion forces, hydrogen bonding, and the formation of protective interfacial films. These mechanisms may operate simultaneously, depending on the inhibitor's molecular structure, the nature of the metal, and the corrosive environment. Computational investigations can help explain these interactions by examining molecular electronic properties, adsorption configurations, and inhibitor–surface binding (Donkor *et al*., 2022). In other words, the inhibitory action of natural extracts is mainly regarded as a intermolecular synergistic effect of the various components rich in aromatic rings, double and triple bonds as well as the heteroatoms (Khadom *et al*., 2022; Lrhoul *et al*., 2023; Barbu *et al*., 2025)

Plant extracts present a particular challenge because their chemical composition varies with species, geographical origin, harvesting conditions, and extraction procedures. Computational studies therefore benefit from chemical profiling using techniques such as gas chromatography–mass spectrometry (GC–MS), liquid chromatography–mass spectrometry (LC–MS), and Fourier-transform infrared spectroscopy (FTIR). These techniques help identify and characterize extract constituents and functional groups that may contribute to adsorption and corrosion protection (Salleh *et al*., 2021). For

example, Obot *et al*. (2021) combined thermodynamic evaluation with quantum-chemical analysis of n-hexane extracts of Costus lucanusianus, showing how a chemically complex botanical material can be linked to candidate molecular descriptors without assuming that one constituent explains the entire extract response.

Reviews by Salleh *et al.* (2021) and other researchers on plant-derived corrosion inhibitors highlight the potential of renewable materials for sustainable corrosion control. Nevertheless, identifying a potentially active compound within an extract does not establish its individual contribution to overall inhibition performance. Differences in constituent concentration, interactions among compounds, and solution chemistry may influence the observed response. Consequently, isolated-compound testing, appropriate computational analysis, and experimental validation remain essential for establishing credible structure–activity relationships (Donkor *et al.*, 2022).

3. Density functional theory in inhibitor discovery

Density functional theory (DFT) is a quantum-mechanical method used to investigate molecular geometry, electronic structure, charge distribution, and chemical reactivity. In corrosion-inhibition research, DFT provides insights into the electronic characteristics of candidate inhibitor molecules and helps identify regions that may participate in interactions with metal surfaces. It is widely used to complement experimental investigations and develop mechanistic explanations for observed inhibition behaviour (Obot *et al*., 2015; Donkor *et al*., 2022; Boekom *et al*., 2020; Ozoemena *et al*., 2024).

3.1. Frontier molecular orbitals and reactivity descriptors

The highest occupied molecular orbital (HOMO) is commonly associated with a molecule's electron-donating tendency, whereas the lowest unoccupied molecular orbital (LUMO) is associated with its electron-accepting tendency. The energy difference between these orbitals, known as the HOMO–LUMO energy gap, is expressed as:

$$\Delta E_{gap} = E_{LUMO} - E_{HOMO}$$

A smaller HOMO–LUMO gap is often interpreted as indicating greater electronic responsiveness or polarizability within a comparable set of molecules. However, this relationship should not be treated as a universal rule for corrosion inhibition: a smaller energy gap does not necessarily imply stronger adsorption, greater surface coverage, or higher experimental inhibition efficiency (Obot *et al.*, 2015; Razali *et al.*, 2024).

Other descriptors commonly employed in DFT studies include electronegativity, chemical hardness, chemical softness, molecular electrostatic potential, atomic charges, and Fukui functions. These parameters provide complementary information about electron distribution, molecular reactivity, and potential adsorption sites. Fukui functions, in particular, can help identify atoms or molecular regions susceptible to electrophilic or nucleophilic interactions. Nevertheless, such descriptors indicate possible reactivity rather than directly establishing the strength or geometry of adsorption at a metal interface (Donkor *et al*., 2022; Razali *et al*., 2024).

The reliability of calculated descriptors depends on factors such as the exchange–correlation functional, basis set, molecular charge, geometry optimization, and treatment of the surrounding solvent. Furthermore, calculations performed on isolated inhibitor molecules do not explicitly represent the metal–inhibitor interface. Consequently, molecular descriptors should be interpreted alongside

surface-based calculations, adsorption-energy analysis, and experimental evidence wherever these are available (Obot *et al.*, 2015; Chen *et al.*, 2025).

3.2. Protonation and solvent effects

Molecular protonation is particularly important when evaluating corrosion inhibitors in acidic environments, including hydrochloric acid (HCl) and sulfuric acid (H_2SO_4). Protonation can alter molecular charge distribution, frontier orbital energies, solubility, and adsorption behaviour. Depending on the molecule and solution conditions, protonated species may interact with the metal interface differently from their neutral forms. Therefore, calculations restricted to neutral molecules may not adequately represent the inhibitor species present under experimental conditions (Donkor *et al.*, 2022; Razali *et al.*, 2024).

A more reliable computational approach evaluates chemically plausible protonation states and incorporates solvent effects where feasible. Continuum-solvation models can account approximately for the influence of the surrounding medium, while explicit solvent and electrolyte models may provide additional information about interfacial interactions. For a more complete description, researchers should distinguish between descriptors calculated for isolated molecules and properties obtained from explicit molecule–surface models, where adsorption configurations and interaction energies can be evaluated directly (Obot *et al.*, 2015; Chen *et al.*, 2025).

Overall, DFT is most useful for generating mechanistic hypotheses, identifying potentially reactive molecular sites, and prioritizing candidate inhibitors for further investigation. Its predictive value improves when electronic descriptors are interpreted collectively and integrated with molecular dynamics simulations and experimental corrosion measurements rather than used individually to estimate inhibition efficiency (Donkor *et al.*, 2022; Razali *et al.*, 2024).

4. Molecular dynamics simulation

Molecular dynamics (MD) simulation is a computational technique that models the time-dependent motion of atoms and molecules by solving their equations of motion under a specified interaction potential. In corrosion-inhibitor research, MD is widely used to investigate adsorption configurations, molecular orientation, interfacial distribution, and the structural stability of inhibitor molecules near metal surfaces. When combined with density functional theory (DFT), MD can provide complementary information about molecular electronic properties and inhibitor–surface interactions, supporting a more comprehensive interpretation of corrosion-inhibition mechanisms (Donkor *et al.*, 2022; Heinz *et al.*, 2008).

A typical MD model comprises a metal slab, inhibitor molecules, and an aqueous environment. Depending on the research objective, the simulation may also include water molecules, dissolved ions, protonated inhibitor species, and other components of the corrosive medium. The selected surface orientation, surface coverage, molecular composition, and electrolyte conditions should reflect the intended application as closely as computationally feasible. These factors influence the predicted adsorption configurations and interfacial organization (Heinz *et al.*, 2008; Donkor *et al.*, 2022).

4.1. Adsorption energy and interfacial behaviour

Adsorption energy is commonly used to assess the energetic favourability of inhibitor association with a model metal surface. One frequently employed expression is:

$$E_{ads} = E_{surface+inhibitor} - E_{surface} - E_{inhibitor}$$

Under this convention, a negative adsorption energy indicates that the combined surface–inhibitor system has lower energy than the corresponding separated reference systems. More negative values may indicate more favourable adsorption energetics when the same computational method, model conditions, and reference states are used. However, adsorption energy is not equivalent to adsorption free energy, which also accounts for entropic and other thermodynamic contributions (Donkor *et al*., 2022).

The interpretation of adsorption energies requires particular care because results may depend on the force field, surface model, solvent representation, and reference-state definition. In aqueous corrosion environments, solvent displacement, molecular rearrangement, temperature, and inhibitor concentration can influence adsorption behaviour. Consequently, adsorption energies obtained using different computational protocols should not be compared directly without establishing their methodological compatibility (Heinz *et al*., 2008; Donkor *et al*., 2022).

Other useful MD outputs include radial distribution functions, molecular density profiles, surface coverage, and residence times. These quantities help characterize the spatial distribution, orientation, and persistence of inhibitor molecules near a metal surface. Nevertheless, they provide evidence of interfacial organization rather than independent proof of chemical bond formation or quantitative prediction of corrosion rates.

4.2. Model reliability and limitations

The reliability of MD predictions depends on the representation of the metal surface, the selected force field, molecular charge assignment, electrolyte composition, temperature, and simulation duration. Idealized iron surfaces may not fully represent practical steel substrates, which can contain alloying elements, surface defects, oxides, and corrosion products. Surface orientation and the presence of water and dissolved ions can also influence the predicted adsorption configurations. Appropriate parameterization of metal–organic and metal–solvent interactions is therefore essential for obtaining meaningful results (Heinz *et al.*, 2008; Donkor *et al.*, 2022).

A further limitation is that conventional classical MD generally employs predefined interaction potentials and does not explicitly describe changes in electronic structure. Consequently, it cannot ordinarily reproduce bond formation, bond breaking, or metal dissolution unless reactive force fields or specialized computational approaches are used. Researchers should justify the selected model and force field, assess equilibration and convergence, and report sufficient methodological details to support reproducibility.

Where feasible, simulations should examine multiple initial configurations and independent trajectories to assess whether the observed adsorption behaviour is robust. The effects of simulation-cell dimensions, surface coverage, solvent representation, and electrolyte composition should also be considered. Combining MD with DFT calculations and experimental measurements can strengthen mechanistic interpretations, although agreement between computational outputs and experimental observations should be demonstrated rather than assumed (Donkor *et al*., 2022).

Overall, MD provides valuable insights into the dynamic organization and adsorption behaviour of green corrosion inhibitors at model metal interfaces. Its greatest contribution lies in complementing electronic-structure calculations and experimental characterization, while recognizing that simulated adsorption behaviour alone cannot establish inhibition efficiency or long-term corrosion protection. Boekom *et al*. (2020) is a relevant regional case study of pyridine adsorption on mild steel in HCl; however, studies should distinguish between quantum-chemical/adsorption analyses and fully specified atomistic MD simulations when comparing methodological depth.

5. Integration of DFT, MD, and experimental measurements

Density functional theory (DFT), molecular dynamics (MD) simulations, and experimental corrosion measurements provide complementary information for the discovery and mechanistic evaluation of green corrosion inhibitors. DFT characterizes molecular electronic structure, reactivity, and potential adsorption sites, whereas MD examines molecular orientation, adsorption configurations, and interfacial organization under specified simulation conditions. Experimental measurements establish whether these predicted interactions correspond to measurable corrosion protection (Obot *et al.*, 2015; Donkor *et al.*, 2022; Boekom *et al.*, 2020; Ozoemena *et al.*, 2024; Ech-chihbi *et al.*, 2025).

An integrated computational–experimental workflow can connect molecular-level predictions with observed inhibition performance. The process begins with the identification and chemical characterization of promising green materials, followed by computational screening and experimental validation. Results from each stage can then be used to refine subsequent investigations.

A practical workflow involves the following stages:

1. Identification and characterization of green materials: Select suitable plant extracts, agricultural residues, or renewable compounds and characterize their chemical composition using appropriate analytical techniques, such as GC–MS, LC–MS, and FTIR.
2. DFT calculations: Optimize molecular geometries and evaluate plausible protonation states, electronic descriptors, charge distributions, and potentially reactive molecular sites.
3. MD simulations: Investigate adsorption configurations, interfacial distributions, and the relative stability of inhibitor molecules near representative metal surfaces in an appropriately modelled environment.
4. Experimental validation: Evaluate corrosion protection using weight-loss measurements, potentiodynamic polarization (PDP), electrochemical impedance spectroscopy (EIS), and suitable surface-characterization techniques.
5. Model refinement: Compare computational predictions with experimental observations and refine molecular structures, surface representations, or simulation conditions where discrepancies arise.

This integrated approach is consistent with the use of computational chemistry to interpret inhibitor–surface interactions and prioritize candidate compounds, while recognizing that experimental evidence remains essential for establishing practical performance (Obot *et al.*, 2015; Donkor *et al.*, 2022; Boekom *et al.*, 2020; Ozoemena *et al.*, 2024).

5.1. *Quantitative comparison with experimental inhibition efficiency*

Experimental inhibition efficiency provides a quantitative measure of the reduction in corrosion under specified conditions. When corrosion current densities are obtained from PDP measurements, inhibition efficiency can be calculated as follows:

$$\eta_{PDP}(\%) = \left[\frac{i_{corr,o} - i_{corr,inh}}{i_{corr,o}} \right] x \ 100$$

where icorr,0 is the corrosion current density of the uninhibited system and icorr, inh is the corrosion current density in the presence of the inhibitor. This expression assumes that both measurements are obtained under comparable experimental conditions. The result indicates the percentage reduction in corrosion current density attributable to the inhibitor (ASTM International, 2023).

For weight-loss experiments, inhibition efficiency is calculated using the corrosion rates or mass losses of the uninhibited and inhibited specimens, provided that exposure times and other relevant conditions are comparable. EIS provides complementary information about interfacial processes, including changes in charge-transfer resistance and coating or surface-film behaviour, depending on the equivalent-circuit model and system investigated (ASTM International, 2023; ASTM International, 2024).

Computational predictions should be compared with experimental measurements obtained under clearly defined and comparable conditions, including inhibitor concentration, temperature, electrolyte composition, exposure duration, and metal-surface characteristics. Agreement between calculated adsorption energies and experimental inhibition efficiency may support a proposed adsorption mechanism, but it does not establish a universal quantitative relationship. Adsorption energy describes an interaction under a specified computational model, whereas inhibition efficiency reflects the overall corrosion response of a real or experimentally modelled system.

5.2. Mechanistic interpretation and validation

Experimental adsorption-isotherm analysis can help characterize relationships between inhibitor concentration and surface coverage. However, a good fit to an adsorption isotherm does not, by itself, conclusively establish a unique adsorption mechanism. Different models may describe similar experimental trends, and estimated surface coverage depends on how it is determined. Mechanistic conclusions are therefore stronger when supported by independent evidence from electrochemical measurements, surface characterization, DFT calculations, and MD simulations (Donkor *et al*., 2022).

Overall, integrating DFT, MD, and experimental measurements provides a more rigorous basis for understanding green corrosion inhibitors than relying on any single technique. This approach can help identify promising molecular candidates, assess proposed adsorption mechanisms, and distinguish computational hypotheses from experimentally demonstrated performance. Its effectiveness depends on transparent reporting, appropriate model selection, reproducibility, and validation under conditions relevant to the intended corrosion-control application. Relevant Nigerian studies further demonstrate complementary parts of this workflow: quantum-chemical and FTIR investigations of isoxazole inhibitors (Essien *et al*., 2023, 2024), extract-based thermodynamic and quantum-chemical analysis (Obot *et al*., 2021), Schiff-base/complex corrosion tests (Ozoemena *et al*., 2023), and computational comparison of Schiff-base structures (Ozoemena *et al*., 2024). These studies are valuable evidence for the molecule and performance stages, although they do not all report the same combination of DFT, MD, and sustainability testing.

Table 1. Selected studies combining DFT and MD in green corrosion-inhibitor research

Researcher(s) and year	Green inhibitor / material	Experimental and computational approach	Major findings	Contribution to the field and limitations
Abdelaziz *et al.* (2021)	Arbutus unedo leaf extract; quercetin and catechin as representative constituents	Weight-loss/electrochemical studies, surface characterization, DFT and MD	Reported a maximum inhibition efficiency of 91.72% at 0.5 g/L and 298 K. MD indicated that quercetin adsorbed spontaneously in a near-	Demonstrated how quantum-chemical descriptors and MD adsorption configurations can help explain experimental inhibition performance. A limitation

			parallel orientation on the iron surface.	is that simulations of selected compounds cannot fully represent the complexity of the whole plant extract.
Berrissoul *et al.* (2022)	Aqueous extract of Origanum compactum Benth.	HPLC-based chemical profiling, weight loss, EIS, PDP, DFT and MD	Reported 92% inhibition efficiency at 0.4 g/L in 1 M HCl. Experimental results and computational predictions supported adsorption-controlled, mixed-type inhibition.	Established a useful experimental–computational workflow for investigating phytochemical inhibitors. Further work is needed to connect individual constituents, extract variability and long-term protective-film stability.
Ramezanzadeh *et al.* (2018)	Nettle (Urtica dioica) leaf extract	EIS, polarization, SEM, AFM, ab initio quantum calculations, Monte Carlo and MD simulations	Reported approximately 92% inhibition efficiency after 2 h in 1 M HCl. Computational results supported adsorption through donor–acceptor interactions and agreement with the experimental evidence.	Illustrates the value of combining quantum calculations, adsorption-energy analysis and surface characterization. Extract composition and the accuracy of idealized surface models remain important considerations.
Al-Moubaraki *et al.* (2022)	Natural plant extracts and their major constituent molecules	Experimental corrosion tests, DFT, density-functional tight-binding (DFTB) and MD	Combined electronic descriptors, including HOMO–LUMO energy gaps, electronegativity and charge-transfer indicators, with simulations of molecular adsorption at metal interfaces.	Advanced multilevel computational interpretation of natural inhibitors. Its broader lesson is that molecular descriptors should be interpreted alongside interfacial simulations and experimental measurements, not used alone to rank inhibitor performance.
Abeng *et al.* (2025)	Natamycin and cefmetazole as potentially more environmentally preferable inhibitor candidates	DFT and MD simulations of electronic properties and adsorption on mild steel	Natamycin exhibited a reported HOMO–LUMO gap of 0.5 eV and adsorption energy of −92.7 kJ/mol; cefmetazole showed a gap of 2.45 eV and adsorption energy of −67 kJ/mol.	Provides a comparative molecular-design approach for assessing adsorption and electronic reactivity. Because these are pharmaceutical compounds, their environmental suitability requires independent toxicity, biodegradability

				and life-cycle assessment rather than being assumed from their computational performance.
Abeng *et al.* (2026)	Eupatorium capillifolium extract; methyleugenol as a major candidate constituent	EIS, PDP, SEM, DFT and MD	Reported a maximum inhibition efficiency of 91.1% at 2.0 g/L in 0.5 M H_2SO_4. Methyleugenol was reported to have a favorable adsorption energy of −98.48 kcal/mol on Fe(110); protonation affected its calculated electronic properties and interaction with iron.	Highlights the importance of protonation state and experimental–computational agreement. Further validation is needed under varied temperatures, electrolyte compositions and longer exposure periods.

Table 2. What these studies reveal about current progress and future challenges

Research theme	Progress demonstrated by researchers	Remaining challenge	Recommended direction for future research
Electronic structure using DFT	HOMO/LUMO energies, energy gaps, charge distribution and reactive sites help explain molecular reactivity	A small energy gap or high HOMO energy does not independently establish strong corrosion inhibition.	Combine molecular descriptors with experimental corrosion rates, adsorption energies and validated interfacial models. Al-Moubaraki *et al*. (2022)
Adsorption configurations using MD	Simulations reveal inhibitor orientation, surface coverage and interactions between organic molecules and iron.	Ideal iron surfaces and simplified solution models may not represent real corroding steel.	Incorporate realistic surface structures, explicit water, hydronium, chloride or sulfate ions, and competing adsorbates. Ramezanzadeh *et al.* (2018)
Extract composition and active species	Chemical profiling combined with DFT and MD can identify candidate compounds responsible for adsorption.	Extracts contain many compounds whose concentrations vary with plant source, season and extraction method.	Use GC–MS/LC–MS profiling, fractionation and testing of isolated constituents and reconstructed mixtures. Abdelaziz *et al.* (2021)
Agreement between experiments and simulations	Several studies report consistency between electrochemical measurements and theoretical predictions.	Agreement may be qualitative, and computed adsorption energies are not directly equivalent to measured inhibition efficiency.	Establish quantitative correlations, uncertainty estimates and independent experimental validation. Berrissoul *et al.* (2022)

Temperature, protonation and electrolyte effects	Studies show that molecular charge state and the chemical environment can influence adsorption and inhibition.	Many studies examine only a narrow range of temperatures, concentrations and solution conditions.	Investigate multiple protonation states, solvent effects, ionic competition and temperature-dependent adsorption. Abdelaziz *et al*. (2021)
Industrial application and sustainability	Natural extracts and selected bio-derived compounds are promising alternatives to conventional inhibitors.	Short laboratory tests do not establish long-term protection, environmental safety or economic viability.	Conduct long-duration corrosion tests, biodegradation and toxicity assessments, life-cycle analysis and pilot-scale trials. Berrissoul *et al.* (2022)

The literature demonstrates that integrating DFT with MD provides a stronger mechanistic basis for green corrosion-inhibitor discovery than relying exclusively on electrochemical measurements or isolated quantum-chemical descriptors. DFT helps identify the electronic characteristics of potentially active molecules, whereas

6. Molecule-to-interface-to-performance-to-sustainability framework

To connect computational chemistry with practical corrosion control, the literature is organized here as four linked stages: molecule, interface, performance, and sustainability. The stages are iterative rather than strictly linear. Chemical profiling informs molecular selection; DFT generates hypotheses about electronic reactivity; MD examines the inhibitor–electrolyte–metal interface; experiments test whether the predicted interactions reduce corrosion; and sustainability assessment determines whether the candidate is suitable for wider use. Disagreement between predicted and measured behaviour should trigger refinement of the molecular form, surface model, electrolyte representation, or experimental design (Donkor *et al.*, 2022; Castillo-Robles *et al.*, 2024).

6.1. Molecule: active-compound identification and DFT descriptors

The molecular stage begins with identifying the potentially active constituents of plant extracts, agricultural residues, or synthesized candidate inhibitors. GC–MS and LC–MS can support chemical identification, while FTIR and other spectroscopic methods can provide evidence of functional groups and changes associated with adsorption. DFT calculations may then examine optimized geometry, HOMO and LUMO energies, the HOMO–LUMO gap, molecular electrostatic potential, atomic charges, dipole moment, electronegativity, hardness/softness, and Fukui functions. These descriptors help generate hypotheses about electron donation, electron acceptance, and possible adsorption sites; they should not be treated as stand-alone predictors of inhibition efficiency (Obot et al., 2015; Donkor et al., 2022).

The studies of Essien et al. (2023, 2024) on 3-methyl-5-phenylisoxazole and 3,5-dimethyl-4-nitroisoxazole provide examples of combining corrosion experiments with quantum-chemical analysis and infrared evidence. Ozoemena et al. (2024) compared a Schiff-base ligand with an analogue through computational modelling, illustrating how structural comparison can support candidate prioritization. Obot et al. (2021) extended this logic to n-hexane extracts of Costus lucanusianus, using thermodynamic and quantum-chemical evaluation to investigate a complex natural feedstock. These

studies contribute to molecular interpretation, but the distinction between a synthetic molecule and a genuinely green inhibitor must be retained: environmental preference requires evidence beyond the presence of heteroatoms or favourable DFT descriptors.

6.2. Interface: MD analysis of adsorption and interfacial stability

The interface stage uses MD to examine how candidate molecules behave near a representative metal surface in a defined electrolyte. Important outputs include adsorption configuration and orientation, inhibitor–surface interaction energy, spatial density profiles, radial distribution functions, surface coverage, residence behaviour, and the displacement or reorganization of interfacial water. The model should include chemically plausible protonation states and, where relevant, explicit water, hydronium, chloride or sulfate ions, and other competing species. Adsorption energies are only comparable when the reference-state definition, surface, force field, solvent representation, and simulation conditions are sufficiently similar (Heinz et al., 2008; Wei et al., 2018; Castillo-Robles et al., 2024).

Boekom et al. (2020) examined pyridine inhibition of mild steel in 0.1 M HCl through kinetic, adsorption, and quantum-chemical analysis, and the work is relevant to discussion of molecular adsorption at the interface. It should not, however, be treated as equivalent to a modern, explicitly documented MD study unless the full methods and trajectory outputs support that classification. This distinction matters because adsorption-isotherm fitting, quantum calculations on isolated molecules, Monte Carlo adsorption configurations, and time-dependent MD trajectories answer related but different questions. Future work should report simulation cells, surface facets, force-field parameters, charge assignment, equilibration, trajectory length, replicate trajectories, and analysis procedures.

6.3. Performance: experimental validation of computational predictions

The performance stage determines whether molecular and interfacial predictions correspond to measurable corrosion protection. Weight-loss measurements estimate average corrosion over an exposure period; potentiodynamic polarization (PDP) evaluates corrosion current and changes in anodic/cathodic behaviour; EIS characterizes interfacial resistance and capacitive response; and surface methods such as SEM/EDS, AFM, FTIR and XPS can provide evidence of surface damage or protective-film formation. These measurements should be performed under clearly reported and comparable conditions, including metal composition, electrolyte, inhibitor concentration, temperature, and exposure time (ASTM International, 2023, 2024).

Several studies supplied for this review are particularly relevant to this validation stage. Ozoemena et al. (2023) investigated a Schiff-base ligand and its metal complexes as inhibitors for ASTM-A36 low-carbon steel in simulated oil- and-gas well-treatment fluid, reporting mixed-type inhibition and surface evidence consistent with a protective layer. Ekiko et al. (2026) evaluated a hydrazone derivative in 1.0 M HCl using 30-day weight-loss testing, PDP and EIS, while Nyong et al. (2026) examined a related hydrazone derivative in oil-field water. These studies provide experimental corrosion evidence, but their results should only be described as DFT- or MD-validated when the respective computational method is explicitly reported in the paper.

At the materials scale, Essien et al. (2026) investigated a calcium oxide/silica nanocomposite for low-carbon-steel protection in concentrated HCl and H_2SO_4. This study broadens the discussion beyond small organic molecules to nanocomposite inhibitors. It can support the performance and materials-design parts of the framework; however, molecular DFT/MD claims should be tied to the methods actually documented in the article. The same principle applies to comparing reported

inhibition efficiencies: values from different acids, concentrations, temperatures and exposure times should not be ranked as if they were obtained under identical conditions.

6.4. Sustainability: environmental safety and industrial feasibility

Sustainability is a separate evidence requirement, not an automatic property of a plant-derived, bio-based, or nanostructured inhibitor. Evaluation should include toxicity to relevant organisms, biodegradation and degradation products, feedstock availability and seasonal variability, extraction-solvent use, life-cycle impacts, production cost, formulation stability, and performance under realistic operating conditions. Metal complexes and nanocomposites also require assessment of metal-ion release, persistence, recovery, and end-of-life fate. Reviews of plant-derived inhibitors emphasize their potential, while also showing why "green" claims require a clearly defined basis (Verma et al., 2018; Salleh et al., 2021; Zakeri et al., 2022).

Essien et al. (2026) reviewed multifunctional nanocomposites for corrosion protection and wastewater treatment, providing adjacent context for evaluating multifunctionality and materials integration. Such multifunctionality may be attractive, but a combined application does not itself demonstrate a lower life-cycle burden. Comparative life-cycle assessment, toxicity testing, biodegradation data, feedstock accounting, and techno-economic analysis are needed to determine whether a candidate is environmentally preferable to an established inhibitor. The CaO-nanoparticle photocatalysis study by Kufre et al. (2025) is relevant to wastewater treatment but does not directly address DFT/MD-based corrosion-inhibitor discovery; it is therefore not used as evidence for the central computational framework.

Table 3. Selected studies mapped to the four-stage framework

Study	Inhibitor / system	Methods reported	Framework stage(s)	Critical relevance / limitation
Boekom et al. (2020)	Pyridine; mild steel in 0.1 M HCl	Gravimetric/kinetic and adsorption analysis; quantum-chemical descriptors; molecular-dynamics wording in title	Molecule / interface	Useful adsorption case; distinguish reported quantum-chemical and adsorption analyses from explicitly documented trajectory-based MD.
Obot et al. (2021)	n-Hexane stem and leaf extracts of Costus lucanusianus	Weight-loss/thermodynamic evaluation and quantum-chemical analysis	Molecule / performance	Links natural-extract performance to molecular descriptors; extract complexity limits attribution to individual compounds.
Essien et al. (2023)	3-Methyl-5-phenylisoxazole; mild steel in HCl	Gravimetric corrosion testing, quantum calculations and IR surface analysis	Molecule / performance	Provides experimental and quantum-chemical evidence for a defined inhibitor; it is not a plant-extract study.
Essien et al. (2024)	3,5-Dimethyl-4-nitroisoxazole; mild steel in HCl	Experimental corrosion testing, quantum-chemical calculations and IR spectroscopy	Molecule / performance	Illustrates how electronic descriptors and spectral evidence can support an adsorption interpretation.
Ozoemena et al. (2023)	Schiff-base ligand and Ni, Cu and Zn	Weight loss, adsorption/thermodyna	Performance	Reported NiL1 inhibition efficiency of 84.29%; "ecofriendly" should be

Study	Inhibitor / system	Methods reported	Framework stage(s)	Critical relevance / limitation
	complexes; ASTM-A36 steel	mic analysis, PDP and SEM		treated as a claim requiring independent environmental testing.
Ozoemena et al. (2024)	Schiff-base ligand and structural analogue	Computational modelling and comparative corrosion-inhibitor evaluation	Molecule / performanc e	Useful example of structure-based comparison; confirm exact computational descriptors and experimental protocols from full text.
Ekiko et al. (2026)	Novel hydrazone derivative; mild steel in 1.0 M HCl	30-day weight loss, PDP and EIS	Performanc e	Shows why long-duration gravimetric and electrochemical measurements are important; the reported response was concentration-dependent.
Nyong et al. (2026)	Hydrazone derivative; mild steel in oil-field water	Experimental corrosion-inhibition evaluation, as described in the supplied citation	Performanc e / application	Potentially useful for service-fluid relevance; detailed methods and computational integration should be confirmed from the full paper.
Essien, et al. (2026)	CaO/SiO_2 nanocomposit e; low-carbon steel in 15% HCl and 15% H_2SO_4	Nanocomposite corrosion-inhibition study	Performanc e / materials design	Extends the framework from molecular inhibitors to nanocomposites; include DFT/MD only if confirmed in the article methods.
Essien et al. (2026)	Multifunctiona l nanocomposit es for corrosion protection and wastewater treatment	Review of emerging materials chemistry	Sustainabili ty / application	Provides adjacent context for multifunctionality; environmental benefits still require toxicity, life-cycle and feasibility evidence.
Abdelaziz et al. (2021); Berrissoul et al. (2022); Ramezanzadeh et al. (2018)	Plant extracts and identified phytochemical s	Experimental corrosion tests integrated with DFT and/or MD/Monte Carlo methods	Molecule / interface / performanc e	Useful comparative cases for connecting molecular descriptors and adsorption modelling with experiments; extract complexity remains a limitation.

Source note: The author-supplied studies are included where they support at least one stage of the framework. The table 3 deliberately avoids attributing DFT, MD, toxicity testing, or life-cycle assessment to a paper unless the cited record or full text confirms that method. “Green” and “ecofriendly” in a title are not, by themselves, proof of environmental safety.

Table 4. Operational questions and recommended evidence for each stage

Stage	Key question	Recommended evidence	Expected output
1. Molecule	Which constituents or structures are potentially active?	GC–MS/LC–MS, FTIR, DFT, protonation-state analysis, HOMO/LUMO, electrostatic potential, charges and Fukui functions	Candidate structures and explicit mechanistic hypotheses
2. Interface	How do inhibitor molecules behave at the metal–electrolyte interface?	MD with specified surface facets, explicit/validated solvent, ions, force fields, multiple trajectories and adsorption analysis	Adsorption configuration, solvent displacement and stability evidence
3. Performance	Does the predicted behaviour reduce corrosion?	Weight loss, PDP, EIS, SEM/EDS, AFM, FTIR/XPS, replicates and uncertainty estimates	Validated corrosion-rate reduction and surface-protection evidence
4. Sustainability	Is the candidate safer and feasible in practice?	Toxicity, biodegradation, leaching, feedstock audit, life-cycle assessment, techno-economics and long-duration service tests	Evidence-based environmental and industrial suitability

7. Future perspectives

Future research should prioritize more realistic metal–electrolyte interfaces, explicit or appropriately validated solvent representations, multiple plausible protonation states, and systematic validation of force fields. Models incorporating surface defects, oxide layers, alloying elements, and competitive adsorption by aggressive ions could provide a more representative description of practical corrosion environments. Where conventional MD sampling is insufficient, enhanced-sampling methods may help characterize adsorption pathways and thermodynamic stability (Castillo-Robles et al., 2024; Donkor et al., 2022).

Free-energy methods, including umbrella sampling and metadynamics, offer opportunities to investigate adsorption thermodynamics beyond static adsorption-energy calculations. These methods can explore free-energy profiles along selected reaction coordinates and provide insights into adsorption barriers and interfacial transitions. Their reliability depends on suitable collective variables, adequate sampling, and appropriate treatment of solvent and surface interactions (Wei et al., 2018).

Integration with machine learning may further accelerate inhibitor discovery by combining molecular fingerprints, DFT-derived descriptors, MD-derived properties, and experimental corrosion data. Data-driven models can help identify structure–property relationships and prioritize candidates for further testing. However, corrosion-inhibition datasets may be small, heterogeneous, and sensitive to experimental conditions. Reliable models require consistent data collection, independent validation, uncertainty assessment, and careful consideration of differences among metals, electrolytes, temperatures, and inhibitor concentrations (Baskin, 2024).

For practical applications, computational screening should be connected to long-term corrosion testing, formulation stability, toxicity assessment, biodegradability, and economic feasibility. Studies should evaluate whether promising laboratory results remain reproducible under conditions relevant to industrial service. Researchers should also share molecular structures, optimized geometries, input files, force-field parameters, simulation settings, and analysis procedures wherever possible. Such transparency would strengthen reproducibility and facilitate meaningful comparisons between studies.

The greatest opportunity lies in developing an iterative workflow in which DFT identifies potentially reactive molecular features, MD investigates interfacial behaviour, experiments establish actual corrosion performance, and sustainability assessment determines environmental and operational suitability. For nanocomposites, the same logic should be extended to the stability of the composite, release of constituent species, and interactions between the organic/inorganic components and the metal surface.

8. Conclusion

DFT and MD are complementary tools for understanding and developing green corrosion inhibitors. DFT provides information about molecular electronic structure, charge distribution, and potentially reactive sites, whereas MD investigates adsorption configurations, solvent effects, and interfacial organization under specified simulation conditions. When integrated with electrochemical measurements and surface characterization, these methods provide a stronger basis for mechanistic interpretation and candidate selection than either computational method alone. However, predictive reliability remains constrained by chemical variability, simplified metal surfaces, force-field accuracy, protonation and solvation effects, and insufficient experimental validation. These works should be integrated critically rather than treated as interchangeable examples: some support quantum-chemical interpretation, some provide adsorption or molecular-simulation evidence, and others chiefly establish experimental corrosion performance. Future progress will depend on clearly documenting which methods each study actually uses and avoiding claims of computational validation or environmental safety without direct evidence. Overall, DFT and MD should guide—not replace—experimental corrosion testing. Their effective integration with validated performance measurements and environmental assessment offers a route towards corrosion inhibitors that are computationally interpretable, experimentally effective, and demonstrably sustainable.

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