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Green corrosion inhibitors for steel: Advanced mechanisms, materials design, and industrial perspectives

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Abstract

The increasing environmental concerns associated with conventional corrosion inhibitors have driven significant research into sustainable alternatives known as green corrosion inhibitors (GCIs). These materials, derived from renewable resources or synthesized through environmentally benign processes, offer a promising route to mitigate steel corrosion in aggressive environments. This comprehensive review provides an in-depth analysis of green corrosion inhibitors with a particular focus on adsorption mechanisms, thermodynamic and kinetic modeling, structure–activity relationships, and performance under industrial conditions. Advanced computational approaches including density functional theory (DFT), Monte Carlo simulations, and molecular dynamics are discussed in relation to inhibitor efficiency. Furthermore, the review evaluates the effectiveness of GCIs in acidic, saline, and CO_2-containing environments, highlighting the role of synergistic effects and hybrid systems. Challenges in scalability, reproducibility, and long-term stability are critically assessed, and future research directions are proposed to accelerate the development of next-generation sustainable corrosion mitigation technologies.

Keywords: Green corrosion inhibitors, steel protection, adsorption mechanisms, density functional theory (DFT), structure–activity relationship

Introduction

Steel corrosion remains one of the most persistent and economically significant problems in modern engineering systems. The intrinsic thermodynamic instability of iron in oxidizing environments leads to spontaneous degradation through electrochemical processes, ultimately resulting in structural failure and loss of functionality. The global economic impact of corrosion is estimated to exceed 2.5 trillion USD annually, corresponding to approximately 3–4% of the global gross domestic product [1]. These losses are not limited to direct material replacement costs but also include maintenance, downtime, environmental contamination, and safety risks.

In industrial systems, corrosion of steel occurs in a wide variety of environments, each characterized by distinct chemical and physical conditions. Acidic environments, such as those encountered in acid pickling, descaling, and oil well acidizing, are particularly aggressive due to the high concentration of hydrogen ions that accelerate the anodic dissolution of iron. In marine environments, chloride ions play a critical role in destabilizing passive films and promoting localized corrosion mechanisms such as pitting and crevice corrosion. Meanwhile, in oil and gas production systems, CO_2 corrosion (commonly referred to as sweet corrosion) arises from the dissolution of carbon dioxide in water, forming carbonic acid that significantly lowers pH and enhances metal dissolution rates [2].

Traditionally, corrosion mitigation has relied heavily on the use of inorganic inhibitors such as chromates, phosphates, and nitrites. While these compounds are highly effective, their environmental and health hazards have led to increasing regulatory restrictions. Chromates, for example, are known carcinogens and have been banned or severely limited in many countries. This has created an urgent need for alternative corrosion inhibitors that are both effective and environmentally benign [3].

Green corrosion inhibitors have emerged as a promising solution to this challenge. These inhibitors are typically derived from natural sources such as plants, biomass, or environmentally friendly synthetic routes. They are characterized by low toxicity, biodegradability, and renewability. From a chemical perspective, most green inhibitors are organic compounds containing heteroatoms (N, O, S, P) and π-electron systems that facilitate adsorption onto metal surfaces. Their inhibition performance is largely governed by their ability to form protective films that block active corrosion sites and reduce electrochemical reaction rates [4].

One of the defining features of green corrosion inhibitors is their multifunctional nature. In addition to adsorption, many of these compounds exhibit antioxidant properties, metal-chelating ability, and radical scavenging activity. These properties contribute to corrosion inhibition by reducing the availability of reactive species and stabilizing the metal surface. Furthermore, the complex molecular structures of natural compounds often enable multiple interaction modes with the metal surface, leading to enhanced adsorption strength and film stability.

Despite significant progress in this field, several challenges remain. The variability in composition of natural extracts, lack of standardization, and limited understanding of molecular-level mechanisms hinder the widespread adoption of green inhibitors in industrial applications. Additionally, their performance under extreme conditions, such as high temperature and pressure, requires further investigation.

This review aims to provide a comprehensive and in-depth analysis of green corrosion inhibitors for steel, focusing on fundamental mechanisms, advanced characterization techniques, and practical considerations for industrial implementation. Special emphasis is placed on adsorption behavior, thermodynamic modeling, quantum chemical analysis, and structure–activity relationships, which are essential for the rational design of next-generation inhibitors.

Electrochemical Fundamentals and Corrosion Kinetics

The corrosion of steel is fundamentally an electrochemical process involving simultaneous anodic and cathodic reactions occurring at the metal–electrolyte interface. The anodic reaction corresponds to the oxidation of iron:

$$Fe \rightarrow Fe^{2+} + 2e^{-}$$

while the cathodic reaction depends on the environment. In acidic solutions, hydrogen evolution dominates:

$$2H^{+} + 2e^{-} \rightarrow H_2$$

In neutral or alkaline environments, oxygen reduction becomes more significant:

$$O_2 + 2H_2O + 4e^{-} \rightarrow 4OH^{-}$$

The overall corrosion rate is determined by the kinetics of these reactions, which are influenced by factors such as temperature, electrolyte composition, and surface condition. Electrochemical techniques such as potentiodynamic polarization and electrochemical impedance spectroscopy (EIS) are commonly used to evaluate corrosion behavior.

The Butler–Volmer equation provides a quantitative description of electrode kinetics:

$$i = i_0 [\exp(\alpha\_aF\eta/RT) - \exp(-\alpha\_cF\eta/RT)]$$

where i represents current density, i_0 is exchange current density, α_a and α_c are anodic and cathodic transfer coefficients, and η is overpotential. Green corrosion inhibitors influence these parameters by modifying the interface, effectively reducing charge transfer rates and shifting corrosion potentials [5].

In practical terms, the efficiency of a corrosion inhibitor is evaluated using inhibition efficiency (η%):

$$\eta\% = [(i\_corr^0 - i\_corr)/i\_corr^0] \times 100$$

Green inhibitors often exhibit mixed-type inhibition behavior, meaning they simultaneously suppress both anodic and cathodic reactions. This is advantageous because it provides broader protection across different corrosion mechanisms. The degree of inhibition depends on the adsorption strength and coverage of the inhibitor molecules on the metal surface.

Electrochemical impedance spectroscopy provides further insight into inhibition mechanisms. The presence of an inhibitor typically increases the charge transfer resistance (R_ct) and decreases the double-layer capacitance (C_dl), indicating the formation of a protective film. These changes reflect the ability of the inhibitor to block active sites and reduce electron transfer processes.

Adsorption Isotherms and Thermodynamic Modeling

Adsorption is the central mechanism through which green corrosion inhibitors protect steel surfaces. The interaction between inhibitor molecules and the metal surface can occur through physisorption, chemisorption, or a combination of both.

Physisorption involves weak electrostatic interactions between charged inhibitor molecules and the metal surface. This type of adsorption is generally reversible and sensitive to temperature changes. Chemisorption, on the other hand, involves the formation of covalent or coordinate bonds between the inhibitor and the metal surface, resulting in stronger and more stable adsorption.

The Langmuir adsorption isotherm is widely used to describe the adsorption behavior of inhibitors:

$$C/\theta = 1/K\_ads + C$$

where θ represents surface coverage and K_ads is the adsorption equilibrium constant. A high value of K_ads indicates strong adsorption and high inhibition efficiency [6].

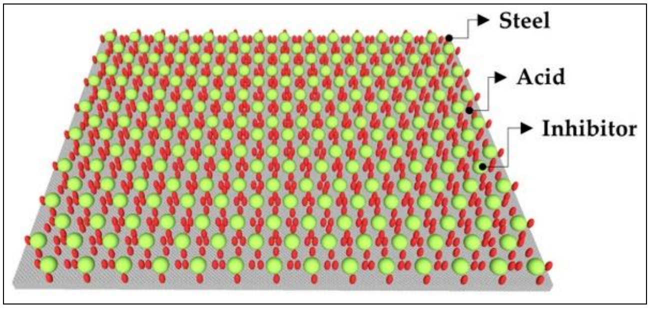
The Gibbs free energy of adsorption is calculated as:

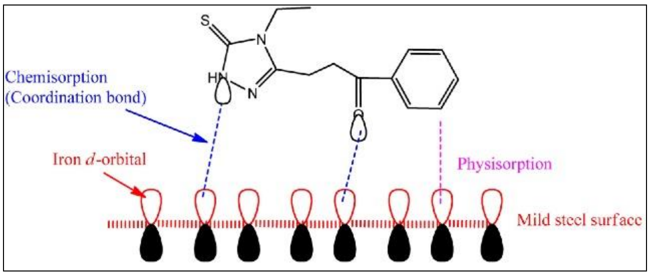
$$\Delta G\_ads = -RT \ln(55.5K\_ads)$$

Values of ΔG_ads provide insight into the nature of adsorption. Typically, values around −20 kJ/mol suggest physisorption, while values around −40 kJ/mol or more negative indicate chemisorption. Many green inhibitors exhibit intermediate values, suggesting mixed adsorption mechanisms [7].

More advanced adsorption models, such as the Temkin and Freundlich isotherms, account for interactions between adsorbed molecules and surface heterogeneity. These models provide a more accurate description of real systems, where ideal assumptions of the Langmuir model may not hold.

Temperature-dependent studies allow the determination of activation parameters, including activation energy (E_a), enthalpy (ΔH), and entropy (ΔS). These parameters provide valuable insights into the adsorption process and inhibition mechanism. For example, a decrease in activation energy in the presence of an inhibitor suggests chemisorption, while an increase indicates physisorption dominance [8].





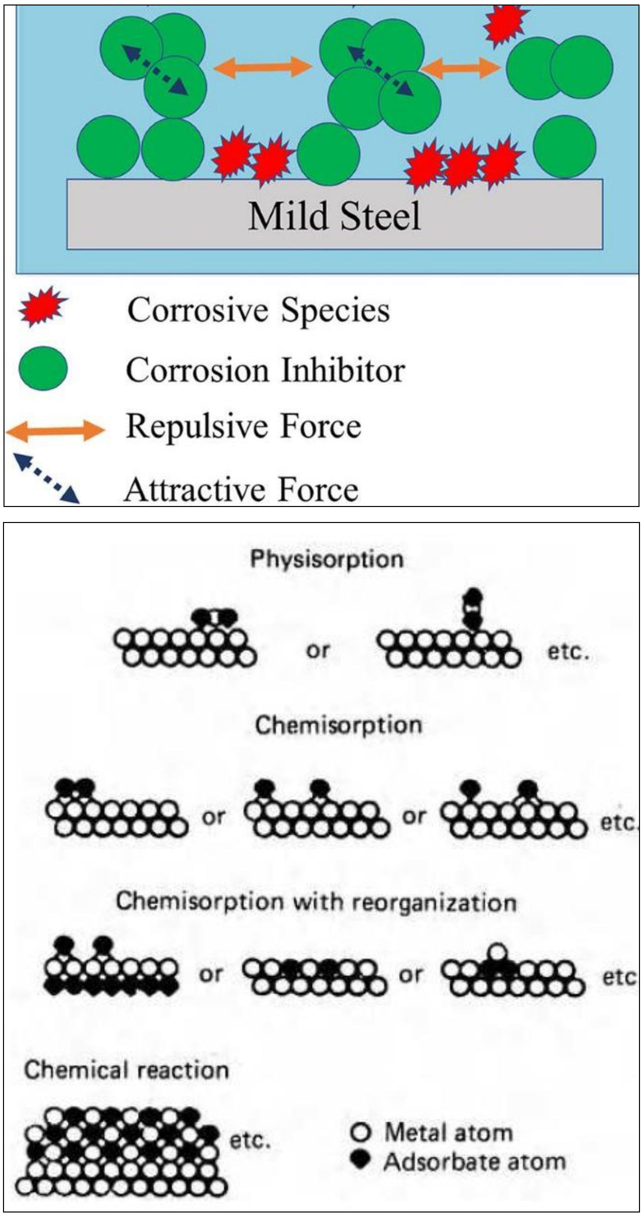


Fig 1: Schematic illustration of adsorption mechanisms of green corrosion inhibitors on steel surfaces, including physisorption (electrostatic interaction) and chemisorption (coordinate bonding), leading to the formation of a protective barrier film [6-8]

Quantum Chemical Analysis and Structure–Activity Relationships

Density functional theory (DFT) has become an essential tool for understanding corrosion inhibition at the molecular level. Key parameters include: HOMO energy (E_HOMO): electron-donating ability; LUMO energy (E_LUMO): electron-accepting ability; Energy gap (ΔE): molecular reactivity; Dipole moment: molecular polarity; Molecules with high E_HOMO and low ΔE tend to exhibit stronger adsorption and higher inhibition efficiency [9].

Fukui functions and Mulliken charge analysis help identify reactive sites within inhibitor molecules, indicating where adsorption is most likely to occur. Typically, heteroatoms and aromatic rings serve as active centers.

Monte Carlo and molecular dynamics simulations provide additional insights into adsorption configurations, binding energies, and film formation. These simulations reveal that flat adsorption orientations maximize surface coverage and enhance protection [10].

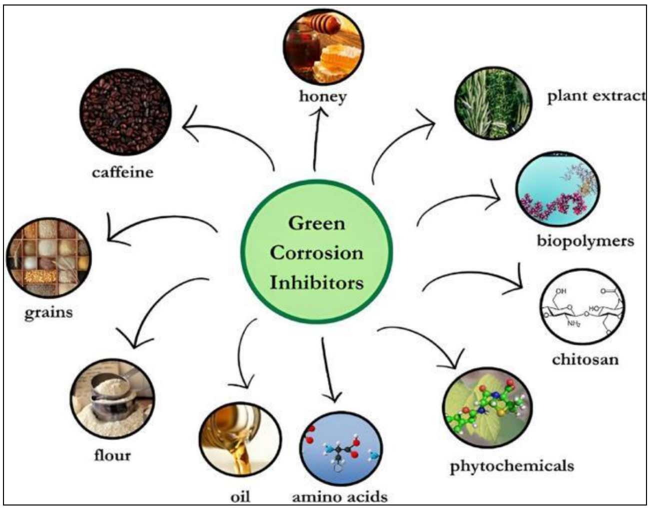
Plant Extracts: Mechanisms, Synergy, and Limitations

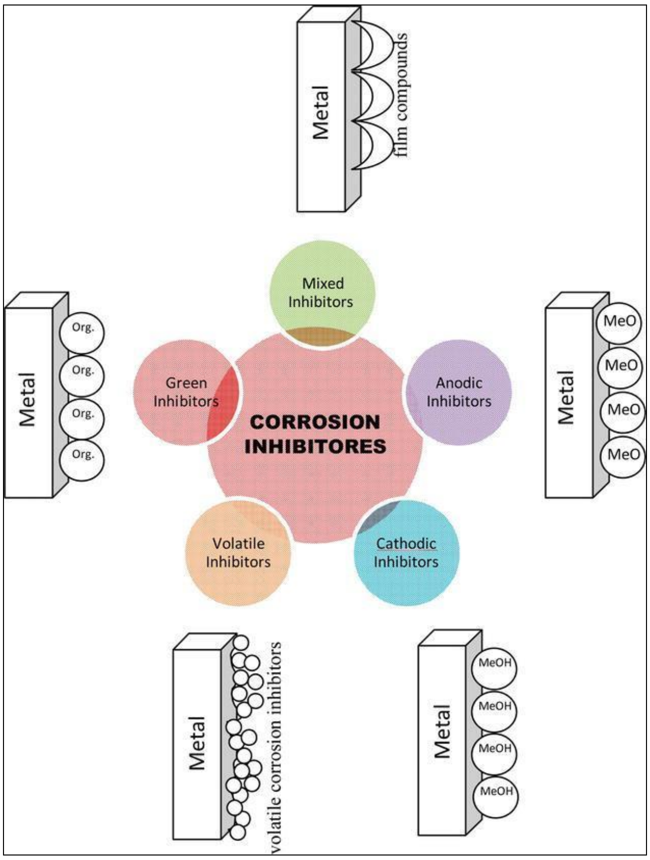
Plant extracts are among the most extensively studied green inhibitors due to their availability and complex chemical composition. They contain multiple active compounds such as flavonoids, alkaloids, tannins, and saponins.

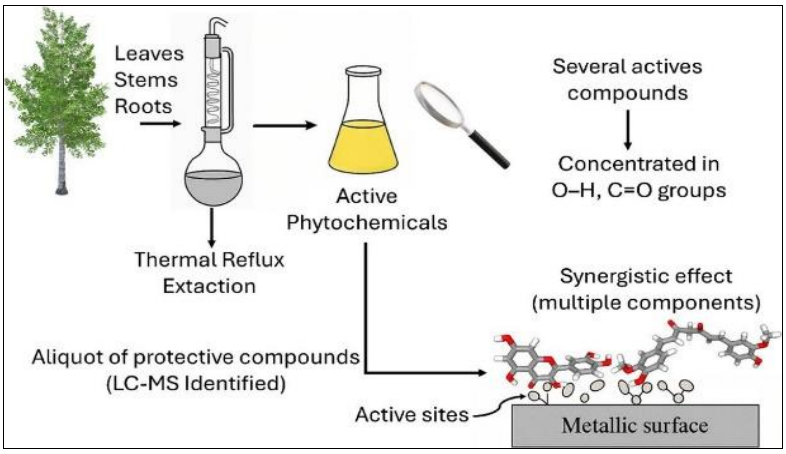
The inhibition mechanism involves adsorption of these compounds onto the steel surface through π-electrons and heteroatoms, forming a protective barrier. The presence of multiple components leads to synergistic effects, where the combined action enhances inhibition efficiency beyond individual contributions [11].

However, plant extracts suffer from variability in composition, which affects reproducibility. Factors such as extraction method, plant species, and environmental conditions influence the chemical profile of the extract [12].

To address this issue, researchers are increasingly focusing on isolating and characterizing individual active compounds or developing standardized extract formulations.







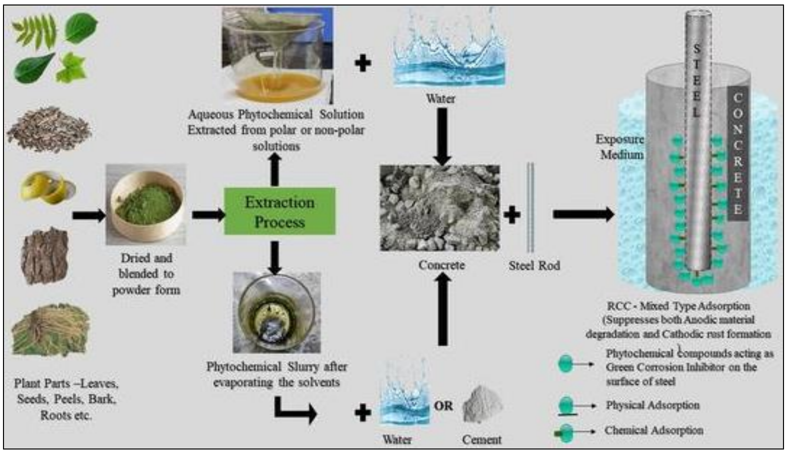


Fig 2: Classification of green corrosion inhibitors for steel, including plant extracts, amino acids, biopolymers, and hybrid systems [9-12]

Amino Acids and Biopolymers

Amino acids are attractive green inhibitors due to their biodegradability and well-defined structures. Their inhibition efficiency depends on the nature of their side chains, with sulfur-containing amino acids showing superior performance.

Biopolymers such as chitosan and cellulose derivatives offer additional advantages due to their high molecular weight and film-forming ability. These materials can create thick protective layers that prevent the diffusion of corrosive species [13].

Chemical modification of biopolymers, such as grafting functional groups or incorporating nanoparticles, can significantly enhance their adsorption strength and stability.

Green Inhibitors in Acidic Environments

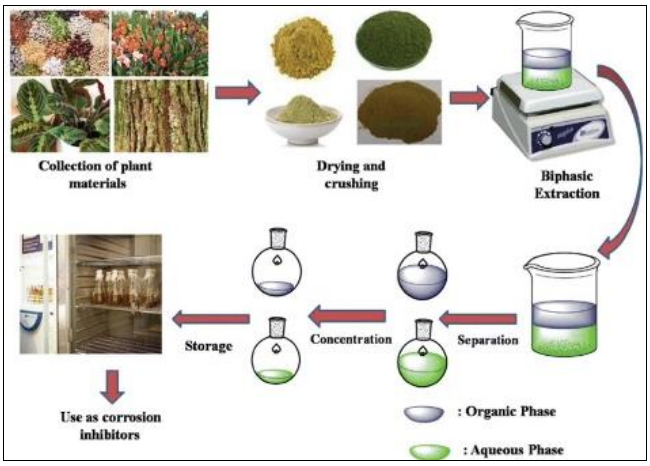
Acidic environments are particularly aggressive due to high proton concentration. Green inhibitors must resist protonation while maintaining adsorption capability.

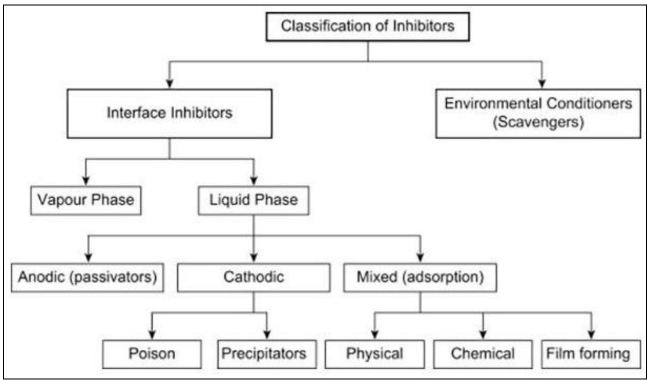
Studies show that many plant extracts and organic molecules achieve inhibition efficiencies above 90% in HCl solutions through strong adsorption and film formation [14].

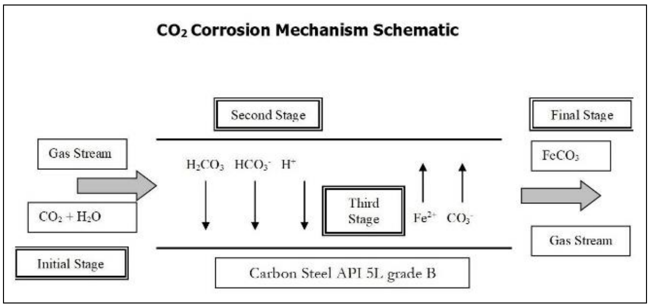
The presence of chloride ions introduces competitive adsorption, requiring inhibitors to have higher affinity for the metal surface than chloride ions.

Marine and Saline Environments

In saline environments, chloride-induced pitting corrosion is a major concern. Green inhibitors must form compact and defect-free films to prevent localized attack. Biopolymer-based coatings and hybrid systems have shown promising results in such environments due to their barrier properties and resistance to chloride penetration [15].







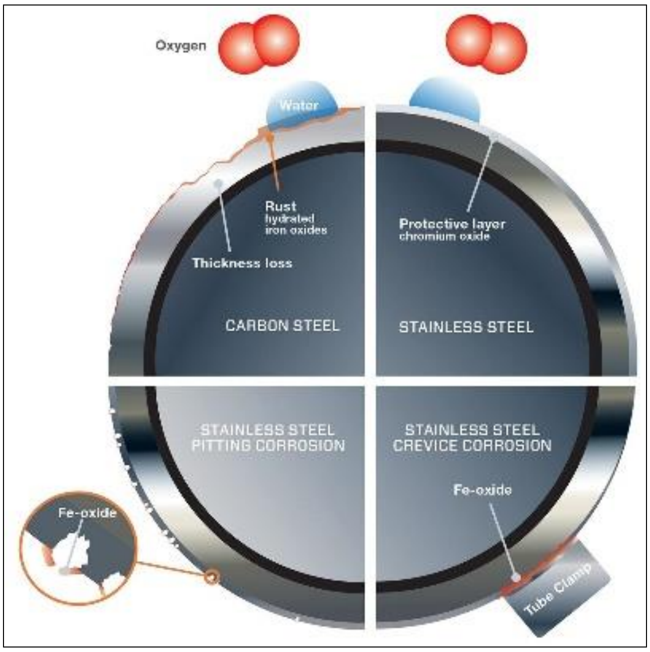


Fig 3: Performance of green corrosion inhibitors in different corrosive environments, including acidic (HCl), saline (NaCl), and CO_2-saturated systems [10-15]

CO_2 Corrosion and Oil & Gas Applications

CO_2 corrosion occurs due to the formation of carbonic acid in aqueous environments. Green inhibitors can mitigate this by forming stable complexes with iron ions and reducing dissolution rates [16].

Field studies indicate that certain plant-based inhibitors and amino acids can achieve significant corrosion reduction in CO_2-saturated systems, although long-term stability remains a challenge.

Nanotechnology and Hybrid Systems

Nanotechnology has significantly advanced the field of corrosion inhibition. Nanoparticles can enhance inhibitor performance by increasing surface coverage and improving film stability.

Hybrid systems combining organic inhibitors with inorganic nanoparticles exhibit synergistic effects, resulting in improved corrosion resistance and durability [17].

Self-healing coatings incorporating green inhibitors represent a promising direction for future research.

Industrial Challenges and Scale-Up

Despite promising laboratory results, several challenges hinder industrial implementation of green inhibitors. These include variability, limited stability under extreme conditions, and economic considerations.

Standardization, process optimization, and large-scale testing are essential for translating laboratory findings into practical applications [18].

Future Directions

Future research should focus on integrating computational modeling, machine learning, and experimental studies to accelerate inhibitor discovery.

The development of smart coatings, multifunctional materials, and hybrid systems will play a crucial role in advancing the field [19].

Conclusion

Green corrosion inhibitors represent a sustainable and effective alternative to traditional inhibitors. Their performance is governed by complex interactions at the molecular level, which can be optimized through advanced design and characterization techniques.

Continued research and technological innovation are expected to overcome current challenges and enable widespread adoption in industrial applications.

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