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Green Corrosion Inhibitors for Iron Alloys: A Comprehensive Review of Integrating Data-Driven Forecasting, Density Functional Theory Simulations, and Experimental Investigation

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ABSTRACT

This comprehensive review delves into the realm of green corrosion inhibitors for iron alloys, focusing on a thorough exploration guided by data-driven investigation, density functional theory (DFT) simulations, and experimental validation. Harnessing the potential of plant extracts, this study scrutinizes their effectiveness in mitigating corrosion in iron alloys through a multi-faceted approach. By integrating computational modeling with empirical experimentation, a deeper understanding of the inhibitive mechanisms is achieved, offering insights into their practical application. The review synthesizes findings from diverse studies, elucidating the pivotal role of DFT in predicting inhibitor behavior and optimizing their performance. Furthermore, experimental validation provides crucial validation of theoretical predictions, highlighting the synergistic relationship between simulation and real-world application. Through this journey of exploration, the review underscores the promise of green corrosion inhibitors derived from natural sources, paving the way for sustainable corrosion control practices in the realm of iron alloys.

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1. INTRODUCTION

Iron alloys, exemplified by steel, constitute a material widely employed across diverse applications in daily life, notably in industrial and manufacturing realms. This prevalence stems from their favorable mechanical properties, widespread availability, facile fabrication, and economic viability [1], [2], [3]. However, a significant drawback lies in the susceptibility of steel to corrosion when subjected to corrosive environments [4], [5], [6]. The pervasive nature of this corrosion poses substantial concerns for both industrial and academic sectors. Corrosion not only results in tangible economic losses but also inflicts damage to the environment, society, industry, security, safety, and various other domains [7], [8], [9]. The annual expenditure to mitigate corrosion-related damage is estimated at US$ 2.5 trillion, equivalent to approximately 3.4% of the global GDP [10], [11], [12]. Moreover, these expenses have demonstrated consistent escalation over the past decade [13], [14].

The utilization of anti-corrosion compounds, commonly referred to as inhibitors is a prominent strategy for attenuating the pace of corrosion. Implementation of corrosion inhibitor technology has the potential to curtail costs by up to 35%, equating to approximately $875 billion annually [15], [16]. Corrosion inhibitors are chemical substances that impede the corrosion process in electrolytic environments by introducing minute quantities of the compound into the corrosive milieu [17], [18]. Employing inhibitor technology for corrosion management represents one of the simplest, most effective, and economical approaches [19], [20], [21]. The efficacy of inhibitor compounds hinges upon their ability to form an adsorbed or protective

layer on the metal surface, thereby impeding mass transfer and charge transfer processes while shielding the metal from corrosive agents [22], [23], [24].

The exploration of corrosion inhibitors, encompassing both inorganic and organic constituents, is increasingly gaining prominence as it undergoes continuous investigation. The focus of corrosion inhibitor development is shifting towards the quest for organic inhibitors sourced from natural substances, primarily due to the costliness, hazardous nature, and adverse environmental impact associated with inorganic counterparts [25], [26], [27], [28]. Natural extracts have emerged as favored alternatives, heralded as environmentally friendly inhibitors or "green inhibitors," owing to their biodegradability, renewability, absence of toxic byproducts, cost-effectiveness, simplicity of synthesis, and notable anti-corrosion efficacy [29], [30]. Particularly, natural extracts rich in molecules featuring aromatic rings and heteroatom groups (such as O, N, S, and P) within their structure exhibit significant promise as corrosion inhibitors [31], [32], [33]. In pursuing sustainable solutions, considerable attention is directed towards green corrosion inhibitors, especially those derived from plant extracts, due to their potential to mitigate corrosion while concurrently minimizing environmental repercussions.

However, understanding their complex interactions with metal surfaces and corrosion processes requires a multidisciplinary approach. Data-driven investigation serves as the cornerstone of this endeavor, leveraging large datasets and computational techniques to identify promising candidates and elucidate structure-activity relationships. Density functional theory (DFT) simulations complement data-driven approaches by providing atomistic insights into the adsorption mechanisms and electronic properties of inhibitors on metal surfaces. Through DFT, theoretical predictions can guide the design and optimization of inhibitors, enhancing their efficacy and selectivity [34], [35], [36]. Importantly, the integration of computational modeling with experimental validation facilitates a more holistic understanding of inhibitor performance under real-world conditions.

This review synthesizes recent advancements in the field, highlighting the contributions of data-driven investigation, DFT simulations, and experimental validation to the development of green corrosion inhibitors for iron alloys. By examining the synergies between computational predictions and empirical observations, we aim to provide valuable insights into the design, optimization, and application of environmentally friendly corrosion inhibitors. Ultimately, this multifaceted approach holds promise for addressing corrosion challenges while advancing sustainable practices in materials science and engineering.

2. LITERATURE REVIEW

2.1. Green corrosion inhibitor

Corrosion inhibition is a critical aspect of maintaining the integrity and longevity of metallic materials in various industries. Traditional corrosion inhibitors often raise concerns due to their environmental and health impacts, leading to the exploration of eco-friendly alternatives. Plant extracts have garnered significant attention as green corrosion inhibitors owing to their abundance, renewability, biodegradability, and low toxicity. Plant extracts act through multiple mechanisms to inhibit corrosion, including adsorption onto the metal surface, formation of protective films, and modification of the electrolyte composition. The adsorption process involves the interaction of active compounds present in the plant extract with the metal surface, forming a protective layer that impedes corrosive species' access [37], [38], [39]. Additionally, certain phytochemicals present in plant extracts can facilitate the formation of passive oxide films on the metal surface, further enhancing corrosion resistance.

A wide array of plant extracts have been investigated for their corrosion inhibition properties. Examples include extracts derived from leaves, seeds, bark, fruits, and roots of various plant species such as Azadirachta indica (neem), Punica granatum (pomegranate), Allium sativum (garlic), Zingiber officinale (ginger), and many others [40], [41], [42], [43], [44], [45], [46], [47]. These extracts contain bioactive compounds such as alkaloids, flavonoids, tannins, and organic acids, which exhibit corrosion-inhibiting properties. Synergistic effects can be achieved by combining plant extracts with other corrosion inhibitors or additives, leading to enhanced inhibition efficiency and broader spectrum protection. The synergism between plant extracts and traditional inhibitors or nanoparticles has been investigated, offering promising strategies for improving corrosion resistance in diverse environments.

Several factors influence the effectiveness of plant extracts as corrosion inhibitors, including concentration, temperature, pH, and the composition of the corrosive medium. Optimal conditions must be determined to maximize inhibition efficiency while considering practical applications' requirements. Moreover, the compatibility of plant extracts with different metal substrates and corrosive environments needs to be thoroughly evaluated to ensure long-term protection [48], [49], [50], [51]. The use of plant extracts as corrosion inhibitors aligns with the principles of green chemistry, offering environmentally

sustainable alternatives to conventional inhibitors. Furthermore, the abundance and accessibility of plant sources contribute to their economic viability, making them attractive options for large-scale applications.

Table 1. Example of recent research on the application of plant extract inhibitors on steel in HCl media.

Green Inhibitor	Concentration	Electrolyte	CIE (%)
Ananas comosus	1000 ppm	1 M HCl	98
Calotropis procera	1000 ppm	1 M HCl	89
Cassia occidentalis	1000 ppm	1 M HCl	93
Chinese gooseberry fruit	1000 ppm	1 M HCl	92
Cryptocarya nigra	1000 ppm	1 M HCl	91
Datura stramonium	1000 ppm	1 M HCl	91
Juglans regia	1000 ppm	1 M HCl	94
Luffa cylindrica	1000 ppm	1 M HCl	88
Mangifera indica leaves	1000 ppm	1 M HCl	92
Papaia	1000 ppm	1 M HCl	92
Pineapple stem	1000 ppm	1 M HCl	97
Plantago	1000 ppm	1 M HCl	94
Plantago ovata	1000 ppm	1 M HCl	94
Poinciana pulcherrima	1000 ppm	1 M HCl	96
Primula vulgaris flower	1000 ppm	1 M HCl	96
Tinospora crispa	1000 ppm	1 M HCl	80
Xantan gum	1000 ppm	1 M HCl	82

Table 1 presents the effectiveness of various green inhibitors, derived from natural sources, in mitigating corrosion in a 1 M HCl (hydrochloric acid) electrolyte at a concentration of 1000 ppm (parts per million) [52], [53], [54], [55], [56], [57], [58], [59], [60], [61], [62], [63], [64]. Corrosion inhibition efficiency (CIE) percentages are provided as indicators of the inhibitory performance of each inhibitor. Overall, the results demonstrate that the majority of the tested green inhibitors exhibit notable corrosion inhibition efficiency in the aggressive acidic environment represented by 1 M HCl. Ananas comosus (pineapple stem) and Pineapple stem extracts exhibit the highest corrosion inhibition efficiency, with CIE percentages of 98% and 97%, respectively. These findings suggest that extracts from pineapple and its stem possess significant potential as effective corrosion inhibitors in acidic environments. Several other natural extracts also demonstrate promising corrosion inhibition capabilities, with CIE percentages ranging from 80% to 96%. These include extracts from Calotropis procera, Cassia occidentalis, Chinese gooseberry fruit, Cryptocarya nigra, Datura stramonium, Juglans regia, Luffa cylindrica, Mangifera indica leaves, Papaia, Plantago, Plantago ovata, Poinciana pulcherrima, and Primula vulgaris flower. These results indicate the diversity of plant sources that can be explored for the development of green inhibitors. However, it is noteworthy that some inhibitors, such as Tinospora crispa and Xantan gum, exhibit comparatively lower corrosion inhibition efficiencies of 80% and 82%, respectively. Further investigation may be warranted to understand the factors influencing the inhibitory performance of these inhibitors and to optimize their effectiveness. The findings underscore the potential of natural extracts as corrosion inhibitors, particularly in acidic environments. The high corrosion inhibition efficiencies observed for several green inhibitors highlight their promising role in corrosion mitigation and underscore the importance of continued research in this area for the development of sustainable and eco-friendly corrosion control strategies.

2.2. Data-driven forecasting

Corrosion inhibition research has seen a growing interest in utilizing data-driven approaches to forecast corrosion rates and evaluate the effectiveness of inhibitors. The quantitative structure-property relationship (QSPR) model based on the machine learning (ML) approach can be used further in investigating different candidate inhibitor compounds because electronic properties and chemical reactivity can be quantified against the chemical structure of compounds [65], [66], [67], [68], [69], [70].

ML modeling involves several steps, from data collection and preprocessing to model training, evaluation, and deployment. Below is a general outline of the procedure:

a) Define the problem
b) Data collection
c) Data preprocessing
d) Model selection
e) Model training
f) Model evaluation
g) Model optimization
h) Model deployment
i) Model maintenance
j) Documentation and Reporting

Feature selection techniques play a crucial role in identifying relevant variables from complex datasets, thereby improving model accuracy and interpretability. Methods like principal component analysis (PCA), recursive feature elimination (RFE), and genetic algorithms help streamline data preprocessing and enhance model performance. Moreover, model optimization techniques, including hyperparameter tuning and cross-validation, ensure robustness and generalizability of predictive models.

To assess inhibitor performance, a variety of ML algorithms have been combined and widely used, including genetic algorithms (GA), multiple linear regressions (MLR), partial least squares (PLS), ordinary least squares regressions (OLS), artificial neural networks (ANN), adaptive neural fuzzy inference systems (ANFIS), and autoregressive with exogenous inputs (ARX). With the use of seven quantum chemical descriptors, the corrosion inhibition potential of eleven thiophene derivatives was predicted by the ANN model, yielding a coefficient of determination (R2) value of 0.96 [71]. Another QSPR study was created to use a mix of non-linear GA-ANN and linear GA-PLS approaches to predict molecules produced from pyridine and quinoline with 20 QCD. Root mean squared error (RMSE) values for the GA-PLS and GA-ANN models are 14.9 and 16.7, respectively, according to [72]. Quadri et al. [73] evaluated 20 pyridazine derivatives with 5 QCD using MLR linear and non-linear ANN models. With an RMSE score of 10.6, the data demonstrate that the ANN model yields more optimal results. OLS linear and non-linear ANN models were also created by Quadri et al. [74] in a different study to predict 40 quinoxaline-derived compounds using five chosen QCDs. With an RMSE value of 5.4, the results indicate that the ANN non-linear model makes a better forecast. The ANFIS and ANN models' performance was reported by Anadebe et al. [24]. For ANN, the two non-linear approaches yielded R2 and RMSE values of 0.91 and 4.4, but for ANFIS, the corresponding values were 0.99 and 1.4. These findings suggest that when assessing 15 salbutamol medication compounds that have expired as inhibitors, the ANFIS model performs better than the ANN model. Furthermore, an RMSE value of 7.0 was obtained in a recent work that developed an ARX model for 250 marketed pharmaceuticals that are utilized as corrosion inhibitors [75].

Despite the promise of data-driven approaches in corrosion inhibition research, several challenges need to be addressed, including the availability of high-quality data, data heterogeneity, model interpretability, and regulatory considerations. Furthermore, the integration of domain knowledge with data-driven techniques remains essential for developing accurate and reliable predictive models. Future research directions in data-driven corrosion inhibition forecasting include the development of hybrid models that combine ML algorithms with mechanistic insights, the utilization of advanced data analytics techniques such as deep learning and reinforcement learning, and the establishment of collaborative platforms for sharing corrosion data and models. Additionally, interdisciplinary collaborations between cor

2.3. DFT simulation

DFT simulation has become increasingly prevalent in corrosion inhibition research due to its ability to provide atomic-level insights into the interactions between inhibitors and metal surfaces. DFT offers a theoretical framework for investigating the electronic structure, energetics, and reactivity of corrosion inhibitors and metal surfaces [76], [77], [78], [79]. By solving the Kohn-Sham equations, DFT calculates the ground-state electronic density and energy, enabling the evaluation of adsorption energies, charge transfer, and bond strengths at the molecular level. Understanding these parameters is crucial for elucidating the mechanisms of corrosion inhibition [80], [81], [82], [83]. Various DFT methodologies are employed in corrosion inhibition studies, including different exchange-correlation functionals, basis sets, and surface models. Hybrid functionals, such as B3LYP and PBE0, are commonly used for their improved accuracy in describing both localized and delocalized electronic states. Additionally, periodic boundary conditions are utilized to simulate metal surfaces and corrosion processes in realistic environments.

DFT simulation has been applied to investigate various aspects of corrosion inhibition. DFT calculations provide insights into the adsorption behavior of inhibitors on metal surfaces, including the orientation, binding strength, and electronic structure of inhibitor-metal complexes. DFT allows for the calculation of electronic properties such as band structures, density of states, and work functions, which influence the corrosion kinetics and stability of inhibitor films [84], [85], [86], [87]. DFT-based QSAR models are developed to predict the corrosion inhibition efficiency of organic compounds based on their molecular descriptors and electronic properties. Despite its utility, DFT simulation in corrosion inhibition research faces challenges such as computational cost, accuracy limitations, and the need for experimental validation. Future research directions include the development of more efficient algorithms, improved exchange-correlation functionals tailored for corrosion studies, and the integration of DFT with experimental techniques for comprehensive mechanistic understanding. Several case studies exemplify the application of DFT in corrosion inhibition research, including the investigation of specific inhibitor-metal systems, the design of novel organic and inorganic inhibitors, and the elucidation of inhibition mechanisms under different environmental conditions [88], [89], [90].

Table 2. Adsorption energy of green inhibitor on iron surfaces

Green Inhibitor	**E_{ads} (kcal/mol)**	**Ref.**
Artichoke	-115.90	[91]
Chamomile flower	-111.17	[92]
Thynus vulgaris	-90.67	[93]

Table 2 presents the energy of adsorption (Eads) values for three different plant extracts - Artichoke, Chamomile flower, and Thymus vulgaris - on iron surfaces. These values provide insights into the strength of interaction between the plant extracts and the iron surface, which is crucial for evaluating their potential as green corrosion inhibitors. Artichoke extract exhibits the highest energy of adsorption (-115.90 kcal/mol) among the three inhibitors considered. This indicates a strong affinity for the iron surface, suggesting effective adsorption and inhibition properties. The high Eads value suggests that Artichoke extract forms a stable and protective adsorbed layer on the iron surface, hindering corrosion processes. Chamomile flower extract shows a slightly lower energy of adsorption (-111.17 kcal/mol) compared to Artichoke extract but still demonstrates a significant interaction with the iron surface. The moderate Eads value suggests that Chamomile flower extract can effectively inhibit corrosion by forming a protective film on the metal surface, albeit slightly weaker than Artichoke extract. Thymus vulgaris extract exhibits the lowest energy of adsorption (-90.67 kcal/mol) among the three inhibitors considered. While still indicating a favorable interaction with the iron surface, the lower Eads value suggests comparatively weaker adsorption compared to Artichoke and Chamomile flower extracts. This may imply that Thymus vulgaris extract provides relatively less effective corrosion inhibition compared to the other two extracts.

The differences in Eads values reflect variations in the chemical composition and surface-active components of the plant extracts. Artichoke and Chamomile flower extracts, with higher Eads values, may contain compounds that promote stronger adsorption and more effective corrosion inhibition. The Eads values provide valuable information for selecting and optimizing corrosion inhibitors for specific applications. Extracts with higher Eads values may be prioritized for further investigation and formulation development as corrosion inhibitors. Further experimental studies, such as electrochemical measurements and surface analysis techniques, are needed to validate the inhibitory performance of these plant extracts under practical corrosion conditions and assess their long-term effectiveness. In summary, the energy of adsorption values presented in the table offers valuable insights into the interaction strength between plant extracts and iron surfaces, aiding in the evaluation and selection of green corrosion inhibitors with potential industrial applications.

2.4. Experimental investigation

Corrosion inhibition plays a crucial role in mitigating material degradation and preserving the integrity of metallic structures in various industries. Experimental investigations on corrosion inhibition utilize a variety of techniques to evaluate the effectiveness of inhibitors and understand the underlying mechanisms. Common methodologies include electrochemical measurements such as potentiodynamic polarization, electrochemical impedance spectroscopy (EIS), and corrosion rate determination. Surface analysis techniques like scanning electron microscopy (SEM), atomic force microscopy (AFM), and Fourier-transform infrared spectroscopy (FTIR) are employed to characterize the morphology and composition of

metal surfaces before and after inhibition [94], [95], [96], [97].

A wide range of corrosion inhibitors, including organic compounds, inorganic salts, and nanomaterials, are tested for their inhibitory properties. Organic inhibitors such as benzotriazole, imidazoles, and quinoline derivatives are commonly studied due to their ability to form protective films on metal surfaces. Inorganic inhibitors like chromates, phosphates, and molybdates are also investigated for their corrosion inhibition potential. Additionally, nanomaterial-based inhibitors, including metal nanoparticles, graphene oxide, and carbon nanotubes, show promise in enhancing inhibition efficiency [98], [99], [100], [101], [102], [103], [104], [105].

Experimental investigations aim to elucidate the mechanisms through which inhibitors mitigate corrosion processes. Adsorption onto the metal surface, formation of protective films, and modification of the electrolyte composition are among the mechanisms studied. Techniques such as surface analysis, spectroscopy, and computational modeling are employed to understand inhibitor-metal interactions, adsorption isotherms, and corrosion kinetics [106], [107], [108], [109], [110].

Various factors affect the effectiveness of corrosion inhibitors, including inhibitor concentration, temperature, pH, and the composition of the corrosive environment. Experimental studies investigate the optimal conditions for inhibition and assess the inhibitor's performance under different operating conditions. Additionally, synergistic effects between inhibitors and other additives are explored to enhance inhibition efficiency and broaden the spectrum of protection [111], [112].

Experimental investigations evaluate the effectiveness of corrosion inhibitors based on parameters such as inhibition efficiency, corrosion rate reduction, and surface morphology analysis. The findings from these studies contribute to the development of practical corrosion mitigation strategies for industrial applications. Inhibitor formulations are optimized, and compatibility with specific metal substrates and corrosive environments is assessed to ensure long-term protection and cost-effectiveness [113], [114].

Despite significant progress, challenges such as inhibitor stability, environmental concerns, and compatibility with existing infrastructure remain to be addressed. Future research directions include the development of eco-friendly inhibitors, advanced characterization techniques for in-situ monitoring of corrosion processes, and the integration of experimental and computational approaches for comprehensive mechanistic understanding.

Table 3. CIE of green inhibitors

Green Inhibitor	CIE (%)	Ref.
Artichoke	99	[115]
Chamomile flower	97	[116]
Thynus vulgaris	95	[117]

Table 3 presents the Corrosion Inhibition Efficiency (CIE) values of three green inhibitors: Artichoke, Chamomile flower, and Thymus vulgaris. These CIE values, expressed as percentages, indicate the effectiveness of each inhibitor in mitigating corrosion on metal surfaces. Artichoke demonstrates a high CIE of 98.7%, as reported by Salmasifar et al. (2021). This indicates that Artichoke extract is highly effective in inhibiting corrosion, with nearly complete protection against metal degradation. The high CIE suggests strong adsorption and formation of a protective barrier on the metal surface, preventing corrosive attacks. Chamomile flower extract exhibits a CIE of 97%, according to Shahini et al. (2021). This indicates excellent corrosion inhibition properties, with a high level of protection against metal corrosion. The CIE value suggests that Chamomile flower extract forms a robust inhibitor film on the metal surface, reducing corrosion rates significantly. Thymus vulgaris extract shows a CIE of 95%, as reported by Lashgari, Bahlakeh, and Ramezanzadeh (2021). While slightly lower than the Artichoke and Chamomile flower, this CIE value still indicates excellent corrosion inhibition performance. Thymus vulgaris extract effectively mitigates corrosion by forming a protective layer on the metal surface, reducing corrosion rates significantly.

The high CIE values for all three green inhibitors suggest their potential as effective corrosion inhibitors for practical applications. The differences in CIE values may be attributed to variations in the chemical composition, concentration, and formulation of the inhibitors, as well as differences in experimental conditions and test methods. The reported CIE values provide valuable guidance for selecting and optimizing corrosion inhibitors for specific industrial applications. Inhibitors with higher CIE values may be prioritized for further investigation and formulation development.

Further studies, including long-term exposure tests and compatibility assessments with different metal substrates and corrosive environments, are needed to validate the inhibitory performance and practical

applicability of these green inhibitors. In summary, the CIE values presented in Table 3 highlight the corrosion inhibition effectiveness of Artichoke, Chamomile flower, and Thymus vulgaris extracts. These green inhibitors show significant potential for mitigating corrosion and protecting metal surfaces in various industrial settings, contributing to the development of environmentally friendly corrosion mitigation strategies.

3. DISCUSSION

Integrating data-driven forecasting, DFT simulation, and experimental investigation offers a comprehensive approach to understanding corrosion inhibition mechanisms, predicting inhibitor performance, and optimizing corrosion mitigation strategies. Each method contributes unique insights and benefits, and their combination can overcome individual limitations while providing a more holistic understanding of corrosion processes.

Data-driven forecasting leverages historical and experimental data to develop predictive models for corrosion inhibition. Machine learning algorithms can identify patterns and relationships within complex datasets, enabling the prediction of corrosion rates, inhibitor efficiencies, and optimal conditions for inhibition. Data-driven models may lack mechanistic insights into corrosion inhibition mechanisms and rely heavily on the quality and quantity of available data. They may also struggle to capture the intricacies of molecular interactions and surface chemistry. Data-driven forecasting provides valuable input parameters for DFT simulations and experimental investigations, guiding the selection of inhibitors, experimental conditions, and optimization strategies.

DFT simulation offers atomic-level insights into inhibitor-metal interactions, electronic properties, and adsorption mechanisms. It provides a theoretical framework for understanding the energetics and kinetics of corrosion processes, enabling the prediction of inhibitor effectiveness and the design of novel inhibitors. DFT calculations are computationally intensive and may be limited by the choice of exchange-correlation functionals and approximations. They may also oversimplify the complexity of real-world corrosion environments and experimental conditions. DFT simulations complement experimental data by providing mechanistic insights into inhibitor adsorption, surface coverage, and film formation. They guide experimental design and interpretation, validating hypotheses and elucidating underlying inhibition mechanisms.

Experimental investigation provides direct measurements of corrosion rates, inhibitor performance, and surface morphology under real-world conditions. Electrochemical techniques, surface analysis, and spectroscopic methods offer valuable insights into inhibitor-metal interactions, film stability, and corrosion kinetics. Experimental studies may be time-consuming, resource-intensive, and subject to variability due to environmental factors and sample preparation techniques. They may also face challenges in quantifying molecular-level interactions and elucidating complex inhibition mechanisms. Experimental data validate and refine predictions from data-driven models and DFT simulations. They provide ground truth measurements for model calibration and validation, confirming the accuracy and reliability of computational predictions. Additionally, experimental findings guide the development of new inhibitors and inform the refinement of theoretical models.

Integrating data-driven forecasting, DFT simulation, and experimental investigation offers a synergistic approach to corrosion inhibition research. By combining quantitative predictions with mechanistic insights and empirical validation, researchers can develop robust and reliable corrosion mitigation strategies tailored to specific applications and environmental conditions. The iterative feedback loop between computational modeling and experimental validation enhances the accuracy and reliability of corrosion inhibition predictions. It allows researchers to refine theoretical models, optimize inhibitor formulations, and address practical challenges in corrosion mitigation. Interdisciplinary collaboration between computational scientists, experimentalists, and corrosion engineers is essential for effectively integrating data-driven, theoretical, and empirical approaches. By leveraging the strengths of each method and fostering collaboration across disciplines, researchers can advance our understanding of corrosion processes and develop innovative solutions for material protection and sustainability.

In summary, integrating data-driven forecasting, DFT simulation, and experimental investigation offers a powerful and comprehensive approach to corrosion inhibition research. By leveraging the strengths of each method and synergistically combining computational modeling with empirical validation, researchers can overcome individual limitations and develop effective corrosion mitigation strategies for diver

4. CONCLUSION

The integration of data-driven forecasting, DFT simulation, and experimental investigation offers a comprehensive approach to corrosion inhibition research. By combining predictive modeling with atomic-level insights and empirical validation, researchers can develop effective corrosion mitigation strategies tailored to specific applications. Interdisciplinary collaboration and iterative feedback between computational and experimental methods enhance the accuracy and reliability of predictions, leading to innovative solutions for material protection and sustainability in various industries.

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