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A Review of Theoretical Techniques in Corrosion Inhibition Studies:

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Abstract: *Studies on corrosion inhibition are essential for preventing and reducing the damaging effects of Corrosion in a variety of sectors. With their ability to provide an understanding of molecular interactions, structure-activity connections, proposal of new inhibitors and the prediction of inhibitor efficacy, theoretical approaches have become important research tools in the field of corrosion inhibition. An overview of the theoretical methods frequently used in investigations on corrosion inhibition is given in this paper. Despite improvements in theoretical methods, problems with accuracy, accessibility to computational tools, large-scale time required for larger molecules and the incorporation of multi-scale modelling strategies still exist. The development of more effective and long-lasting corrosion inhibitors is made possible by theoretical methodologies, which have the potential to have a considerable impact on corrosion inhibition research. In this review, theoretical methods are viewed as an avenue for the provision of knowledge of molecular interactions, prediction of inhibitor function, and useful insights into corrosion inhibition investigations. The use of theoretical approaches allows for the understanding of molecular interactions, the prediction of inhibitor activity, and the optimization of inhibitor design. It is the view of the authors that likely, future theoretical developments will significantly advance corrosion prevention techniques and improve the toughness and dependability of materials and structures in a variety of industrial applications. Consequently, the advantages, challenges and the way forward on the derivation of theoretical results closely analogous to those from experiments are enumerated in this work. The authors considered this view the considerations of the popular and relatively developed methods that apply to corrosion studies. These include density functional theory (DFT), molecular dynamics (MD) simulations, Monte Carlo (MC) simulations, and quantum chemical calculations, etc. These techniques are now essential for the creation, improvement, and comprehension of corrosion inhibitors.*

Keywords: *Corrosion, analytical methods, experimental and computational methods.*

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1.0 Introduction

In a variety of industries, including oil and gas, aerospace, fertilizer, automotive, and metallurgical industries, Corrosion offers

severe challenges that can lead to their closure if not handled effectively. Corrosion can be defined as an electrochemical process that operates to progressively degrade metals due to interactions with some chemicals or components of the environment. C environment—poses serious problems. Studies on corrosion inhibition are essential because they can recommend remediation measures that can curb damages to industrial facilities and consequent reduction of economic costs that may not be bearable to the industries and the environment. Experimental methods have historically been the main method used to study corrosion inhibition. To understand and build efficient corrosion inhibitors, however, theoretical approaches have become potent tools that complement and augment experimental efforts (Al-Amiery *et al.,* 2021; Etim et al., 2022).

In order to study corrosion processes at the atomic and molecular level, researchers use theoretical methodologies, which cover a wide spectrum of computational techniques. The interactions between inhibitors and corroding surfaces, as well as the fundamental causes of Corrosion, are all usefully revealed by these techniques (Eddy and Ita, 2011b).

With the success of computational tools based on quantum backgrounds, scientists can pre-screen possible inhibitor candidates and gain a basic understanding of their inhibition processes by using theoretical approaches, which also save time, money, and effort. Molecular modelling is one of the popular theoretical approaches utilized in corrosion inhibition investigations (Eddy *et al*., 2018). Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations are two techniques included in molecular modelling packages (Etim *et al*., 2020a,b,c). With the aid of DFT, corrosion systems' electronic structure, energetics, and reactivity may be precisely calculated, giving vital details on bond strengths, adsorption energies, and reaction routes. By giving dynamic insights into the behavior of inhibitors and the corrosion interface, MD simulations, on the other hand, enable the study of corrosion processes throughout time (Al-Amiery *et al.,* 2021). By offering invaluable insights into the molecular-level interactions, structure-activity connections, and inhibition mechanisms, theoretical approaches have transformed investigations of corrosion inhibition. These techniques, which include molecular modelling, high-throughput screening, data mining, machine learning, molecular docking, and computational electrochemistry, can be used in conjunction with experimental research to discover and enhance corrosion inhibitors. It is possible to considerably develop corrosion inhibition strategies and lessen the detrimental impacts of Corrosion in several industrial applications by combining theoretical and experimental methodologies. This article's goal is to model, predict, and understand how corrosion inhibitors behave and how they interact with metallic surfaces using computational methods like molecular dynamics simulations, quantum chemical calculations, density functional theory, Monte Carlo simulations, structure-property relationships, data mining and machine learning techniques, and molecular docking and binding energy calculations (Al-Amiery *et al.,* 2021).

2.0 Theoretical & Computational Methods in Corrosion Inhibition Studies

Some of the computational methods commonly employed in corrosion research are highlighted in this section.

2. 1. Molecular dynamics simulations

A powerful tool for comprehending corrosion processes and judging the effectiveness of corrosion inhibitors is molecular dynamics (MD) simulations. MD simulations, which provide atomistic-level insights into the behavior of molecules and materials over time, enable the study of corrosion mechanisms,

inhibitor adsorption, and interactions at the metal surface and electrolyte contact. (Xiong *et al.,* 2021). Investigation of inhibitor adsorption and its impact on the corrosion behavior of metal surfaces, such as the effect on the adsorption behavior of poly (aspartic acid) and poly (glutamic acid) on Fe (110) surface and carbon steel in salt spray, is one application of Molecular Dynamics (MD) simulations in corrosion as shown in Fig 1.

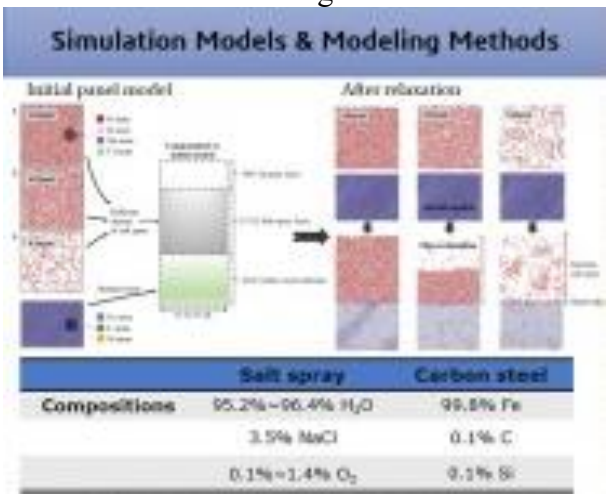

Fig. 1: Molecular dynamics simulations of carbon steel in salt spray. (Source: 1-s2.0-S0927025621008041-ga1.jpg (373×200) (els-cdn.com))

In Fig. 2, the schematic diagram is displayed. Six layers of Cu (111) surface atoms made up the bottom layer, while the intermediate layer was made up of 300 H2O, 5 H3O+, 5 Cl, and 1 inhibitor molecule (a blank group lacking an inhibitor molecule). The software makes provisions that employ the periodic boundary conditions, (the upper layer was built as a 25-layer) to account for some expected environments.

In MD simulations, quantum mechanical potentials or classical force fields are used to describe how atoms and molecules behave. According to Gao *et al.* (2018), these potentials include empirical parameters that represent bonded and non-bonded atom-to-atom interactions. The motion equations are then numerically solved, enabling the simulation of the system's dynamics. The adsorption behavior of inhibitors on metal surfaces, the stability of inhibitor-metal complexes, and the diffusion of inhibitors in the electrolyte are just a few of the topics that MD simulations can shed light on concerning studies on corrosion inhibition.

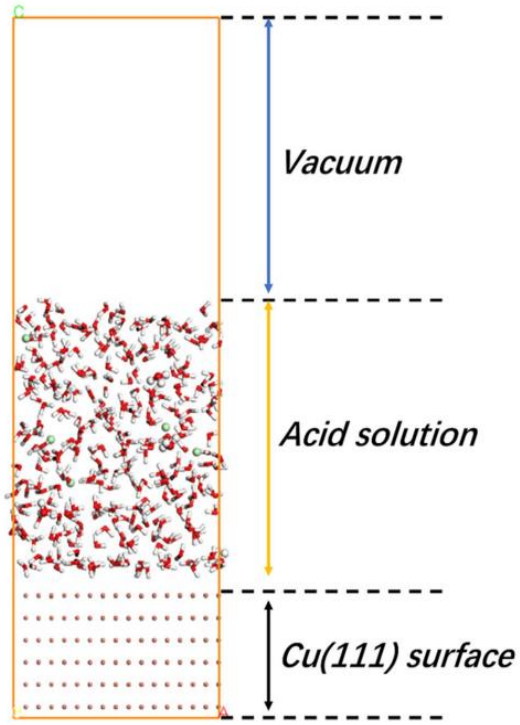

Fig. 2.0 Schematic diagram of the MD simulation model (Source: Xu, *et al.*, 2022)

Researchers can learn more about the fundamental principles regulating corrosion inhibition by simulating the behavior of corrosion systems under various variables, such as temperature, pH, and inhibitor concentration. MD simulations have been used in several investigations to look into corrosion inhibition. For instance, Gao *et al.* (2018) used MD simulations to examine the adsorption characteristics of an inhibitor of corrosion based on imidazoline on an iron surface. The simulations shed light on the inhibition mechanism by showing the intricate molecular interactions between the inhibitor molecules and the metal surface.

2.2 Quantum chemical calculations

The electronic structure, energetics, and reactivity of corrosion systems and corrosion inhibitors are crucially understood through the use of quantum chemical simulations. These computations, which are based on quantum mechanics concepts, offer insightful knowledge about the interactions between atoms and molecules and enable the prediction of molecular characteristics and behavior (Ser, *et al.,* 2021; Etim *et al.*, 2017a,b; Shinggu *et al.*, 2023; Ushie *et al.*, 2017). One of the popular quantum chemical approaches for the study of corrosion inhibition is density functional theory (DFT). By employing an exchange-correlation function to solve the Schrödinger equation, DFT determines a system's electronic structure. The understanding of the adsorption behavior and reactivity of corrosion inhibitors requires knowledge of the molecular orbitals, energy levels, charge distributions, and bonding properties, all of which are revealed by DFT simulations (Etim *et al.*, 2021).

The adsorption energies, corrosion potentials, and reaction barriers are just a few of the features that may be predicted using quantum chemical calculations that are important to the prevention of corrosion. These forecasts support rational design and screening of candidate inhibitors, enabling the discovery of compounds with advantageous corrosion-inhibiting capabilities. For instance, Guo *et al.* (2017) investigated the inhibitory effects of pyrazoline derivatives using DFT simulations. The computed molecule orbital and adsorption energies shed light on the inhibitory mechanism and explained the experimentally detected trends. A case study of the quantum chemical approach is Imidazoline derivatives as corrosion inhibitors for carbon steel. The investigated methodologies included the following: Based on the structural variety of the compounds and prior experimental research, a group of imidazoline derivatives with possible corrosion-inhibitory abilities was selected. The calculations were done using density functional theory (DFT), a popular quantum chemistry technique. The electronic structure and characteristics of molecules may be efficiently and precisely calculated using DFT. DFT computations were used to optimize the imidazoline derivatives' molecular structures (Liu and Gao, 2019). To achieve the compounds' most stable structures, this stage involved minimizing the overall energy of the compounds. The lowest unoccupied molecular orbital (LUMO), the highest occupied molecular orbital (HOMO), and the energy gap of the imidazoline derivatives were all calculated using DFT. These characteristics shed light on the compounds' reactivity, stability, and charge transfer abilities. Through the use of DFT adsorption calculations, the interaction between the imidazoline derivatives and the carbon steel surface was examined. Adsorption energies were established to calculate the strength of the inhibitor-metal interaction. Charge density difference calculations were also performed to observe the charge redistribution during adsorption (Xiong et al., 2021). The quantum chemical simulations helped to clarify the mechanism of action of the selected imidazoline derivatives on carbon steel corrosion. Electronic properties, including HOMO, LUMO, and energy gaps, revealed stability, reactivity, and charge transfer (Liu and Gao, 2019).

2.3. Density Functional Theory (DFT)

Density functional theory (DFT) is a regularly used theoretical technique in research on corrosion inhibition. For analyzing the energetics, electronic structure, and properties of molecules and materials (Eddy and Ita, 2011a). The DFT method can provide a strong foundation for several corrosion processes. It offers a helpful approach for resolving the many-electron Schrödinger equation by substantially approximating the exchange-correlation functionals, which describe the electron-electron interactions. Several characteristics, such as adsorption energies, charge distributions, and electronic properties,

that are essential to inhibitor effectiveness in corrosion inhibition studies can be predicted using DFT simulations. These estimates take into account the reactivity of inhibitor molecules, the stability of inhibitor-metal complexes, and the adsorption behavior of inhibitors on metal surfaces (Li et al., 2020; Onen *et al.*, 2017). DFT computations can be used by scientists to examine the atomic-level interactions between corrosion inhibitors and metal surfaces. This helps to understand the process of adsorption, the strength of inhibitor-metal interactions, and the stability of the adsorbed species. The electronic features obtained by DFT calculations, such as the frontier molecular orbitals and electronic density of states, convey information about the inhibitory activity of the molecules and their ability to donate or absorb electrons. The DFT computations and molecular dynamics simulations are routinely coupled to study the behavior of corrosion systems over time. The inclusion of DFT-derived parameters in force fields or potentials improves simulation accuracy and enables the study of larger systems and longer periods. Li *et al.,* (2020). Numerous studies on corrosion inhibition have utilized DFT calculations. For instance, Li *et al.* (2020) used DFT calculations to examine the adsorption behavior of thiazole derivatives as corrosion inhibitors on a copper surface. The projected adsorption energies and electrical properties provide insights into the inhibition process and clarify the structure-activity correlations of the inhibitors.

2. 4. Monte Carlo (MC) simulations

Studies on corrosion inhibition often make use of Monte Carlo (MC) simulations, another useful theoretical method. Through the random selection of configurations from a set of possibilities according to a specified probability distribution, MC simulations offer a statistical method to model the behavior of complex systems. MC simulations are frequently used in corrosion inhibition studies to examine the thermodynamic and adsorption characteristics of corrosion inhibitors. The MC simulations packages have offered researchers the opportunity to probe into the conformational space of inhibitor chemicals and how they attach to metal surfaces. The simulations, which can account for the effects of temperature, pH, and inhibitor concentration, can provide insights into the thermodynamics of the adsorption process. By examining the probability distribution of alternative configurations, MC simulations can predict the equilibrium adsorption isotherms and the surface coverage of inhibitors (Martinez *et al*., 2017). The free energy of adsorption can be determined by the use of MC simulations in conjunction with the necessary force fields or potentials, providing numerical data on the inhibitory effects of compounds. The design and optimization of corrosion inhibitors depend heavily on this information. The impact of molecular structure, functional groups, and environmental factors on the adsorption behavior of inhibitors can also be studied using MC simulations. MC simulations enable the exploration of the chemical space and the identification of molecular properties that contribute to effective inhibition by sampling a large number of potential configurations (Wu *et al.,* 2019).

Wu *et al.* (2019) study employed MC simulations to examine the adsorption behavior of an amino acid-based corrosion inhibitor on a steel surface. The understanding of the inhibition mechanism was aided by the simulations' insights into the coverage, orientation, and interactions of the inhibitor molecules.

2.5. Structure-Property Relationship (SPR)

SPR analysis is yet another essential component of theoretic methods in corrosion inhibition investigations. Quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) models are created as part of SPR analysis. These models relate the effectiveness

of corrosion inhibitors to molecular characteristics, including electronic, steric, and hydrophobic properties. Researchers can estimate the efficiency of possible inhibitors by identifying these correlations, which helps with the logical design and optimization of corrosion inhibitors. The subject of corrosion inhibition has undergone a revolution because of high-throughput screening technologies and theoretical theories (González-Olvera *et al.,* 2021). To find prospective inhibitor candidates, virtual screening, a ligand- or structure-based method, rapidly screens vast chemical libraries. Combinatorial chemistry approaches enable the synthesis and screening of many inhibitor libraries, allowing researchers to efficiently investigate a broad variety of chemical space. The prediction of corrosion inhibition efficiency of pyridines and quinolines using quantitative structure-property relationship models is an example of a structure-property relationship. It describes the development of linear and non-linear QSPR models to predict corrosion inhibition efficiency for a series of 41 pyridine and quinoline N-heterocycles.

2.6. Data mining and machine learning techniques

Studies on corrosion inhibition have seen a rise in the use of data mining and machine learning approaches. These methods enable the extraction of significant patterns and correlations from big datasets that include experimental and computational data. Researchers can forecast inhibitor performance, discover critical variables affecting inhibition effectiveness, and gain insights into the intricate relationship between molecular characteristics and corrosion inhibition by training machine learning models on these datasets (Ser*, et al.,* 2020). A method using machine learning to model measurements of carbon steel corrosion rates as a function of time when corrosion inhibitors are added in various dosages and dose schedules is machine learning modelling of time-dependent corrosion rates of carbon steel in the presence of corrosion inhibitors. We have found out that Random Forest, with mean squared errors ranging from 0.005 to 0.093, was the best algorithm for predicting the complete time profile of corrosion rates. The trained Random Forest model makes accurate predictions about how corrosion rates will fluctuate in response to changes in environmental variables. (Aghaaminiha *et al.,* 2021).

2.7. Molecular docking and binding energy calculations

The interactions between inhibitors and corroding surfaces are examined using molecular docking and binding energy estimates. These methods shed light on the main interactions between the inhibitor molecules and the metal surface as well as their binding affinities and ways of binding. According to Moussaoui and Mernari (2020), such knowledge facilitates the logical design of inhibitors with enhanced binding and inhibitory characteristics. Researchers can also examine the electrochemical behavior of corrosion inhibitors using computational electrochemistry methods, including diffusion-controlled reaction simulations and Electrochemical Impedance Spectroscopy (EIS) modelling. These methods aid in the interpretation of experimental electrochemical data and offer a fuller knowledge of the inhibitory mechanisms. In investigations on corrosion inhibition, combining theoretical and experimental methods has become standard practice. Researchers can improve inhibitor designs, optimize synthesis pathways, and increase confidence in the effectiveness of corrosion inhibitors by fusing theoretical hypotheses with experimental validations (Moussaoui and Mernari, 2020).

3.0 Conclusion

The use of theoretical methods has transformed research on corrosion inhibition by illuminating the interactions at the molecular

level, the structure-activity correlations, and the inhibition processes.

A robust framework for examining the electronic structure and characteristics of molecules and materials is provided by DFT calculations. Researchers can gain knowledge about the adsorption behavior and reactivity of corrosion inhibitors by using DFT calculations to forecast crucial features such as adsorption energies, charge distributions, and electronic properties. The atomic level analysis of inhibitor-metal interactions made possible by DFT simulations helps to clarify the adsorption process and stability of inhibitor-metal complexes. Additionally, to analyze the evolution of corrosion systems and get dynamic insights into the interactions and behavior of inhibitors, DFT calculations and MD simulations are frequently combined. MD simulations offer atomistic-level insights into the behavior of molecules and materials throughout time. These models enable the study of inhibitor adsorption, corrosion processes, and interactions at the metal-electrolyte interface. Researchers can learn more about the underlying principles driving corrosion inhibition by modelling corrosion systems under various situations. We can explore larger systems and longer time scales using MD models, which helps us better understand the dynamics and kinetics of corrosion processes. A thorough knowledge of the interactions and behavior of corrosion inhibitors is made possible by the combination of MD simulations and DFT calculations.

A statistical method for examining the thermodynamic and adsorption characteristics of corrosion inhibitors is provided by MC simulations. by randomly selecting configurations from a probability distribution. MC simulations shed light on the adsorption behavior and equilibrium surface coverage of inhibitors. The thermodynamics of the adsorption process can be learned from these simulations, which take into consideration the effects of temperature, pH, and inhibitor concentration. Using MC simulations, it is possible to investigate the conformational space of inhibitor molecules and pinpoint the specific chemical characteristics that contribute to efficient inhibition. To comprehend the electronic structure, energetics, and reactivity of corrosion systems and inhibitors, quantum chemical calculations such as DFT and other quantum mechanical approaches are used. These calculations help in the molecular level property and behavior prediction by shedding light on the interactions between atoms and molecules.

Overall, theoretical methods contribute significantly to research on corrosion inhibition by enhancing experimental work and providing a greater knowledge of the molecular-level mechanisms underlying corrosion processes. These methods help with the design and optimization of corrosion inhibitors, the prediction of inhibitor performance, and the clarification of structure-activity connections. The improvement of inhibitor designs, optimization of synthesis pathways, and verification of theoretical hypotheses are all made possible by the merging of theoretical and experimental methodologies. Likely, future theoretical developments will significantly advance corrosion prevention techniques and improve the toughness and dependability of materials and structures in a variety of industrial applications.

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Declarations

The authors declare that they have no conflict of interest.

Data availability

All data used in this study will be readily available to the public.

Consent for publication

Not Applicable

Availability of data and materials

The publisher has the right to make the data Public.

Competing interests

The authors declared no conflict of interest.

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Authors' contributions

HSS, UNM and UNM were involved in literature review, writing and drafting, revision and editing while GJ and EEE were involved in conceptualization, writing and drafting, revision and editing.