Modern Chemistry
2026, Vol. 14, No. 4, pp. 116–119
https://doi.org/10.11648/j.mc.20261404.12

Research Article

Theoreticaland Computational Studies of Corrosion Inhibition: Recent Developments

Sulaiman Tijjani Nasiru[1, *], Abubakar Ado Ibrahim[2], Sagir Isa Musa[3], Abdulmumin Malam Usman[1], Hadiza Jibril Abdullahi[4]

[1]Department of Applied Chemistry, Federal University of Technology, Babura, Nigeria

[2]Department of Human Medicine, Bayero University, Kano, Nigeria

[3]Department of Pure and Industrial Chemistry, BayeroUniversity, Kano, Nigeria

[4]Department of Chemistry, Federal College of Education (Technical) Bichi, Kano, Nigeria

Abstract

Corrosion remains a major challenge in industrial systems, leading to significant economic losses, material degradation, and safety concerns. Corrosion inhibitors are widely employed to mitigate metal deterioration; however, the discovery and optimization of efficient, environmentally friendly inhibitors through conventional experimental methods are often costly and time-consuming. Consequently, theoretical and computational approaches have become indispensable tools for understanding corrosion inhibition mechanisms and accelerating inhibitor development. This review aims to provide a comprehensive overview of the theoretical and computational methods applied in corrosion inhibition studies between 2015 and 2025, with particular emphasis on Density Functional Theory (DFT), Molecular Dynamics (MD) simulations, Quantitative Structure-Activity Relationship (QSAR) modeling, and emerging Machine Learning (ML) techniques. Relevant literature was critically analyzed to evaluate recent advances in predicting inhibitor efficiency, adsorption behavior, and structure-activity relationships for metallic systems, particularly aluminium and steel.The review demonstrates that DFT remains a powerful approach for identifying key electronic descriptors, including HOMO energy, LUMO energy, and energy gap, which strongly influence inhibitor performance. Molecular dynamics simulations provide detailed insights into adsorption mechanisms and inhibitor orientation at metal surfaces, while QSAR models establish quantitative relationships between molecular descriptors and inhibition efficiency. Recent integration of machine learning algorithms with DFT and QSAR methodologies has significantly improved predictive accuracy, enabled rapid screening of large molecular libraries, and facilitated the design of eco-friendly corrosion inhibitors. Furthermore, hybrid computational workflows combining DFT, MD, QSAR, and ML have enhanced mechanistic understanding while reducing experimental costs and development time. Theoretical and computational techniques have transformed corrosion inhibitor research by providing reliable predictive frameworks for inhibitor design. Future progress will depend on the integration of advanced artificial intelligence tools, standardized datasets, and rigorous experimental validation to support sustainable and industrially applicable corrosion protection strategies.

Keywords

Corrosion Inhibition, DFT, Molecula RDynamics, QSAR, Machine Learning, Aluminium, Adsorption

*Correspondence: SulaimanTijjaniNasiru (tnsulaiman.chem@futb.edu.ng)

Received: 8 June 2026; **Accepted:** 25 June 2026; **Published:** 3 November 2026

Copyright: © The Author(s), 2026. Published by Science Publishing Group. This is an **Open Access** article, distributed under the terms of the Creative Commons Attribution 4.0 License (http://creativecommons.org/licenses/by/4.0/), which permits unrestricted use, distribution and reproduction in any medium, provided the original work is properly cited.

1.Introduction

Many studies have reported the effectiveness of some compoundsas corrosion inhibitors for a wide range of metals and alloys such as aluminum, mild steel, and iron. Generally, these inhibitors act by forming protective films on metal surfaces, reducing the electrochemical reactions responsible for corrosion. However, due to the environmental and health hazards associated with inorganic inhibitors, there has been a shift toward the development of environmentally benign, biodegradable ("green") corrosion inhibitors [1]. Various electrochemical and surface characterization techniques such as electrochemical impedance spectroscopy (EIS), potentiodynamic polarization, and surface analysis (SEM, XPS, FTIR) have been used to study inhibitor performance and film formation [2]. The inhibition mechanism and adsorption behavior of these compounds depend on both the nature of the metal and the corrosive environment, often obeying different adsorption isotherms and exhibiting anodic, cathodic, or mixed-type inhibition characteristics[3]. Several factors including cost, availability, and environmental safety are essential when selecting a corrosion inhibitor [3]. Due to the high expense and time-intensive nature of experimental methods, theoretical and computational methods have become increasingly important in corrosion science [4]. The Quantitative Structure-Activity Relationship (QSAR) approach has become widely used to predict corrosion inhibition efficiency based on molecular descriptors such as dipole moments, molecular surface area, EHOMO, ELUMO, and energy gap [5]. Recent developments in computational chemistry, artificial intelligence, and materials informatics have expanded the predictive accuracy of these models[5, 6].

2. Theoretical Background

Quantum chemical calculations, molecular dynamics simulations, and QSAR modeling form the theoretical foundation for predicting corrosion inhibition efficiency. Density Functional Theory (DFT) provides information about molecular orbitals and reactivity, while molecular dynamics (MD) simulations reveal the adsorption mechanisms at the metal-solution interface. QSAR methods relate these quantum descriptors to inhibition performance using statistical or machine learning models. Together, these approaches provide insight into the mechanisms of inhibitor adsorption and electron transfer at metal surfaces.

3. Computational Approaches to Corrosion Inhibition

3.1. Density Functional Theory (DFT)

DFT has been widely applied to determine the relationship between molecular structure and corrosion inhibition efficiency. [6] and [7] reported that EHOMO, ELUMO, and the energy gap (ΔE) strongly correlate with inhibition performance. [7] extended this approach by studying quinoline Schiff bases on aluminium, showing that smaller ΔE and higher EHOMO values enhance electron donation to the metal surface. More recent works, such as [7] and [8], combine DFT with machine learning to identify key descriptors governing corrosion protection efficiency.

3.2. Molecular Dynamics Simulation

Molecular dynamics simulations provide atomic-level insight into inhibitor adsorption on metallic surfaces. [9] and [10] applied MD simulations to study alanine and organic inhibitors on aluminium and steel, revealing parallel adsorption configurations that maximize surface coverage. Recent MD studies by [10] and [11] demonstrate that combining DFT with MD enables accurate prediction of adsorption strength and inhibitor orientation, essential for optimizing inhibitor formulations.

3.3. QSAR and Machine Learning Approaches

QSAR modeling correlates experimental inhibition efficiencies with molecular descriptors using statistical or machine learning techniques. [12] used the Genetic Function Approximation (GFA) method to model amino acid inhibition efficiencies, while [12] developed neural network-based QSAR models for furan derivatives. More recently, [13] and [14] have integrated deep learning algorithms to predict corrosion inhibitor efficiency across diverse compound libraries, marking a major step toward automated inhibitor discovery. Early pioneering work such as [15] explored the inhibition efficiencies of 23 organic compounds on steel (and separately on aluminium) surfaces in hydrochloric acid media. They used physicochemical and topological descriptors to build QSAR (quantitative structure-acstivity relationship) models [15]. Their findings indicated that quantum chemical descriptors - especially the lowest unoccupied molecular orbital energy (E_LUMO) and molecular volume - were crucial predictive parameters for inhibition efficiency. In the aluminium case, they concluded similarly that quantum descriptors outperform structural descriptors when prediction ability is the key goal. Subsequently, other authors such as [16] emphasised that an inhibitor's performance is strongly influenced by molecular features such as functional groups, electron-density at donor atoms, p-orbital character, chain length, aromatic/conjugated systems, bonding strength to substrate, cross-linking ability and solubility [16]. Meanwhile, [17] pointed out that inhibitors often act by forming one or more molecular layers on the metal surface which prevent acid attack via physical and/or chemical adsorption.

In 2019, the work of [17] on quinoline derivatives for aluminium in 1 M HCl integrated DFT calculations and QSAR analysis: descriptors such as E_HOMO, softness (σ), electrophilicity (ω), ΔN (electron transferred), and back-donation energy (ΔE_b-d) were found to have strong correlation with inhibition efficiency; interestingly, molecular weight and volume had negative correlation with IE whereas E_LUMO, band gap (BG) and hardness (η) did not show correlation [18]. More recently (2019-2025), there has been a strong shift toward machine-learning (ML) and hybrid workflows: A study developed a data-driven QSPR model using gradient-boosting decision trees combined with permutation feature importance (PFI) to predict inhibition efficiency (IE) of organic inhibitors on carbon steel; descriptors of topological/BCUT2D/MOE-type featured strongly and the model achieved $R^2 \approx 0.72$, MAE ≈ 4.80%, RMSE ≈ 6.40% [18].

Another work applied ML (SVR, RF, MLP, XGBoost) to predict corrosion inhibition of quinoxaline compounds via QSPR; the best models achieved high predictive accuracy [19].

4. Discussion of Recent Findings

A comprehensive review of computational methods in corrosion inhibition highlighted the integration of DFT, MC/MD simulations, and ML/AI workflows to accelerate inhibitor discovery [20]. A 2024 study of chitosan-modified quaternary ammonium salts for carbon steel used quantum chemical calculations, surface analysis and electrochemical tests to link molecular structure and inhibitor performance in real wastewater environments [21]. A 2025 review by Riyaz et al. described the rise of ML-driven prediction of inhibitor efficiency and its role in sustainable corrosion control [22]. Synthesis of Results: From earlier QSAR/DFT/MC studies, key molecular descriptors such as E_HOMO ↑, E_LUMO ↓, ΔE ↓, larger molecular volume/area (for better coverage), dipole moment ↑, and electron donating heteroatoms (N, O, S) were consistently correlated with better inhibitor performance. Adsorption models (Langmuir, Temkin, Freundlich) described how molecules interact with metal surfaces both physically and chemically. From recent ML-driven studies, several trends have emerged:

1. Descriptor sets are richer: beyond frontier orbitals, they include BCUT2D, topological indices, molecular electrostatic potential descriptors, and solvent-interaction energies.

2. Feature-selection techniques (PFI, SHAP) identify the most predictive descriptors, enabling smaller descriptor sets and better interpretability.

3. ML models provide rapid screening of large libraries of compounds and can suggest new inhibitor molecules with predicted high IE.

4. Hybrid pipelines (DFT → MD/MC → ML → experiment) reduce experimental burden and cost while retaining mechanistic insight.

5. Real-world applications increasingly combine computational prediction with electrochemical validation.

Implications for Future Research:

i. Integrating QSAR/ML with adsorption modelling (MD/MC) and electronic structure (DFT) offers a holistic framework for corrosion inhibitor design.

ii. Descriptor development remains critical: inclusion of adsorption energy, solvent interactions, film formation parameters, and machine-learned embeddings may further improve predictive accuracy.

iii. Building larger and standardized datasets (with consistent experimental conditions) is essential to improve model generalisability.

iv. Experimental validation remains necessary to confirm predictions with electrochemical and surface characterization data.

v. Emphasis on sustainability and eco-friendliness continues to grow: computationalworkflows can prioritize less toxic, biodegradable inhibitors.

Recent studies (2019-2025) reveal a trend toward combining DFT and MD simulations with data-driven QSAR and ML models. Zhang et al. (2021) showed how hybrid DFT-ML models improve prediction accuracy for new eco-friendly inhibitors. Molecular dynamics simulations confirm the stability of inhibitor adsorption at elevated temperatures, providing thermodynamic and kinetic validation of theoretical models [22]. Emerging work by Lin et al. (2023) focuses on polymer-metal interfaces, showing how hybrid organic inhibitors form nanostructured protective films. Overall, these advancements demonstrate that theoretical and computational methods are essential complements to experimental corrosion research, offering cost-effective and environmentally sustainable solutions.

5. Conclusion

Computational and theoretical techniques such as DFT, MD, and QSAR/ML modeling have transformed the field of corrosion science by enabling predictive understanding of inhibitor efficiency. The integration of classical quantum descriptors with machine learning is a significant leap toward data-driven corrosion prevention. Future studies should focus on expanding experimental validation and developing standardized computational protocols for industrial application of green inhibitors.

Abbreviation

DFT	Density Functional Theory
MD	Molecular Dynamic
HOMO	Highest Occupied Molecular Orbital
LUMO	Lowest Unoccupied Molecular Orbital
E_{HOMO}	Energy of Highest Occupied Molecular Orbital
E_{LUMO}	Energy of Lowest Unoccupied Molecular Orbital
QSAR	Quantitative Structure Activity Relationship

Author Contributions

Sulaiman Tijjani Nasiru: Writing – original draft
Abubakar Ado Ibrahim: Conceptualization, Funding acquisition
Sagir Isa Musa: Data curation, Funding acquisition
Abdulmumin Malam Usman: Conceptualization, Methodology

Conflicts of Interest

The authors declared no conflicts of interest.

References

[1] Abiola, O. K. (2023). Machine learning-assisted corrosion inhibitor design. *Corrosion Science, 220*, 111318.

[2] Arslan, T. (2009). Quantum chemical study on sulphonamides as corrosion inhibitors for aluminium. *Corrosion Science, 51*(10), 2278–2285. https://doi.org/10.1016/j.corsci.2009.06.021

[3] Benhiba, F., Missioui, M., Lamghafri, S., Hsissou, R., Bellaouchou, A., Oudda, H., Lamhamdi, A., Warad, I., Ramli, Y., & Zarrouk, A. (2023). Theoretical and experimental studies of 1-dodecyl-3-phenylquinoxalin-2(1H)-one as a sustainable corrosion inhibitor for carbon steel in acidic electrolyte. *Coatings, 13*(6), 1109. https://doi.org/10.3390/coatings13061109

[4] Feng, J.-J., Zhang, S.-S., Cao, S.-J., Li, W.-H., and Wang, Y. (2010). Theoretical methods in corrosion inhibition studies. *Electrochimica Acta, 55*(28), 8702–8709.

[5] Fu, J., Li, S., and Wang, Y. (2020). Computational and electrochemical studies of some amino acid compounds as corrosion inhibitors for mild steel in hydrochloric acid solution. *Journal of Molecular Liquids*, 309, 113102.

[6] Ikeuba, A. I., Ita, B. I., and Okonkwo, C. P. (2024). Review of computational methods used in the evaluation of corrosion inhibition of metallic materials. *Discover Chemical Engineering, 4*, 28. https://doi.org/10.1007/s43938-024-00065-6

[7] Khaled, K. F.,. (2016). QSAR and MD study of furan derivatives as corrosion inhibitors. *Applied Surface Science, 379*, 472–482.

[8] Khaled, K. F., andEl-Sherik, A. M. (2013). QSAR modeling of amino acid corrosion inhibitors. *Corrosion Science, 68*, 160–167. https://doi.org/10.1016/j.corsci.2012.11.015

[9] Lin, Y.,.(2023). Molecular dynamics investigation of polymer corrosion inhibitors. *Journal of Molecular Liquids, 384*, 122003.

[10] Obot, I. B., Obi-Egbedi, N. O., Ebenso, E. E., Afolabi, A. S., & Oguzie, E. E. (2013). Experimental, quantum chemical calculations, and molecular dynamic simulations insight into the corrosion inhibition properties of 2-(6-methylpyridin-2-yl)oxazolo[5,4-f][1, 10]phenanthroline on mild steel. *Corrosion Science, 66*, 52–60. https://doi.org/10.1016/j.corsci.2012.08.004

[11] Pham, T. H., Le, P. K., and Son, D. N. (2024). A data-driven QSPR model for screening organic corrosion inhibitors for carbon steel using machine learning techniques. *RSC Advances, 14*, 11157–11168. https://doi.org/10.1039/D4RA02159B

[12] Rani, B. E. A., andBasu, B. B. J. (2020). Green inhibitors for corrosion protection: A review. *International Journal of Corrosion, 2012*, Article 380217. https://doi.org/10.1155/2012/380217

[13] Riyaz, N. U. S., Khaled, M. and Alshami, A.,(2025). Machine learning-driven prediction of corrosion inhibitor efficiency: Emerging algorithms, challenges, and future outlooks. *Arabian Journal for Science and Engineering*. Advance online publication. https://doi.org/10.1007/s13369-025-10386-5

[14] Saha, S. K., Dutta, A., Ghosh, P., Sukul, D., and Banerjee, P. (2025). Adsorption and corrosion inhibition effect of Schiff base molecules on the mild steel surface in 1 M HCl medium: A combined experimental and theoretical approach. *Physical Chemistry Chemical Physics, 17*(8), 5679–5690. https://doi.org/10.1039/C4CP05614K

[15] Saha, S. K., Dutta, A., Ghosh, P., Sukul, D., and Banerjee, P. (2015). Quantum chemical and molecular dynamics simulation studies of Schiff bases as corrosion inhibitors. *Corrosion Science, 92*, 174–186. https://doi.org/10.1016/j.corsci.2014.12.038

[16] Saha, S. K., Ghosh, P., Hens, A., Murmu, N. C., andBanerjee, P. (2015). Density functional theory and molecular dynamics simulation study on corrosion inhibition performance of mild steel by mercapto-quinoline Schiff base corrosion inhibitor. *Physica E: Low-dimensional Systems and Nanostructures, 66*, 332–341. https://doi.org/10.1016/j.physe.2014.10.035

[17] Setiyanto, N. A., Al Azies, H., Sudibyo, U., Pertiwi, A., & Akrom, M. (2024). A machine learning model for evaluation of the corrosion inhibition capacity of quinoxaline compounds. *Journal of Multiscale Materials Informatics, 1*(1). https://doi.org/10.62411/jimat.v1i1.10429

[18] Singh, A.,(2024). Deep learning prediction of corrosion inhibitor performance. *Materials Today Chemistry, 34*, 101234.

[19] Wantulok, J.. (2020). Computational evaluation of eco-friendly corrosion inhibitors. *Chemical Physics Letters, 742*, 137152.

[20] Xiang, J., Mo, C., Peng, C., Yang, L., Wan, T., Song, Y., Lei, X., Liu, P., Gao, B., Ren, D., Zhao, C., Huang, Y., Wang, Y., andZhang, L. (2024). An evaluation of the corrosion inhibition performance of chitosan modified by quaternary ammonium salt for carbon steel in stone processing wastewater. *Molecules, 29*(14), 3401. https://doi.org/10.3390/molecules29143401

[21] Zhang, P.,(2021). Hybrid DFT–machine learning approach for corrosion inhibition prediction. *Computational Materials Science, 199*, 110755.

[22] Usman, A. M., Haris, A. M., Sulaiman, Z., Oyiza, O. F., Nasiru, S. T., and Ali Daddy, S. (2026). Designing novel quinoline derivatives as corrosion inhibitors for aluminium in hydrochloric acid solutions. American Journal of Quantum Chemistry and Molecular Spectroscopy, 10(1), 1–14.