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Computational Modeling and Simulation in Corrosion Research: From Atomic Scale to Lifetime Prediction

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ABSTRACT

Computational modeling and simulation have emerged as indispensable tools for understanding corrosion phenomena across multiple length and time scales, bridging the gap between atomistic mechanisms and component-level lifetime prediction. This comprehensive review systematically examines the multiscale computational framework for corrosion research, from electronic structure calculations to continuum-scale predictive models. Density functional theory (DFT) provides quantum-level insights into corrosion inhibitor adsorption, with frontier molecular orbital analysis revealing that a lower energy gap (ΔE = ELUMO - EHOMO) correlates with enhanced inhibition efficiency through increased molecular reactivity. Reactive molecular dynamics (ReaxFF) enables tracking of chemical reactions, bond formation and breaking during initial corrosion stages, though time scales remain considerably shorter than realistic corrosion phenomena. Multiscale approaches integrating atomistic insights with finite element method have emerged, preserving grain boundary crystallography while enabling realistic large-scale simulations of corrosion-induced intergranular strain. Phase-field modeling has become a powerful mesoscale tool for simulating autonomous evolution of corrosion pits, capturing the complex interactions between electrochemical processes and mechanical deformation. Machine learning applications have revolutionized lifetime prediction, with hybrid models achieving R^2>0.99 for corrosion rate forecasting and service life prediction. The review concludes that next-generation corrosion modeling requires integrated frameworks combining physics-based mechanistic understanding with data-driven approaches.

Introduction

Corrosion, the electrochemical degradation of metallic materials, represents one of the most pervasive and economically burdensome challenges confronting modern industry, with annual global costs exceeding $2.5 trillion [1]. The complexity of corrosion phenomena spanning electronic structure at the atomic scale, microstructural evolution at the mesoscale, and component degradation over years of service demands sophisticated modeling approaches capable of capturing the fundamental physics while providing practical engineering predictions [2].

Computational modeling and simulation have emerged as indispensable tools to meet this challenge, enabling understanding of corrosion mechanisms, design of protective strategies, and prediction of remaining service life [3]. The multiscale nature of corrosion necessitates a hierarchical modeling framework. At the atomic scale, density functional theory (DFT) provides quantum-level insights into electronic structure and chemical bonding, enabling prediction of inhibitor

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adsorption energies and identification of reactive sites. Molecular dynamics (MD) simulations, particularly with reactive force fields (ReaxFF), extend the time and length scales to capture chemical reactions and interfacial processes during initial corrosion stages [4-10]. At the mesoscale, phase-field modeling has emerged as a powerful technique for simulating autonomous evolution of corrosion pits and localized corrosion morphologies, capturing the complex interactions between electrochemical processes and mechanical deformation [11-20]. Continuum-scale models, including computational fluid dynamics (CFD) for flow-accelerated corrosion and finite element methods for stress-corrosion cracking, enable prediction of component-level degradation. Machine learning approaches have revolutionized data-driven corrosion prediction, capturing nonlinear relationships among environmental variables, alloy composition, and corrosion rates with exceptional accuracy [21-30]. This comprehensive review aims to synthesize current knowledge on computational modeling and simulation in corrosion research, systematically examining techniques from atomic to continuum scales. The review is structured to first establish the theoretical foundations of each modeling approach, followed by critical evaluation of their applications, strengths, and limitations [31-40]. Particular attention is devoted to emerging integrated frameworks combining physics-based mechanistic understanding with data-driven approaches that promise transformative advances in corrosion prediction and management.

Literature Review

Historical Evolution of Corrosion Modeling:

The application of computational methods to corrosion research has evolved substantially over the past four decades, reflecting advances in computational power and theoretical understanding. Early corrosion modeling relied primarily on empirical correlations and semi-empirical rate equations, such as the parabolic rate law for oxidation kinetics and the Stern-Geary relationship for electrochemical measurements [41-50]. The introduction of finite element methods in the 1970s enabled first-principles modeling of diffusion-controlled processes, though computational constraints limited system sizes and time scales. The 1990s witnessed the emergence of atomic-scale modeling techniques in corrosion research. Density functional theory (DFT), building on the Hohenberg-Kohn theorems and Kohn-Sham equations, enabled quantum-level investigation of metal surfaces, oxide films, and inhibitor adsorption. The development of reactive force fields (ReaxFF) in the 2000s enabled molecular dynamics simulations of chemical reactions, including bond formation and breaking, without predefining reaction paths [51-60]. The computational cost and efficiency of DFT calculations have improved significantly with advanced algorithms, making it a popular tool for designing anticorrosive materials. The past decade has witnessed transformative advances through integration of multiscale approaches and machine learning [61-70]. Multiscale modeling coupling atomistic, mesoscale, and continuum methods has emerged as the dominant paradigm for corrosion simulation, enabling prediction across length scales from nanometers to meters. Phase-field modeling has matured as a robust technique for simulating autonomous evolution of corrosion pits and localized corrosion morphologies [71-80]. Machine learning applications have grown exponentially, with algorithms including artificial neural networks, support vector regression, and ensemble learning applied to predict corrosion rates from multivariate datasets.

Atomic-Scale Modeling: DFT and Molecular Dynamics:

Density Functional Theory (DFT) has become an essential tool for understanding corrosion inhibition at the molecular level. DFT operates on the principles of molecular/electronic structure, using electron density as the main carrier of information in the molecular ground state. The frontier molecular orbitals highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are critical parameters for assessing molecular reactivity [81-90]. A lower energy gap ($\Delta E = E_{LUMO} - E_{HOMO}$) indicates higher molecular reactivity and typically correlates with enhanced corrosion inhibition efficiency. DFT studies of quinoxalinone derivatives on Fe (110) surfaces revealed that protonated molecules demonstrate stronger surface affinity, primarily interacting through oxygen atoms and conjugated systems, with parallel adsorption configurations being more stable than perpendicular modes.

Mesoscale Modeling: Phase-Field and Cellular Automata:

Phase-field modeling has emerged as a powerful mesoscale technique for simulating autonomous evolution of corrosion pits and localized corrosion. The phase-field method represents the metal-electrolyte interface through a diffuse order parameter, eliminating the need for explicit interface tracking that complicates sharp-interface formulations. Recent developments include grand-potential formulations that decouple interface width and energy, enabling efficient simulation of corrosion in multiphase alloys. Phase-field models coupled with smoothed boundary methods have been used to study the effect of overpotential on pitting corrosion in low-carbon steel, revealing that the system stays in the charge transfer-controlled regime at lower overpotentials and transits to ohmic resistance-controlled regime at higher overpotentials. Phase-field fracture modeling extends the capability to simulate pressure-induced cracking in corrosion pits [91-100]. By integrating corrosion-induced pit morphology with phase-field fracture models, researchers have shown that increasing pit depth in multiphase systems significantly reduces the critical relative pressure required for crack initiation and propagation. These models demonstrate how phase boundaries and local topology influence degradation through pitting and subsequent micro-crack formation, providing insights relevant to structural components in industrial environments where corrosion and internal pressure coexist.

Continuum-Scale Modeling and Computational Fluid Dynamics:

Computational Fluid Dynamics (CFD) has been extensively applied to model flow-accelerated corrosion (FAC) in power plants and pipeline systems. Numerical models demonstrate capability to predict FAC profiles across multiple power plant components, though increased turbulence in the flow significantly contributes to prediction errors, emphasizing the need for advanced turbulence models in numerical simulations of FAC [101-110]. Understanding the intricate relationship among flow dynamics, environmental factors, and corrosion reactions is essential for developing effective prediction and mitigation strategies.

Finite Element Method (FEM) combined with 3D digital representations of multi-grain microstructures enables investigation of texture effects on corrosion. Studies of pitting corrosion in stainless steel demonstrate that texture significantly affects corrosion rate and causes various irregular pit growth patterns in granular microstructures, consistent with DFT and reactive force field molecular dynamics simulations [111-122]. This multiscale methodology does not suffer from common limitations of quantum-based computational approaches in time and space while providing comparable accuracy with orders of magnitude less computational cost.

Machine Learning and Data-Driven Modeling:

Machine learning has revolutionized corrosion prediction and lifetime assessment, capturing complex relationships among environmental variables, alloy composition, and corrosion rates that traditional empirical models cannot address. Regression and classification models developed using large pipeline failure databases enhanced with weather data have achieved R-squared values exceeding 90%. Hybrid models combining extreme learning machine (ELM) with metaheuristic optimization algorithms (Bald Eagle Search integrated with Lévy flight and simulated annealing) have demonstrated mAP approaching 95% and R^2 of 0.9926 for corrosion rate prediction.

Machine learning approaches have also been applied to service life prediction of reinforced concrete structures, where algorithms can grasp complex relationships among key factors impacting deterioration and offer precise evaluations without relying on traditional empirical models. SHAP (SHapley Additive exPlanations) analysis has enabled identification of key predictors, revealing that weather conditions significantly affect time left till pipeline failure. However, limitations persist, including data scarcity, no standardized descriptor selection, and insufficient physical interpretability of many reported ML-based corrosion models.

Methodology

This comprehensive review was developed through systematic analysis of peer-reviewed literature indexed in major scientific databases including Scopus, Web of Science, ScienceDirect, and Google Scholar. The search strategy employed combinations of keywords including "computational modeling," "corrosion simulation," "density functional theory," "molecular dynamics," "phase-field modeling," "machine learning corrosion," "multiscale modeling," and related terms. Particular emphasis was placed on studies published between 2019 and 2026, while seminal earlier works were included were mechanistically or historically significant. The literature screening process involved identification of peer-reviewed research articles, review papers, and conference proceedings. Studies were selected based on relevance to the review scope, methodological rigor, completeness of reported computational details, mechanistic significance, and applicability to industrial contexts. Representative studies for comparative analysis were chosen based on clear presentation of computational methodology, validation approaches, and performance metrics. Publications lacking sufficient methodological detail or quantitative performance data were excluded.

Quantitative data synthesis focused on computational performance metrics including prediction accuracy (R^2 values), computational efficiency, and validation approaches. For DFT and MD studies, specific attention was given to adsorption energies, frontier molecular orbital parameters, and simulation conditions.

Methodological approaches evaluated based on their theoretical foundations, practical applicability, and limitations for different corrosion systems. Integration strategies across scales were assessed through analysis of multiscale coupling approaches reported in the literature. Environmental and industrial context considerations were examined through analysis of application case studies across oil and gas, marine, and infrastructure sectors.

Results

Table 1. Computational Modeling Approaches for Corrosion Research: Capabilities and Limitations

Modeling Approach	Length Scale	Time Scale	Key Parameters	Advantages	Limitations	Development Status
Density Functional Theory (DFT)	Atomic (~nm)	Electronic (fs)	EHOMO, ELUMO, ΔE, adsorption energy	Quantum accuracy, electronic structure insight	System size limited (<500 atoms); static mostly	Mature
Molecular Dynamics (ReaxFF)	Nanoscale (~nm-μm)	Molecular (ps-ns)	Force field parameters, charge distribution	Chemical reactions, dynamic processes	Time scale too short for realistic corrosion	Mature
Multiscale (ReaxFF+FEM)	Atomic to Macroscopic	ns to s	Grain boundary properties, strain	Upscales atomistic to continuum	Coupling complexity	Emerging
Phase-Field	Mesoscale (~μm-mm)	Seconds to days	Interface mobility, overpotential, diffusivity	Autonomous interface evolution	Computational demand; parameter calibration	Emerging/Commercial
Computational Fluid Dynamics	Macroscopic (mm-m)	Seconds to years	Flow velocity, turbulence, mass transfer	Realistic flow conditions	Turbulence modeling challenges	Mature
Phase-Field Fracture	Mesoscale (~μm-mm)	Mechanical timescales	Fracture toughness, pressure, morphology	Pit-to-crack transition	Decoupled from corrosion kinetics	Research
Machine Learning (ELM, ANN, RF)	System-level	Data-driven	Multiple environmental features	$R^2 > 0.99$, nonlinear relationships	Data quality, physical interpretability	Emerging/Commercial

Data compiled from references.

Analysis of Table 1: The comparative analysis reveals the hierarchical nature of computational corrosion modeling, with each approach operating at distinct length and time scales while offering complementary capabilities. DFT provides fundamental quantum-level understanding of molecular interactions, with frontier molecular orbital parameters (EHOMO, ELUMO, ΔE) serving as key descriptors for predicting inhibition efficiency. However, system size limitations and static nature constrain application to simplified models. ReaxFF-based MD enables dynamic simulation of chemical reactions at the nanoscale, tracking bond formation and breaking through charge update at each time step. While extending beyond DFT in time scale, the microsecond-nanosecond range remains orders of magnitude shorter than realistic corrosion phenomena, necessitating multiscale approaches.

Multiscale modeling combining ReaxFF with FEM represents an emerging advance, preserving grain boundary crystallography while enabling realistic large-scale simulations of corrosion-induced intergranular strain. Phase-field modeling has matured as a powerful mesoscale technique, enabling autonomous simulation of corrosion pit evolution through diffuse interface representation. The computational demand and parameter calibration challenges are being addressed through improved formulations and coupling with experimental validation. CFD provides continuum-scale prediction of flow-accelerated corrosion, though turbulence modeling remains challenging. Machine learning has demonstrated exceptional prediction accuracy ($R^2 > 0.99$) at the system level, capturing nonlinear relationships among environmental variables, though data quality and physical interpretability limitations persist.

Table 2. DFT and Molecular Dynamics Studies for Corrosion Inhibition

Inhibitor System	Metal Surface	DFT Key Findings	MD/ReaxFF Findings	Adsorption Energy (kJ/mol)	Key Descriptors
Quinoxalinones on Fe (110)	Fe (110)	Parallel adsorption > perpendicular; protonated stronger affinity	Charge transfer Fe(3d)-molecule	-190 to -230	Protonation enhances electrostatic interactions; methyl substitutions not significant
Quinoxaline Derivatives	Fe (110), Cu (111), Al (110)	HOMO/LUMO energies, ΔE correlate with inhibition	Adsorption energies: Q6 > Q2 > Q3	-150 to -220	Lower ΔE = higher reactivity; protonated Q6 strongest
Rosmarinus officinalis Polyphenols	XC48 Steel	Carnosic acid > carnosol inhibition	Parallel adsorption on surface	-160 to -200	Electron donation to metal surface
Amino Acids	Cu (111)	Protonated forms more reactive	Parallel adsorption; π-electron interaction	-120 to -180	N atoms interact with Cu surface

Data compiled from references.

Analysis of Table 2: DFT and MD studies provide complementary insights into corrosion inhibition mechanisms. DFT analysis of quinoxalinones on Fe (110) surfaces revealed that protonated molecules demonstrate stronger surface affinity, primarily interacting through oxygen atoms and conjugated systems. The parallel adsorption configuration was more stable than the perpendicular mode, with enhanced electrostatic interactions and charge transfer mechanisms driving adsorption. Notably, methyl substitutions did not significantly enhance adsorption strength, as reduced steric interference maintained molecular planarity. Projected density of states (PDOS) and electron density difference analyses confirmed the importance of charge transfer between active sites and iron 3d orbitals in stabilizing adsorption.

Quinoxaline derivatives across multiple metal surfaces (Fe, Cu, Al) showed that inhibition efficiency increases with decreasing energy gap between frontier orbitals. The protonated state of Q6 exhibited high reactivity, low stability, and strong adsorption, making it a potential candidate for further exploration. Rosmarinus officinalis polyphenols demonstrated that among the most abundant constituents, carnosic acid has a greater inhibiting effect compared with carnosol. The theoretical approaches provide crucial insights for the conceptual development of new and powerful corrosion inhibitors through identification of structure-activity relationships.

ReaxFF MD simulations enable tracking of chemical reactions during initial corrosion phases. Application of electric fields (50 MV/cm) at 300 K led to considerable diffusive and chemical processes, with grooving of grain boundaries and changes in grain morphology. The ReaxFF potential used in these studies has been effectively applied to passive layer formation and breakdown, as well as crystallographic effects on pitting corrosion expansion patterns in metallic polycrystalline materials.

Table 3. Phase-Field Modeling Applications and Key Findings

Corrosion System	Model Type	Key Parameters	Findings	Validation Approach	Application
Low-Carbon Steel (S355) in Seawater	Butler-Volmer + Phase-Field	Overpotential (+250 mV to +840 mV), jcorr = 5.8×10^{-6} A/cm²	System in charge transfer-controlled regime <+250 mV; pit growth 246 μm in 1000 s	PDP tests; comparison to field coupons	Pit growth acceleration; offshore wind
Stainless Steel Pitting	Grand-Potential Phase-Field	Interface mobility, pressure conditions	Pit morphology determines pressure threshold	Analytical solutions; numerical benchmarks	Pit-to-crack transition; pipelines

			for crack initiation		
Multiphasic Microstructures	Grand-Potential Phase-Field	Interfacial mobility, phase boundaries	Phase boundaries intensify failure variability; critical pressure reduced with pit depth	Comparative phase-field framework	Structural alloys; geothermal systems
AlTiVCr and $Al_{0.9}FeCrCoNi$ CCAs	Oxidation Phase-Field	Temperature, composition	AlTiVCr higher mass gain; $Al_{0.9}FeCrCoNi$ Al_2O_3 spalling	Experimental validation	High-temperature alloys

Data compiled from references.

Analysis of Table 3: Phase-field modeling has enabled significant advances in understanding pitting corrosion and pit-to-crack transition. For low-carbon steel in seawater, phase-field simulations revealed that the system stays in charge transfer-controlled regime when overpotential is less than +250 mV vs. OCP and transits to ohmic resistance-controlled regime at higher overpotentials. The model predicted pit growth of 246 μm in depth under +840 mV overpotential in 1000 s, which was utilized to guide potentiation polarization tests. Comparison with field coupons confirmed that the acceleration mechanism effectively produced surface conditions closely resembling naturally pitted steel.

Grand-potential phase-field formulations have been extended to simulate corrosion in multiphase systems and pressure-driven cracking. The results demonstrate that increasing pit depth in multiphase systems significantly reduces the critical relative pressure required for crack initiation and propagation, demonstrating the strong linkage between morphology and mechanical failure. Interfacial mobility controls pit evolution and failure susceptibility, while polycrystalline microstructures intensify corrosion-driven failure variability. The framework advances mesoscale corrosion-mechanics understanding by integrating grand potential-driven dissolution with pressure-dependent fracture analysis.

Phase-field modeling of compositional complex alloys (CCAs) reveals distinct oxidation behavior, with AlTiVCr demonstrating higher mass gains due to Ti-rich and V-rich oxide formation, while $Al_{0.9}FeCrCoNi$ forms Al_2O_3 scales with notable spallation propensity. The models enable prediction of oxide scale formation, spallation, and alloy performance across temperature ranges from 700–1000°C.

Table 4. Machine Learning Performance Metrics for Corrosion Prediction

ML Model	Application	Dataset Size	Performance Metric	Key Predictors	Validation Approach
Extra Trees Regression	Pipeline service life prediction	PHMSA + Weather data	R^2=90.35%	Temperature, precipitation (SHAP)	Cross-validation; test split
Extra Trees Classification	Failure classification	PHMSA + Weather data	F1=85%	Weather conditions significantly affect failure timing	Cross-validation
LSBES-ELM	Buried pipeline corrosion rate	Extensive corrosion database	mAP=94.83%; R^2=0.9926	Multi-environmental factors	Benchmark against BES-ELM, ELM, BPNN
LSBES-ELM-MCS	Pipeline reliability evolution	Extensive corrosion database	RE=0.0274 - 0.0761	Corrosion rate influence factors	Monte Carlo Simulation
ANN	Corrosion behavior	Electrochemical + environmental	R^2>0.85	Good experimental trend agreement	Cross-validation
Traditional Empirical Models	RC service life	Limited experimental data	$R^2 \approx 0.60$-0.75	Corrosion rate, cover depth, diameter	Limited field validation

Data compiled from references.

Analysis of Table 4: Machine learning models demonstrate superior predictive capability for corrosion rate and service life prediction compared to traditional empirical approaches. The extremely randomized trees (extra trees) algorithm achieved R^2=90.35% for regression and F1 score of 85% for classification, leveraging enhanced datasets incorporating weather data (temperature and precipitation). SHAP analysis identified that weather conditions significantly affect the time left till pipeline failure, highlighting the importance of environmental factors often overlooked in traditional models. The LSBES-ELM hybrid model, combining Lévy flight-enhanced Bald Eagle Search with Extreme Learning Machine, achieved mAP=94.83% and R^2=0.9926 for corrosion rate prediction, surpassing both baseline ELM-based models and non-optimized neural networks. The model was extended with Monte Carlo Simulation (LSBES-ELM-MCS) for dynamic assessment of pipeline reliability evolution across various buried soil conditions, projecting optimal inspection intervals of 21-24 years for target reliability levels. This represents significant advancement over traditional probabilistic models that rely on simple linear or power function assumptions and underestimate the impact of numerous complex factors. Machine learning captures complex relationships among key factors impacting deterioration and offers precise evaluations of remaining service life without relying on empirical models, though limitations persist in data standardization and physical interpretability.

Discussion

Bridging the Scale Gap: From Atoms to Engineering:

The fundamental challenge in corrosion modeling lies in bridging the enormous gap between atomic-scale processes and component-level lifetime prediction. DFT and molecular dynamics simulations provide unprecedented insights into electronic structure and chemical bonding at the atomic scale, but the time scales of these simulations' picoseconds to nanoseconds for DFT, nanoseconds to microseconds for ReaxFF MD are orders of magnitude shorter than the hours to years relevant to realistic corrosion phenomena. While applied electric fields can accelerate physical processes during simulation, this acceleration must be carefully validated against experimental observations.

Multiscale modeling has emerged as the primary strategy to bridge this gap, integrating atomistic insights with continuum-scale computational efficiency. Reactive molecular dynamics coupled with finite element methods enables preservation of grain boundary crystallography while enabling realistic large-scale simulations of corrosion-induced intergranular strain. This approach captures the critical influence of microstructure on corrosion phenomena, particularly grain boundaries that serve as short-circuiting paths for diffusion and sites for localized corrosion initiation. The experimental tracking of localized corrosion expansion patterns is challenging due to rapid expansion and coverage by corrosion products, making multiscale modeling a valuable complement to experimental techniques like scanning vibrating electrode technique (SVET). Phase-field modeling operates at the mesoscale, capturing the autonomous evolution of corrosion pits and localized corrosion morphologies without explicit interface tracking. The grand-potential formulation enables efficient simulation of corrosion in multiphase alloys, while sequential coupling with phase-field fracture models captures pit-to-crack transitions. The computational demand of phase-field models remains significant, but recent advances in algorithms and computational power are enabling practical applications to industrial problems.

Data-Driven Discovery and Machine Learning Integration:

Machine learning has transformed corrosion prediction capabilities, capturing nonlinear relationships among environmental variables, alloy composition, and corrosion rates that traditional empirical models cannot address. The exceptional predictive performance R^2>0.99 achieved by hybrid LSBES-ELM models represents a paradigm shift in corrosion rate forecasting. Integration of weather data (temperature, precipitation) has significantly enhanced prediction accuracy for pipeline service life, revealing that environmental factors often overlooked in traditional models are critical drivers of failure timing. SHAP analysis provides model interpretability, enabling identification of key predictors and their contributions to failure timing.

However, several challenges persist in ML-based corrosion modeling.

Validation and Integration Challenges:

Validation remains a critical challenge across all computational corrosion modeling approaches. DFT and MD predictions require comparison with experimental measurements for confirmation. The limited time scale of atomistic simulations creates challenges for direct experimental validation, though studies have demonstrated consistency between ReaxFF simulations and DFT calculations. Phase-field models require calibration against experimental electrochemical data, with parameters such as corrosion current density and Tafel slopes derived from potentiodynamic polarization tests. The validation of phase-field predictions against field coupon data represents a significant advance, enabling correlation between accelerated laboratory corrosion and actual long-term exposure. CFD models of flow-accelerated corrosion have been evaluated against experimental measurements, though increased turbulence in flow significantly contributes to prediction errors, emphasizing the need for advanced turbulence models.

The integration of different modeling approaches presents both opportunities and challenges. Sequential coupling of corrosion and fracture models enables isolation of mechanistic effects while reducing computational complexity, but fully coupled treatment of chemo-mechanical interactions would provide more comprehensive predictions. The development of integrated frameworks combining physics-based mechanistic understanding with data-driven approaches represents the next frontier. Digital twin technologies, combining physical modeling with real-time monitoring and predictive analytics, offer transformative potential for infrastructure integrity management, though development requires validation across diverse operational conditions.

Emerging Technologies and Future Directions:

Several emerging technologies promise to advance computational corrosion modeling capabilities. Physics-informed machine learning architectures incorporating electrochemical rate expressions and structural constraints can enhance interpretability and improve generalization beyond original training domains. Generative design frameworks combining DFT, MD, and ML could accelerate discovery of novel corrosion inhibitors and protective materials. Four-dimensional impedance analysis enables time-varying characterization for non-stationary systems, with applications to additively manufactured metals. The integration of molecular biology approaches multi-omics and gene editing with computational corrosion modeling offers systems-level understanding of microbiologically influenced corrosion. The development of standardized open datasets, explicit solvation and interfacial modeling, uncertainty-aware ML, and generative design frameworks capable of coherently linking quantum chemistry, interfacial dynamics, and data-driven prediction are essential requirements for future progress. Addressing these challenges will require interdisciplinary collaboration across materials science, electrochemistry, data science, and industrial engineering. The transition toward predictive, data-driven, and digitally integrated corrosion management offers potential for significant cost reduction, improved safety, and extended asset life across industrial sectors.

Conclusion

This comprehensive review has systematically examined computational modeling and simulation in corrosion research, spanning techniques from atomic-scale quantum chemistry to data-driven lifetime prediction. DFT and molecular dynamics simulations provide atomistic insights into corrosion inhibition mechanisms, with ReaxFF enabling dynamic simulation of chemical reactions during initial corrosion stages. Frontier molecular orbital analysis has established that a lower energy gap ($\Delta E = E_{LUMO} - E_{HOMO}$) correlates with enhanced inhibition efficiency through increased molecular reactivity. Multiscale modeling approaches integrating atomistic insights with finite element methods have emerged as a robust methodology, preserving grain boundary crystallography while enabling realistic large-scale simulations. Phase-field modeling has matured as a powerful mesoscale technique for simulating autonomous evolution of corrosion pits and localized corrosion morphologies. Grand-potential formulations enable efficient simulation of corrosion in multiphase alloys, while sequential coupling with phase-field fracture models captures the linkage between pit morphology and mechanical failure. CFD provides continuum-scale prediction of flow-accelerated corrosion, though advanced turbulence modeling remains a priority.

Machine learning has revolutionized corrosion prediction, with hybrid models achieving $R^2>0.99$ for corrosion rate forecasting and service life prediction. Integration of environmental data has significantly enhanced predictive accuracy, revealing that weather conditions critically influence failure timing. However, challenges persist in data standardization, physical interpretability, and model generalization. Future progress requires integrated frameworks combining physics-based mechanistic understanding with data-driven approaches, interdisciplinary collaboration, and development of standardized open datasets. With continued innovation, computational modeling and simulation offer transformative potential for corrosion management, enabling proactive protection, optimized maintenance, and extended infrastructure service life.

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Authors' Contributions

All authors contributed to data analysis, drafting, and revising of the paper and agreed to be responsible for all the aspects of this work.

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