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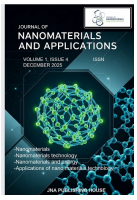

Recent advances in the application of Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations to elucidate metal corrosion mechanisms

Umut Saraç [1,*], Lam Vu Truong [2], Dung Nguyen Trong [3,*], and Hoang Thi Phuong [4], Ştefan Ţălu [5]

[1] Bartın University, Department of Science Education, 74100, Bartın, Türkiye.

[2] Department of Advanced Materials and Metallurgical Engineering, Sunchon National University, Suncheon, Jeonnam 540-742, Republic of Korea.

[3, 4] University of Transport Technology, 54 Trieu Khuc Thanh Xuan, Hanoi, Vietnam.

[5] The Directorate of Research Development and Innovation Management (DMCDI) Technical University of Cluj-Napoca, 15 Constantin Daicoviciu Street Cluj-Napoca 400020, Cluj County, Romania.

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Corresponding author*:

Umut Saraç

E-mail address:

usarac@bartin.edu.tr

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Abstract: Over the past decade, atomistic simulation techniques, particularly Density Functional Theory (DFT) and Molecular Dynamics (MD), have become essential for understanding metal corrosion at electronic and atomic scales. DFT offers quantitative insight into adsorption energetics, electronic structure evolution, and reaction pathways governing metal–environment interactions, whereas MD enables dynamic modeling of ion transport, inhibitor adsorption, and passive film stability under realistic conditions. Recent studies show that integrating DFT and MD significantly improves predictive understanding of corrosion involving aggressive species (Cl^-, SO_4^{2-}, H^+), oxide film growth, alloying effects, and inhibitor performance. Moreover, multiscale approaches linking atomistic simulations with continuum models allow quantitative prediction of corrosion kinetics and material degradation. This review summarizes advances in DFT- and MD-based corrosion modeling from 2020 to 2025, discusses key methodological limitations, and highlights emerging trends such as reactive force fields, ab initio molecular dynamics, and machine learning-assisted simulations, with emphasis on validation and predictive reliability.

Keywords: Metal corrosion; Density functional theory; Molecular dynamics simulation; Multiscale model

1. Introduction

Corrosion of metals is considered a spontaneous phenomenon in which chemical or electrochemical reactions between metals and their surroundings occur, leading to the gradual deterioration of the

mechanical, chemical and electrical properties of the material. According to the World Corrosion Organization, the global economic losses due to metal corrosion have been estimated at 2.5–3.0 trillion USD per year, equivalent to 3–4% of global GDP [1]. In addition to economic losses, serious safety risks have also been recorded in the energy, aviation, defense and infrastructure sectors, where high requirements for reliability and longevity of materials are placed. Previous experimental methods such as electrochemical measurements, electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), scanning electron microscopy (SEM) and X-ray spectroscopy (XPS) have been widely used to determine the corrosion rate, surface morphology and corrosion product composition. However, these methods mainly reflect phenomena at the macroscopic or mesoscopic level, while the actual corrosion mechanisms are initiated by electron, adsorption, diffusion and chemical reaction processes at the atomic level. Therefore, in the last two decades, computational simulation has been considered as an indispensable complementary tool to help elucidate the microscopic nature of the corrosion process. In the field of simulation, Density Functional Theory and Molecular Dynamics (MD) simulation have been recognized as the two most widely applied key techniques. With DFT, an advanced quantum mechanical method, the electronic structure, adsorption energy, charge density and energy levels of molecules or ions on the metal surface have been accurately determined. Through this, the adsorption mechanisms, the passive film formation process, and the role of alloying elements in enhancing corrosion resistance have been elucidated [2,3]. In addition, MD, a classical simulation tool based on Newton's equation of motion, has been used to observe the time evolution of atoms and molecules, thereby allowing dynamic processes such as ion diffusion (Cl^-, SO_4^{2-}), inhibitor adsorption, or the formation and destruction of protective oxide layers to be investigated in detail under different environmental conditions [4]. The combination of DFT and MD has been shown to provide the ability to explain the microscopic mechanism and predict corrosion behavior at the macroscopic level through multiscale modeling. During the period, a large number of works were published, thereby confirming the central role of DFT and MD in the research of anti-corrosion materials. For example, Oukhrib et al. (2021) [5] applied a combination of DFT, Monte Carlo and MD to simulate the adsorption of pyrazolylnucleosides on the Cu (111) surface, thereby determining the binding energy and stability of the organic inhibitor layer. Similarly, Wang et al. (2023) [6] used DFT to analyze the corrosion mechanism of acetic acid on X80 steel, thereby demonstrating that the undissociated acid molecules mainly act as proton sources rather than direct oxidants. Despite significant advances, DFT- and MD-based corrosion simulations still face fundamental challenges related to accessible time and length scales, realistic representation of electrochemical environments, and quantitative experimental validation. Although reactive force fields, ab initio molecular dynamics, and hybrid DFT-based approaches have been developed to address specific limitations of classical models [7,8], constraints in system size, simulation duration, and the treatment of surface defects, electrolyte effects, and applied potentials continue to limit predictive accuracy. Recently, the integration of machine learning with DFT and MD has emerged as a promising strategy to enhance predictive capability and accelerate materials screening [9,10]. Therefore, a systematic synthesis of recent progress (2020–2025), methodological limitations, and emerging developments is essential to critically evaluate the current state of the field and guide the rational design of corrosion-resistant materials. This review does not present new experimental measurements; instead, it systematically integrates experimental data such as EIS, XPS, SEM, and AFM reported in recent literature to validate and interpret DFT- and MD-based corrosion models.

2 Theoretical basis

2.1. Density functional theory

Density functional theory (DFT) was developed as a quantum mechanical method to describe many-electron systems through electron density functions, instead of through the complicated wave functions as in traditional methods. The foundation of DFT is based on two theorems Hohenberg–Kohn (1964), in which the first theorem states that the energy of a quantum system is determined solely by the electron density, and the second theorem shows that the most accurate electron density is the density that minimizes the total energy of the system.

To describe the interacting electron system, the Kohn–Sham equation was established. In this framework, a hypothetical electron system consisting of independent electrons is used to replace the real electron system, provided that the two systems have the same electron density. Thanks to this approach, the complex multi-particle problem is simplified into a set of single-particle equations, allowing the total energy of the system to be determined through the expression:

$$E[n(r)] = T_s[n(r)] + E_{ext}[n(r)] + E_H[n(r)] + E_{xc}[n(r)] \quad (1)$$

In which: T_s: is the kinetic energy of the non-interacting electron system, E_{ext}: is the interaction energy between the electron and the external field (such as the ion nucleus or the electric field), E_H: is the Coulomb energy due to the classical electron–electron interaction, E_{xc}: is the exchange–correlation energy, the most important part that determines the accuracy of the simulation.

In the field of corrosion research, Density Functional Theory (DFT) is often applied as an effective computational tool to elucidate the interactions occurring at the atomic level along with changes in the electronic structure. Through DFT, the basic characteristics of the interaction between metals and the corrosive environment have been determined, including:

(1) The adsorption energy of typical molecules or ions such as H_2O, O_2, Cl^-, SO_4^{2-} and organic inhibitors on the metal surface has been calculated to evaluate the corrosion resistance and the tendency to form a protective passive film;

(2) The electronic structure (density of states – DOS) has been analyzed to clarify the nature of the bond between the metal and the adsorbent, thereby reflecting the degree of chemical interaction and the distribution of electron density at the surface;

(3) The chemical reaction mechanism and reaction pathway of oxidation, reduction or protonation processes on the metal surface have been determined, helping to understand the kinetic and thermodynamic nature of the reaction stages [11–13].

A typical example is reported in the study of Gattinoni and Michaelides (2015) [13], in which DFT was used to elucidate the adsorption mechanism of benzotriazole on Cu(111) surface. The simulation results showed that Van der Waals interactions, hydrogen bonding and electrostatic forces play a dominant role in determining the most stable adsorption configuration of the inhibitor molecule. In addition, recent works [14,15] have shown that the addition of dispersion correction (DFT-D3, vdW-DF) or the use of implicit solvent models significantly improves the accuracy of simulating realistic corrosive environmental conditions. For material systems containing d or f electrons (such as oxides of Fe, Ni, Ti), extended methods such as DFT+U or hybrid functionals (HSE06, PBE0) have been applied to more accurately describe the strong correlations between local electrons. In these studies, adsorption distances, electron density distributions and HOMO–LUMO energy differences are often used as characteristic quantities to evaluate the inhibitor effectiveness or corrosion resistance of materials.

Despite its extensive application, density functional theory inherently relies on approximations that may influence the accuracy of corrosion-related predictions. Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA), particularly the widely used PBE functional, often underestimate band gaps and may inadequately describe strongly correlated d-electron systems in transition metal oxides. This limitation is especially critical when modeling passive films such as Fe_2O_3 or Cr_2O_3, where electronic localization governs protective behavior. Although hybrid functionals (e.g., HSE06) and DFT+U approaches improve electronic structure descriptions, they significantly increase computational cost and remain sensitive to parameter selection. Furthermore, conventional DFT calculations are typically conducted at 0 K and neglect entropic contributions, which can lead to discrepancies when comparing with experimental corrosion phenomena under realistic temperature and electrochemical conditions.

2.2. Molecular Dynamics (MD) simulations

The molecular dynamics (MD) simulation method is based on classical Newtonian mechanics, in which the motion trajectory of each atom is determined by integrating the equations of motion over time:

$$m_i \frac{d^2 r_i}{dt^2} = -\Delta U\left(r_1, r_2 \ldots r_N\right) \qquad (2)$$

where: ΔU is the potential energy of the system, which depends on the position of the atoms.

In corrosion research, molecular dynamics (MD) simulations are often applied to reproduce at the atomic level the mechanisms occurring on the metal surface. Through MD, the adsorption and orientation of corrosion inhibitor molecules on the metal surface are simulated; the diffusion of ions such as H^+, Cl^-, and OH^- in the near-surface electrolyte layer is investigated; the formation, dissolution, and destruction of the passive oxide film are reproduced; at the same time, the influence of environmental conditions such as temperature, pH, ion concentration, and potential is also analyzed in detail. Current MD models are often established as slab models, in which a metal surface (e.g., Fe(110), Cu(111), or Al(100)) is covered by a solvent layer representing the corrosive environment (H_20, Cl^-, metal, etc.). From these simulations, important parameters such as the average adsorption energy (E_{ads}), radial distribution function (RDF), self-diffusion coefficient (D), and structural stability of the adsorbed layer are extracted and analyzed to elucidate the nature and interaction mechanism between the corrosive environment and the metal surface. MD methods are generally classified into three main types. First, classical molecular dynamics simulations (Classical MD) are performed based on empirical potentials such as COMPASS, CHARMM, or OPLS-AA. Second, reactive molecular dynamics simulation (ReaxFF) is used when it is necessary to simulate the formation and breaking of chemical bonds, which is especially useful in studying oxidation and oxide film formation [16]. Third, quantum molecular dynamics simulation (Ab initio MD) is implemented when the forces acting between atoms are calculated directly from density functional theory (DFT), which allows for a more accurate description of electronic properties but requires high computational costs [17]. A typical demonstration of the effectiveness of this method is noted in the study of Bala et al. (2025) [18], in which the adsorption process of imidazole compounds on steel surfaces in acidic environments was simulated using MD. The configuration parallel to the metal surface was determined to be the most stable adsorption state, and the resulting adsorption energy showed a clear correlation with the corrosion inhibition efficiency observed experimentally.

2.3. Integration and comparison between DFT and MD

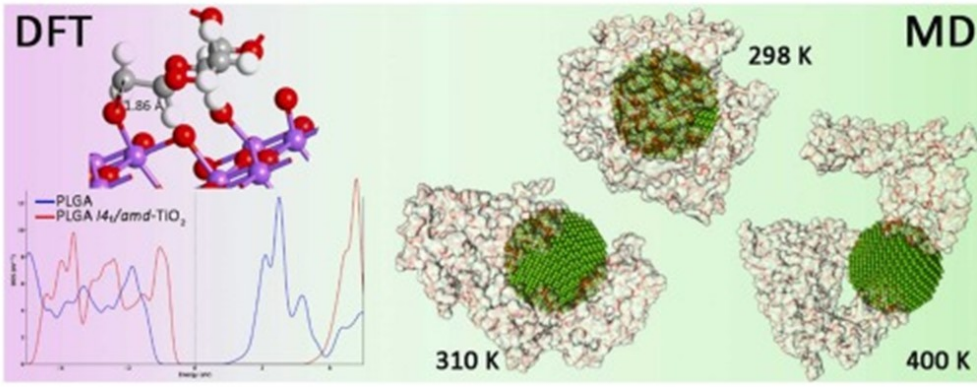

Figure 1. Illustration of the connection between DFT and MD together to evaluate the properties of materials. From the electronic structure in DFT combined with the molecular interactions at specific temperatures in MD will give insights into the behavior of materials in different corrosive environments. (Source: E. et al., Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2023, 667, 131388 [23])

Although DFT and MD are different in nature and simulation scale, the combination of these two methods (DFT–MD coupling) provides a more comprehensive view of the metal corrosion mechanism. DFT provides accurate information on the energy and electronic structure at the quantum level, while MD simulates atomic dynamics on a longer time scale. The combination of DFT and MD is usually carried out in three main directions: Sequential coupling: The results from DFT (such as adsorption energy, binding parameters, atomic charges) are used as input to MD, helping to simulate the adsorption process and atomic motion more accurately [19]. Concurrent coupling: The reaction zone is simulated by DFT, while the surrounding environment is simulated by MD – also known as QM/MM hybrid model [20]. Parameter correction (DFT-informed force field): Experimental potentials in MD (especially in the ReaxFF method) are trained directly from DFT data, helping to better simulate complex systems such as oxides, alloys or composite materials. The integrated DFT-MD method has proven effective in describing oxide film formation, local corrosion mechanisms and predicting corrosion resistance of alloys. Recently, studies by Zhao et al. (2024) [21] and Castillo-Robles et al. (2025) [22] also combined DFT–MD with machine learning to determine adsorption energy and reconstruct virtual corrosion surfaces, opening up a new direction for predictive materials modeling.

3. Application of density functional theory (DFT) in metal corrosion research

3.1. Adsorption Energy and Reactivity Descriptors

One of the most basic and common applications of DFT in corrosion research is to calculate the adsorption energy (Eads) of corrosive molecules or ions (Cl^-, H_2O, H^+, O_2) and corrosion inhibitors on metal surfaces. The adsorption energy is determined by the formula:

$$E_{ads} = E_{sys} - (E_{surf} + E_{mol}) \quad (3)$$

Where E_{sys} is the total energy of the system when the molecule is adsorbed onto the surface, E_{surf} is the energy of the bare metal surface, and E_{mol} is the energy of the free molecule in vacuum.

An E_{ads} value < 0 indicates an exothermic (stable) adsorption process, and a more negative value indicates a stronger binding between the adsorbent and the metal surface. Electronic reactivation indices are also commonly used to complement the analysis of the adsorption

mechanism, including: HOMO–LUMO energy gap (ΔE): determines the electron transfer ability; Electronegativity (χ) and chemical hardness (η): related to the tendency to electron reactivity; Fukui index indicates the site with the strongest tendency to accept or donate electrons in the molecule [24]. Studies show a close correlation between the adsorption energy calculated by DFT and the experimentally measured inhibition efficiency. For example, Bala et al. (2025) [25] used DFT to calculate the adsorption energy of a series of imidazole compounds on carbon steel, finding that molecules with -OH and -NH_2 substituents gave larger negative adsorption energies and exhibited higher inhibition efficiency in electrochemical experiments. Other works [26,27] have shown that molecules with high HOMO energy levels (easily donating electrons) often form stronger bonds with the metal surface, while molecules with low LUMO levels (easily accepting electrons) increase the electrostatic adsorption capacity. Thus, DFT not only helps explain the inhibition mechanism but also guides the design of new inhibitor molecules based on the principle of "simulation-guided inhibitor design".

3.2. Modeling of metal surfaces and interactions with intruding ions

In corrosion studies, simulation of metal surfaces is considered an important step to accurately reproduce the interaction mechanism with intruding ions. By DFT, slab models consisting of 3–5 layers of metal atoms are usually established; in which, the top two layers are optimized for free geometry, while the lower layers are fixed to simulate the bulk crystal. Metal surfaces such as Fe(110), Cu(111), Al(100), Ni(111) and Mg(0001) are often chosen because of their high atomic density and high energy stability. Through DFT simulations, the breakdown of the passive oxide film has been attributed to the influence of Cl^- ions, which is considered the main agent causing localized corrosion (pitting corrosion) [28]. In the study of Chen et al. (2025) [29], the competitive adsorption between Cl^- and H_2O on the Fe(110) surface was simulated using DFT. The negative adsorption energy of Cl^- (-2.34 eV) was determined to be larger than that of H_2O (-0.95 eV), indicating that the metal surface tends to be more susceptible to Cl^-, leading to the destabilization of the protective oxide layer. Similarly, Wang et al. (2023) [30] showed that the presence of Cl^- reduces the energy barrier for proton extraction from acetic acid, resulting in a significant increase in the corrosion rate of X80 steel. In addition to Cl^-, the role of SO_4^{2-}, NO_3^-, and CO_3^{2-} ions has also been considered in recent studies [31]. The analysis of charge density and density of states (PDOS) shows that SO_4^{2-} generally has a weaker interaction than Cl^-, so it is less likely to cause damage to the protective oxide film.

3.3. Simulation of passive oxide film formation

In corrosion research, simulation of passive oxide film formation is considered an important direction to understand the natural protection mechanism of metals. By DFT method, the formation process of oxide systems such as Fe_2O_3, Al_2O_3, TiO_2 and Cr_2O_3 has been simulated to elucidate their role in preventing the diffusion of ions and electrons, thereby slowing down the metal oxidation process. In the study by Zhao et al. (2024) [32], a hybrid DFT method was used to simulate the formation of TiO_2 film on the titanium surface. The redistribution of electron density at the metal-oxide interface was identified as a key factor in stabilizing the passive layer.

Similarly, Li et al. (2024) [33] showed that in the Fe-Cr system, the presence of Cr promotes the formation of a more stable Cr_2O_3 layer, thereby improving the corrosion resistance of stainless steel. The formation energy and energy barrier values obtained from DFT were used to determine the rate-controlling stage of the oxide film formation process. In addition, the application of the continuum solvation model was carried out to simulate the influence of the electrolyte environment, helping the simulation results reflect the experimental conditions more accurately [34].

3.4. Influence of alloying elements and crystal structure

In corrosion research, the DFT method is widely applied to evaluate the influence of alloying elements on the corrosion resistance of materials. Elements such as Cr, Ni, Mo, Si and N are believed to have the ability to change the local electronic structure of the metal surface, thereby affecting the formation of oxide film or interacting with corrosive environment ions such as Cl^-, O^{2-}, SO_4^{2-},....

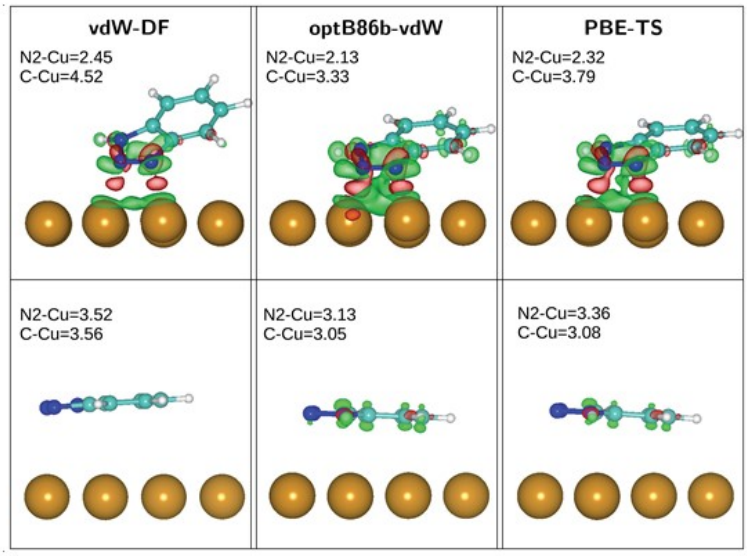

Figure 2. DFT simulation of the adsorption mechanism of corrosive ions and inhibitors on metal surfaces.

Electron density difference plots for the 'Tilted' (top row) and 'Flat' (bottom row) BTAH/Cu structures using three representative vdW-inclusive functionals. Green represents the region of charge density depletion and red regions of accumulation. The isosurface level is 0.002e/a03 for all structures. The distances between the azole N2 and the surface and between the center of the benzene-like ring and the surface are given in Å. In the study of Arachchige et al. (2020) [35], the addition of Cr to the Fe–Ni system was shown to reduce the density of states at the Fermi level, causing the electron donation-acceptance process. Figure 1 schematically illustrates the hierarchical integration of density functional theory and molecular dynamics simulations for corrosion studies, highlighting the complementary roles of electronic-level and atomistic-scale modeling. In addition, Figure 2 presents representative electron density distributions and adsorption configurations obtained from DFT calculations, which provide fundamental insights into the interaction mechanisms between aggressive ions, inhibitor molecules, and metal surfaces.

4.Application of molecular dynamics (MD) simulation in metal corrosion research.

4.1.Molecular dynamics (MD) simulation method

MD is used as an important tool to study corrosion mechanisms in real environmental conditions, where electrochemical reactions occur simultaneously with the diffusion and chaotic motion of ions and molecules. Unlike DFT, which describes the static electronic state, MD allows direct observation of the time evolution of particles in the system, reflecting more accurately the kinetics and interaction mechanism between the material and the corrosion environment [36]. A typical MD model for corrosion research is usually established with three main parts: Metal slab: built from 3–5 atomic layers, often using Fe(110), Cu(111), Al(100), Mg(0001) or Ni(111) surfaces. Solvent layer: contains H_2O molecules with the correct density in reality to simulate the corrosive environment. Corrosive/inhibiting molecules or ions: including Cl^-, SO_4^{2-}, H^+ or inhibitory organic compounds such as benzotriazole, imidazole, pyrazole, triazine, etc. The simulation process is usually conducted in three stages: (i) Geometry optimization,

(ii) Equilibration at a specified temperature and pressure, (iii) Production simulation (production run) lasting from tens to hundreds of nanoseconds. From this process, important physical quantities are determined including the average adsorption energy (Eads, avg), radial distribution function (RDF), diffusion coefficient (D) and orientation angle of the inhibitor molecule relative to the metal surface. A prominent advantage of the MD method is the ability to simulate complex experimental conditions that are difficult to handle with DFT, such as the effects of temperature, ion concentration, potential, or solvent fluctuations. Thanks to that, MD allows visual description of the adsorption-desorption process, molecular rearrangement in the protective layer, as well as the stability of the inhibitor film in an aggressive environment. While molecular dynamics simulations provide valuable insights into the dynamic evolution of corrosion processes, several intrinsic limitations should be acknowledged. Classical MD simulations are highly dependent on the quality and transferability of empirical force fields, which may not accurately capture charge transfer, polarization effects, or complex chemical reactions at metal–electrolyte interfaces. In addition, the accessible simulation timescale, typically limited to nanoseconds, is several orders of magnitude shorter than real corrosion processes that occur over hours, days, or even years. Consequently, MD results often represent accelerated or idealized corrosion scenarios and should be interpreted primarily in a comparative or mechanistic context rather than as direct quantitative predictions.

4.2. Simulation of adsorption and orientation of corrosion inhibitors

A typical application of the MD method is the analysis of the adsorption configuration of corrosion inhibitor molecules on metal surfaces. By examining the radial distribution function (RDF) between the active atoms in the inhibitor molecule (N, O, S, π-ring) and the metal atoms (Fe, Cu, Al), the optimal adsorption distance can be determined, which is usually in the range of 1.5–3.5 Å for chemical adsorption and 3.5–5.0 Å for physical adsorption [37]. For example, Bala et al. (2025) used MD to examine the adsorption of imidazole on the Fe(110) surface. The results showed that the molecule was oriented parallel to the surface, thereby maximizing the π–d interaction and increasing the coverage area. Similarly, Oukhrib et al. (2021) [20] simulated the adsorption of pyrazolylnucleoside derivatives on Cu(111), finding that the –OH and $–NH_2$ groups form hydrogen bonds with the surface, stabilizing the protective layer and preventing the penetration of Cl^- ions. Another important quantity in the analysis is the interaction energy, which is averaged over the entire simulation time to evaluate the bond strength between the inhibitor and the metal surface [38,39]

$$E_{int} = E_{total} - (E_{surface} + E_{inhibitor} + E_{solution}) \quad (5)$$

The more negative the E_{int} value, the more stable the inhibitor layer. These simulations can be directly compared with the adsorption energy obtained from DFT, helping to verify the accuracy of both methods [40].

4.3. Reactive Force Field

ReaxFF (Reactive Force Field) marks a major step forward in corrosion simulation, allowing for dynamic chemical bond formation and breakdown, which is not possible with classical MD. In corrosion research, ReaxFF is used to simulate the oxidation of metal surfaces, oxide film formation, as well as interactions with water and Cl^- ions. Nevertheless, the predictive reliability of ReaxFF simulations strongly depends on the quality of parameterization. Force fields developed for specific metal–oxygen–hydrogen systems may lack transferability to different alloys, surface terminations, or electrolyte environments without careful reparameterization. In some cases, overparameterization can result in artificially enhanced reaction rates or unrealistic oxide growth kinetics. Therefore, ReaxFF-based corrosion simulations should be systematically benchmarked against first-principles calculations and experimental observations to ensure physical consistency. For example, Du et al. (2021) [41] used ReaxFF to investigate the oxidation of Fe(110) surfaces in aqueous environments. The results showed that the Fe_2O_3 film was formed through the diffusion of O atoms from water molecules into the metal surface, and then restructured into a stable oxide network. Similarly, Zhao et al. (2024) [42] applied ReaxFF to simulate the dissolution of TiO_2 oxide films in acidic environments, and found that the breakage of Ti–O bonds occurred mainly at low-energy surface defects. In addition, ReaxFF was also exploited to study the electrochemical corrosion mechanism through the reaction between the metal and protons (H^+) or between Cl^- ions and the oxide layer. These simulation results contributed to the construction of a quantitative corrosion rate model, showing good agreement with experimental electrochemical data [43].

4.4. Ab Initio MD (AIMD) simulation

Ab Initio Molecular Dynamics (AIMD) is a hybrid method between DFT and MD, in which the forces acting on atoms are calculated directly from DFT at each time step. This approach allows for the simulation of dynamic changes in the electronic structure during the evolution of the system, which is particularly useful for studying the formation of the initial oxide film and the complex electronic interactions between the metal and the etching molecules [44]. Zhao et al. (2024) [45] applied AIMD to simulate the early stages of TiO_2 film formation, observing the redistribution of the electron density within a few picoseconds, leading to stable Ti–O bonds. In addition, AIMD was used to investigate the metal–water interface, providing detailed information on the structure of the first hydration layer – a factor that determines the electrochemical stability of the metal surface. Despite the outstanding accuracy of AIMD, the very high computational cost remains a major limitation, limiting the simulation range to a few hundred atoms and the time to less than 50 picoseconds. However, the development of machine learning potentials is gradually overcoming this barrier, opening up the possibility of AIMD simulations at nanosecond scale with more reasonable computational costs [46].

4.5. MD applications in the prediction of anti-corrosion properties

Molecular dynamics (MD) simulations are not only used to describe corrosion mechanisms at the atomic level, but also have the ability to predict the predictive corrosion performance of materials and inhibitors. Parameters obtained from simulations such as interaction energy, coverage, ion diffusion coefficient, or adsorption layer thickness can be used to quantitatively evaluate the protective ability of inhibitors under specific environmental conditions. For example, Castillo-Robles et al. (2025) [11] combined MD

simulation with a deep neural network (DNN) to build a model to predict the inhibitory effect of more than 50 organic molecules on the Fe(110) surface. This hybrid MD-ML model showed a prediction error of less than 5% compared to experimental data, demonstrating high reliability and generalizability. The above results confirm the potential of automating the corrosion inhibitor design process, moving towards the trend of "simulation-machine learning-synthesis-validation" in modern computational materials science.

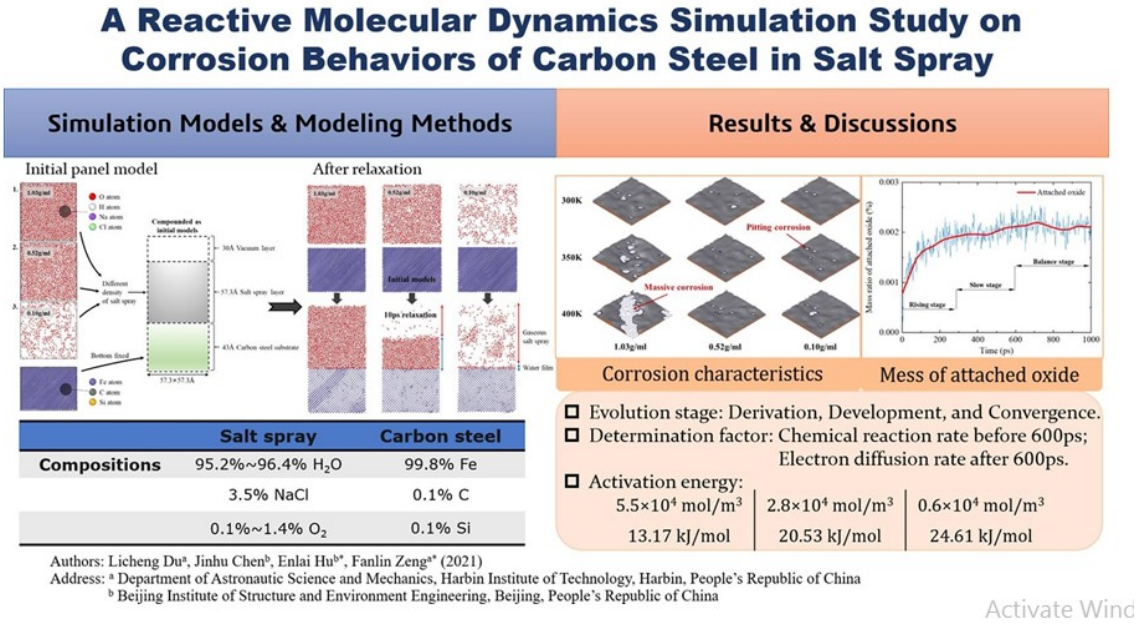

Figure 3. Illustration of the initial configuration and the results obtained when using MD for steel surface corrosion simulation.

5. MULTI SCALE INTEGRATED MODELING (DFT, MD, MACROSCOPIC)

5.1. Need for integrated modeling in corrosion research

Metal corrosion research is considered a multiscale problem, in which microscopic (electron movement, atomic bonding), mesoscopic (adsorption, ion diffusion) and macroscopic (material degradation, corrosion product formation) phenomena interact closely. No single simulation method - such as DFT or MD - can fully cover the time and space scales of the corrosion process. Therefore, the current trend in computational materials science is to develop multiscale integrated modeling, in which DFT, MD and macroscopic models (such as continuum models, phase-field models or finite element method – FEM) are linked sequentially or simultaneously to simulate the corrosion process more comprehensively. This approach not only helps to elucidate the corrosion reaction mechanism at the atomic level, but also allows for quantitative prediction of macroscopic quantities such as corrosion rate, material life, and inhibitor protection efficiency, contributing to narrowing the gap between simulation and experiment.

5.2. Information Linkage Between Simulation Scales

The linkage between models in corrosion studies is often established in a "bottom-up" approach, in which quantum data from DFT are used as input for MD simulations, and the MD results are further transferred to macroscopic models to describe the corrosion process at larger scales. Specifically: From DFT → MD: Parameters such as adsorption energy, bond strength, atomic charge, and force constant are extracted from DFT results to calibrate the force field parameters in MD. For example, modern ReaxFF potential sets such as Fe/O/H 2021 or Ni/Cr/O/H 2024 have been trained directly on the DFT database [48,49].

From MD → macroscopic model: Data obtained from MD, including diffusion coefficient (D), surface reaction rate (k), or average oxide film thickness (d), are transformed into input parameters for corrosion kinetics or finite element models (FEM) at the macroscopic level [50]. Two-way coupling (DFT ↔ MD ↔ Continuum): Some advanced integrative models also allow for feedback, in which when environmental conditions (such as pH, potential, or ion concentration) change, the macroscopic model updates the boundary conditions for MD or DFT, creating a closed feedback loop. This approach allows for the simulation of adaptive corrosion evolution, reflecting the dynamic and nonlinear nature of metallic systems in real environments [51].

5.3. DFT–MD–Phase Field Model for Localized Corrosion Prediction

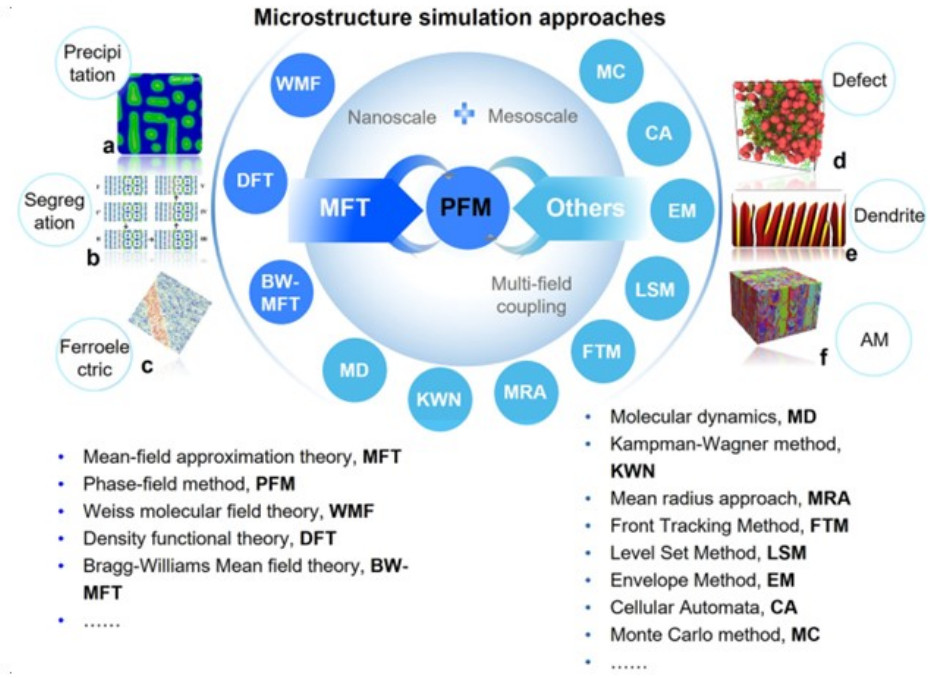

Figure 4. The diagram illustrates the relationship between DFT, MD and PFM simulation methods.

An advanced approach that is being strongly developed today is to integrate DFT and MD into a phase field model (PFM) to simulate localized corrosion processes such as pitting or crevice corrosion. In this model, the simulation scales are closely connected in a series: -DFT is used to determine the surface energy, the reaction potential barrier of oxidation-reduction processes, as well as the electronic characteristics of the defect region on the metal surface. -MD is used to simulate the diffusion of Cl^- and H^+ ions, and to monitor the formation of the initial oxide cluster, reflecting the dynamic interactions in the electrolyte environment.

-PFM takes on the task of describing the spatiotemporal evolution of the pit or oxide layer using the extended Ginzburg–Landau equation, in which the energy and diffusion parameters are taken from DFT and MD. Zhao et al. (2024) [52] successfully demonstrated a DFT-MD-PFM model for the Fe-Cl system, which accurately reproduced the pit growth morphology initiated by atomic surface defects. This model not only allowed for simulation of pitting dynamics, but also predicted pit growth rates with deviations of less than ±10% from experimental data, demonstrating the quantitative prediction potential of multiscale simulation in metal corrosion research.

6. COMBINATION OF DFT–MD WITH EXPERIMENTAL DATA (EXPERIMENTAL VALIDATION)

6.1. The role of experimental validation in simulation of corrosive materials

One of the core requirements of simulation studies is to ensure validation. The results obtained from DFT or MD are only scientifically meaningful when verified by experimental data, to confirm that the simulation model correctly reflects the physical and chemical nature of the system. In corrosion research, the comparison between simulation and experiment is often done through three main groups of techniques:

Electrochemical analysis: including electrochemical impedance spectroscopy (EIS), Tafel polarization curve, determination of corrosion current density (Icorr) and corrosion potential (Ecorr); Surface analysis: using XPS spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM) and atomic force microscopy (AFM) to investigate the morphology and chemical composition of the surface; Chemical analysis: applying FTIR, Raman, UV–Vis to identify the functional groups or chemical bonds of the inhibitor after adsorption. The integration of DFT–MD simulation and experiment not only plays a role in verifying the corrosion and adsorption mechanism, but also helps to calibrate and optimize the model, thereby improving the reliability and predictability in anti-corrosion material studies [54].

6.2. Comparison of simulated adsorption energy and experimental inhibition efficiency

A common validation method in corrosion simulation studies is to compare the adsorption energy (Eads) obtained from DFT/MD calculations with the corrosion inhibition efficiency (η%) determined through electrochemical measurements. Several works have shown that there is a near linear correlation between |Eads| and η%, in which a more negative adsorption energy indicates a higher protection of the metal surface [55]. For example, Al-Amiery, et al. (2025) [56] studied a series of imidazole compounds on Fe(110) surfaces using DFT and compared them with EIS (Electrochemical Impedance Spectroscopy) results. The results showed that the compound with Eads = -1.95 eV achieved 94% inhibition efficiency, while the compound with Eads = −0.88 eV achieved only 67%. The strong correlation (R^2 = 0.92) between simulation and experimental data demonstrates the reliable prediction ability of this method for new inhibitors, even before synthesis. It is important to emphasize that such correlations are not universally applicable. In several reported studies, DFT calculations tend to overestimate adsorption energies due to the neglect of explicit solvent effects, surface roughness, temperature fluctuations, and electrochemical potential. These simplifications may lead to optimistic predictions of corrosion inhibition performance that are not fully realized under experimental conditions. Consequently, adsorption energy should be regarded as a qualitative descriptor for screening purposes rather than a sole quantitative predictor of inhibitor efficiency. Similarly, Wang et al. (2023) [6] compared the interaction energy between Cl^- ions and the X80 steel surface calculated by DFT with the experimental corrosion rate obtained from Tafel measurements. The simulation model accurately reproduced the increasing trend of corrosion rate with increasing Cl^- concentration, with an error of less than 8%, thereby confirming the validity of the combined simulation-experiment method in predicting corrosion behavior.

6.3. Surface structure analysis by XPS and electron density simulation

XPS spectroscopy is considered a powerful tool to determine the oxidation state and chemical bonding nature on the material surface after the adsorption of inhibitors or the formation of protective oxide film. Meanwhile, DFT plays a role in supplementing quantitative information through the analysis of electron density difference and Mulliken or Bader charge distribution, allowing direct comparison with experimental XPS peaks. In the study by Zhao et al. (2024) [2], the DFT method was used to calculate the electron density distribution on the Ti surface after the formation of the TiO_2 film. The simulation results

showed that the electron density transfer from Ti atoms to O at the interface layer corresponded exactly to the Ti $2p_3/_2$ = 458.7 eV peak in the experimental XPS spectrum – confirming the reliability and consistency of the DFT model. Similarly, Chen et al. (2025) [11] studied the adsorption of benzotriazole (BTA) molecules on the Cu(111) surface and found that the N 1s and Cu 2p peaks shifted in the direction of Cu–N chemical bond formation. These results are in good agreement with the electron density and local electronic distribution of states (PDOS) simulations, thereby confirming the ability of DFT to explain in detail the interaction mechanism between the inhibitor and the metal surface.

6.4. Comparison of simulated adsorption structures and AFM/SEM images

Molecular dynamics (MD) and reactive force field (ReaxFF) simulations allow visual observation of molecular adsorption and the formation of the inhibitor film on the metal surface. The obtained results are often compared with experimental images from AFM or SEM, to confirm the morphology and continuity of the protective layer. In the study of Shashirekha et al. (2024) [57], MD simulations showed that imidazole molecules arranged themselves in parallel layers on the Fe(110) surface, forming a protective film about 1.2 nm thick. This result is consistent with the experimental AFM image, which shows a reduction in surface roughness from 95.4 nm to 27.8 nm after inhibitor treatment. In addition, the SEM image shows a reduction in the pit density of more than 80%, which corresponds to the ReaxFF simulation predicting that the inhibitor film significantly inhibited the diffusion of Cl^- ions into the steel surface.

6.5. Integration of simulation-experimental data in material lifetime assessment

Simulation (DFT-MD) and experimental data (EIS, XPS, SEM) are now integrated into lifetime prediction models. This approach allows quantifying the relationship between electronic properties, microstructure, and corrosion rate at the macroscopic scale. For example, Xiaohong Ji et al. (2022) [58] developed an integrated model using adsorption energy from DFT, interaction energy from MD, and polarization resistance from EIS to predict the lifetime of epoxy-TiO_2 coatings. The model results accurately estimated the corrosion onset time with an error of less than 6% compared to the experiment, demonstrating the effectiveness of the multi-data modeling approach in predicting material durability. Despite the increasing accuracy of DFT–MD models, uncertainty quantification and reproducibility remain underexplored. Variations in exchange–correlation functionals, force field parameterization, and simulation protocols can lead to non-negligible discrepancies across studies. Establishing standardized benchmarking datasets and reporting guidelines is therefore essential to enhance the transparency and comparability of corrosion simulations.

7. RESEARCH TRENDS AND PROSPECTS

7.1. Research trends and future perspectives

Although recent studies increasingly report strong agreement between simulation results and experimental observations, not all corrosion phenomena can be reliably captured by current DFT–MD frameworks. Factors such as microstructural heterogeneity, grain boundaries, surface defects, and long-term electrochemical aging remain challenging to model accurately at the atomistic scale. Addressing these issues requires not only increased computational resources but also the development of standardized validation protocols and uncertainty quantification strategies in corrosion simulations. In the early stages, DFT and MD simulations were mainly used to explain the corrosion mechanism at the atomic level, including ion adsorption, oxide film formation, or inhibitor protection. However, in recent decades, the research focus has shifted from “descriptive simulation” to “predictive simulation” [59]. The

development of high-performance computing (HPC) and parallel algorithms has significantly shortened the simulation time, allowing thousands of structures to be processed in just a few hours. As a result, the design of anti-corrosion materials can be carried out entirely on the simulation platform, before actual synthesis and testing. Currently, large material databases such as Materials Project, Open Quantum Materials Database (OQMD) and NOMAD Repository have integrated corrosion data, facilitating the retrieval, analysis and training of machine learning models for predictive material design [60].

7.2. Application of artificial intelligence (AI) and machine learning

AI and machine learning (ML) are becoming the mainstream direction in computational materials for corrosion protection. Instead of simulating individual compounds, deep learning models can learn the relationship between electronic properties – structure – inhibition efficiency from thousands of data samples, helping to quickly predict hundreds of potential inhibitor molecules [61]. Prominent research directions include: Simulation-informed ML: Combining DFT (adsorption energy, PDOS) and MD (coverage, diffusion coefficient) data as input to ML models – allowing prediction of inhibition efficiency with an error of less than 5% [62]. AI supports the design of new inhibitor molecules: Generative AI models based on GAN or Transformer networks can generate new molecular structures with high predicted adsorption energy – aiming at the design of "automatic corrosion inhibition" [63].

7.3. Smart coating materials and self-healing mechanisms

A prominent research direction today is smart corrosion-resistant materials, especially self-healing materials. These materials are capable of self-healing cracks or pits through a controlled release mechanism of inhibitors, triggered by environmental factors such as pH, Cl^- ions or surface potential [64]. In this area, DFT and MD play a central role in simulating the micromechanism of self-healing, including:
(i) Release of inhibitors from microcapsules or metal–organic frameworks (MOFs); (ii) Interaction between inhibitors and metal surfaces; (iii) Re-formation of bonds, passive oxide films after damage. For example, Li et al. (2024) [65] used MD simulations to investigate the release of 2-mercaptobenzothiazole (MBT) from epoxy–MOF coatings in high Cl^- ions concentrations. The results showed that the diffusion rate of MBT increased threefold when the pH decreased to 4, allowing the membrane to recover its passivation in just 20 min in good qualitative with the experimental EIS results.

7.4. Corrosion simulation in complex environments and new materials

Most previous studies focused on corrosion in neutral or mildly acidic aqueous environments. However, the current trend has expanded to more harsh environments, including seawater, ionic liquids, plasma, and high radiation environments [66]. In parallel, many advanced materials are being interested in corrosion simulation, typically: High-Entropy Alloys (HEA): have complex crystal structures and superior corrosion resistance, but the protection mechanism has not been fully elucidated; 2D materials such as graphene, MoS_2, MXene: potential to become ultra-thin anti-corrosion coatings; Conductive polymers and inorganic-organic hybrid films: combine waterproofing, adhesion and conductivity, helping to reduce electrochemical polarization [67]. Modern DFT-MD models allow for atomic-level description of surface structure and reaction, thereby predicting protection mechanisms and optimizing coating structures, contributing to the design of new generation anti-corrosion materials.

7.5. Development of Open Corrosion Databases

To promote global collaboration and data standardization, many research groups have developed Open Corrosion Databases, integrating both simulation and experimental data. These databases store comprehensive information such as adsorption energies from DFT, MD data (diffusion coefficients,

interaction energies), and experimental EIS, XPS, AFM results. This approach is transforming corrosion simulation from a manual, case-by-case approach to automated data mining, an important step towards digitalized materials science.

7.6. Overview

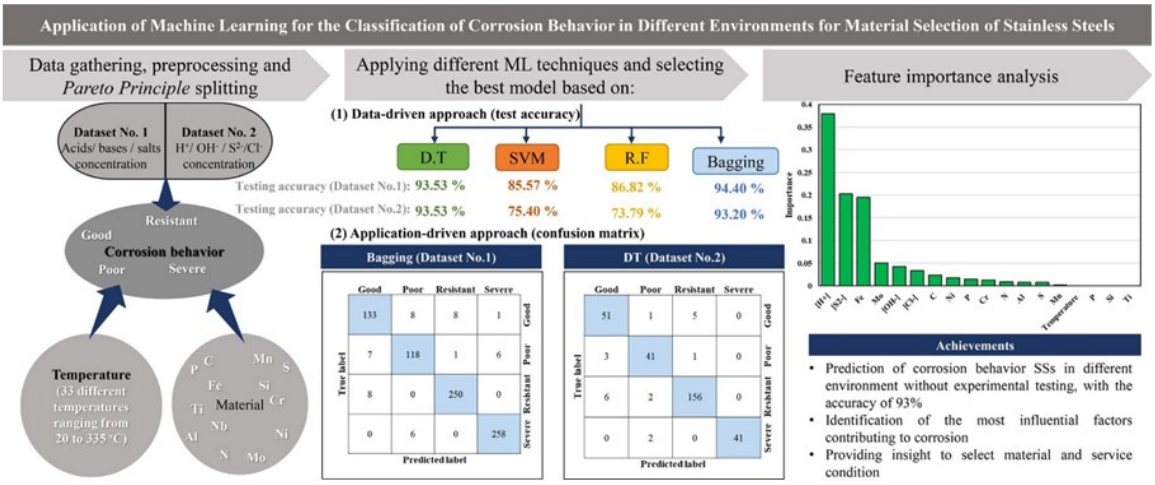

Figure 5. Schematic illustration of the integration of artificial intelligence (AI) with DFT and MD simulations for corrosion behavior classification and material selection. Simulation-derived descriptors and experimental data are used to train machine learning models for predicting corrosion performance under different environments.

In the next decade, corrosion simulation research is expected to develop strongly towards the comprehensive integration of DFT-MD-AI-experiment, forming a closed cycle of "simulation prediction verification optimization". In addition, real-time corrosion models will be developed, allowing data to be updated directly from sensors and environmental conditions. The emergence of cloud-based simulation platforms opens up the possibility of collaboration, sharing data and global computing resources, significantly reducing research costs and time. Finally, when multi-scale simulation is combined with 3D printing technology and nanomaterials, the design of anti-corrosion coatings with optimal structures at the atomic level will become a reality, marking the transition from basic simulation to predictive material design. Application of AI in the study of stainless steel corrosion (Source: S. Hakimian et al., Computational Materials Science, 2023 [68]).

8. Conclusion

Over the past decade, significant advances in Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations have enabled new insights into corrosion mechanisms and the development of corrosion-resistant materials at the atomic scale. DFT provides accurate descriptions of electronic structures, adsorption energies, and reaction barriers on metal surfaces, while MD captures the kinetics of adsorption, ion diffusion, and oxide film formation under near-experimental conditions. Their combined use offers a multiscale framework linking atomic, mesoscopic, and macroscopic behaviors, thereby deepening the quantitative understanding of corrosion processes. When integrated with experimental techniques such as EIS, XPS, SEM, and AFM, DFT–MD models can achieve prediction errors below 10%, highlighting their reliability and practical applicability. Furthermore, the rapid growth of artificial intelligence and machine learning has driven the emergence of predictive corrosion materials science, where DFT–MD data are used to design and optimize alloys, inhibitors, and self-healing coatings. The development of open corrosion materials databases further supports data sharing, reuse, and

automated materials design. Overall, DFT and MD have evolved from fundamental research tools into strategic platforms for designing smart, sustainable, and environmentally friendly corrosion-resistant materials. Beyond summarizing recent advances, this review critically evaluates the strengths, limitations, and validation challenges of atomistic simulations, providing practical guidance for their rational application in corrosion science.

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