JOURNAL OF NANOMATERIALS AND APPLICATIONS

Journal of Nanomaterials and Applications

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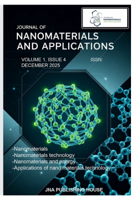

Atomistic simulations of two dimensional materials: insights from first principles and molecular dynamics methods

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Review info

Type of paper:
Review article

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Received: 26 September 2025
Revised: 25 October 2025
Accepted: 26 October 2025
Published: 30 October 2025

Abstract: Computational methods have become indispensable tools for the discovery and characterization of two-dimensional (2D) materials. This review focuses on the powerful synergy between Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations in understanding these atomically thin systems. We highlight how DFT serves as the cornerstone for predicting fundamental electronic properties such as band structure, defect states, and electronic transport in 2D materials like graphene and transition metal dichalcogenides (TMDs). Concurrently, MD simulations with accurately parameterized force fields provide critical insights into their mechanical resilience, thermal transport, and defect-driven fracture mechanisms. The integration of these two methods enables a multiscale approach to material design, from predicting quantum phenomena at the nanoscale to modeling large-area mechanical performance. This review demonstrates the pivotal role of atomistic simulations in unlocking the vast potential of 2D materials for next-generation electronics, energy, and sensor technologies.

Keywords: 2D Materials ; DFT ; Graphene ; Mechanical Properties; Molecular Dynamics.

1. Introduction

Two-dimensional (2D) materials have emerged as one of the key research directions with many breakthroughs in recent years. Since the discovery of graphene [1], this field has opened a new era, arousing strong interest due to its unique electronic, optical, mechanical and chemical properties that only appear at the atomic scale. The outstanding features of 2D materials lie in their planar structure and large specific surface area, which make them fundamentally different from traditional bulk materials [2]. Graphene, known for its remarkable stiffness and resistance to mechanical stress, has attracted researchers who are currently studying the prospect of replacing conventional silicon technology with these special materials [3]. The advent of graphene has spurred a wave of exploration into many other families of two-dimensional (2D) materials, including: graphyne, graphdiyne, graphenelene, dodecagon, and other 2D carbon variants; transition metal dichalcogenides (TMDs, e.g., molybdenum disulfide MoS_2, tungsten disulfide WS_2); hexagonal boron nitride (hBN); phosphorene (single layer black phosphorus); MXenes (2D transition metal carbides, nitrides, or carbonitrides) [4]; as well as oxide-based 2D materials. Each material exhibits a distinct set of properties: TMDs possess a direct band gap in their monolayer form, opening up prospects in nanoelectronics; hBN is an insulator with exceptional thermal stability [5]; while MXenes display high electrical conductivity and great potential for energy storage applications. The strength of 2D materials lies in their tunable properties, which can be modulated by varying the number of layers, applying mechanical strain, introducing defects, or incorporating elemental doping. For example, MoS_2 transitions from an indirect band gap in its bulk form to a direct band gap in the monolayer form, significantly enhancing photoluminescence efficiency [6]. To date, extensive experimental research has focused on the synthesis and characterization of 2D materials. However, at the experimental level, achieving materials with high purity, precise control over the number of layers, and large-area sample fabrication remains challenging [7,8]. Meanwhile, at the theoretical level, understanding electronic mechanisms, defect dynamics, and interactions with the surrounding environment requires simulation tools with high accuracy and multiscale capabilities [9].

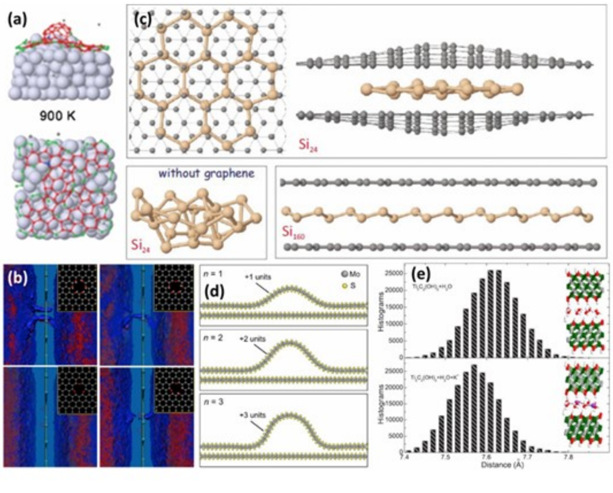

Figure 1. Application of simulation to 2D materials research [14].

Consequently, the development of data-driven simulation methods has played an important role in elucidating atomic level mechanisms, thereby enhancing the understanding of the morphology, structure, and properties of 2D materials and supporting the control of complex synthesis processes and structural modulation. In this context, atomic-scale simulation methods such as Density Functional Theory (DFT) and Molecular Dynamics (MD) have become the mainstays for the discovery, prediction, and design of 2D materials, playing a crucial complementary role to experiments and shortening the transition from research to practical applications [10]. DFT is recognized as an efficient and accurate quantum mechanical method for investigating the electronic, mechanical, and optical properties of materials, though it is typically limited to systems containing several hundred atoms [11]. In contrast, MD simulations can handle much larger systems and longer timescales, but they cannot describe energy and electronic properties in as much detail as DFT [12,13]. Therefore, integrating DFT and MD has become an inevitable trend in 2D material research, enabling researchers to leverage the strengths of each method while mitigating their individual limitations. Recently, numerous studies have successfully combined DFT and MD to explore the intrinsic properties of 2D materials. In this work, we synthesize and analyze the applications of numerical simulations in 2D material research and highlight the current limitations, as illustrated in Figure 1.

2. Overview of computational methods

2.1. First principles calculation

The foundation of the first-principles method lies in quantum mechanics, which describes the behavior of electrons and atomic nuclei under all conditions. The Schrödinger equation (Equation 1) is the central equation used in these calculations. However, its major limitations stem from its mathematical complexity and the high computational cost associated with systems containing more than one electron. In multi-electron systems, interactions among electrons give rise to the many-body problem.

$$\hat{H}\Psi = E\Psi \tag{1}$$

where $\hat{H}$ is the Hamiltonian, Ψ is the wave function and E is the energy of the system.

To solve the complex Schrödinger equation, several approximations have been developed, such as the Born–Oppenheimer approximation, Kohn–Sham formulation, exchange–correlation (XC) functionals, and pseudopotential methods [15,16]. The DFT method has been widely used to calculate the electronic structure of molecules and 2D materials [17,18]. Several review papers on DFT are available in the literature, discussing in detail its theoretical framework, approximations, and applications across various systems [19,20].

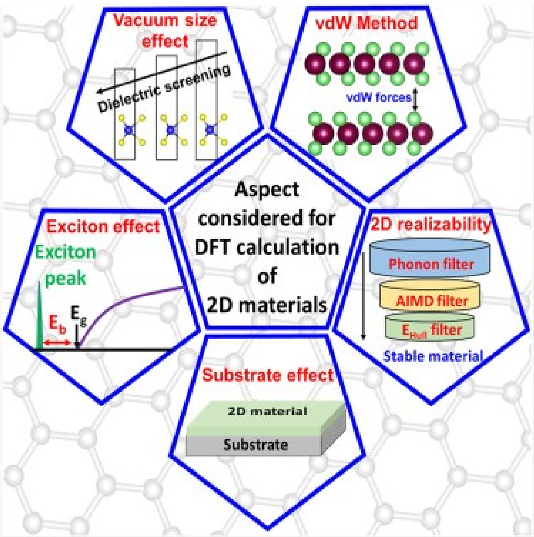

Figure 2. Application of DFT in 2D materials research [25].

Therefore, we do not discuss the DFT method in detail here but briefly highlight some key approximations commonly employed in DFT calculations to achieve more accurate results. For instance, conventional DFT calculations based on standard XC functionals often underestimate the band gap values of semiconductors compared to experimental results [21]. To address this issue, several modified approaches have been developed, including DFT + U (DFT with on-site Coulomb correction), hybrid functionals (e.g., SX Screened Exchange, PBE0 Perdew Burke Ernzerhof hybrid, HSE Heyd Scuseria Ernzerhof), the GW approximation (Green's function + screened Coulomb interaction), and DMFT (Dynamical Mean-Field Theory), as illustrated in Figure 2 [22–25].

2.2. Molecular dynamics

Molecular Dynamics (MD) is one of the most important computational simulation tools in materials science, chemistry, and biology. The basic principle of MD is to track the time evolution of a many-body system (atoms or molecules) based on classical mechanics, primarily Newton's laws of motion. In this approach, the force acting on each atom is determined from the interatomic potential, which is then used to update the acceleration, velocity, and position of atoms at small time steps. The MD method was originally developed in the 1950s to solve the classical many body problem, extending beyond the limitations of traditional theoretical approaches [26]. By analyzing the motion of individual particles through interatomic potentials, MD can reproduce the collective dynamics of a system, thereby enabling the explanation, prediction, and design of experimentally observed phenomena [27]. The MD simulation process typically involves: (i) constructing the simulation system and defining boundary conditions; (ii) selecting the interaction force field or potential, for example, the Embedded Atom Method (EAM) potential for metals or the Reactive Force Field (ReaxFF) for complex chemical reaction systems; (iii) integrating the equations of motion (e.g., Verlet or Velocity Verlet algorithms); and (iv) analyzing the results to obtain quantities such as energy, pressure, diffusion coefficients, and radial distribution functions (RDFs), as well as insights into kinetic mechanisms and structural transformations [28]. The molecular interaction potentials are typically defined using functions such as the Tersoff potential [29–31] or ReaxFF [32]. In contrast, interlayer molecular interactions are often represented by Lennard–Jones potentials in van der Waals multilayers. The MD-based simulation package LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [33] is one of the most widely used tools for modeling nanoscale processes, including nanoindentation experiments. The main advantage of MD is its ability to provide detailed, atomistic information in real time something difficult to achieve experimentally. However, MD also has limitations, such as relatively short simulation times (typically on the order of nanoseconds to microseconds), system sizes constrained by computational resources, and accuracy that strongly depends on the choice of potential energy function. With the advancement of supercomputing and optimization algorithms, MD has become an increasingly powerful tool for bridging computational simulations and experiments, contributing significantly to the discovery, design, and optimization of new materials.

3. Applications

3.1. DFT: Practical applications

This section discusses the application of DFT based computational methods to the study of 2D materials. By calculating wave functions and particle behavior within the framework of quantum mechanics, DFT can provide highly accurate predictions of thermodynamic properties, stability across different crystal structures, and various mechanical, electronic, and optical properties.

3.1.1. Electronic structure prediction

DFT provides the ability to simulate in detail the energy band structure and band gap of 2D materials [25]. For example, for materials such as graphene, MoS_2, and hBN, DFT has accurately determined their electronic properties, including whether they exhibit a direct or indirect band gap an important factor in the design of electronic and optoelectronic devices. Recent studies have employed DFT to predict and analyze these properties, providing a solid theoretical foundation for the development of new 2D materials. Understanding the electronic structure of 2D materials is crucial. The electronic properties often change between the bulk and 2D states due to structural splitting and bond modifications. For instance, bulk MoS_2 (space group: $P6_3/mmc$) is an indirect-band-gap insulator with a gap of 0.91 eV, where the valence band maximum (VBM) is located at Γ and the conduction band minimum (CBM) lies between Γ and K, as shown in Figures 3A–3B. In contrast, monolayer MoS_2 is a direct-band-gap insulator with a gap of 1.9 eV according to DFT calculations. Similarly, the band gap of phosphorene decreases from 1.49 eV in the monolayer to 0.33–0.87 eV as the number of layers increases (Figures 3C–3D).

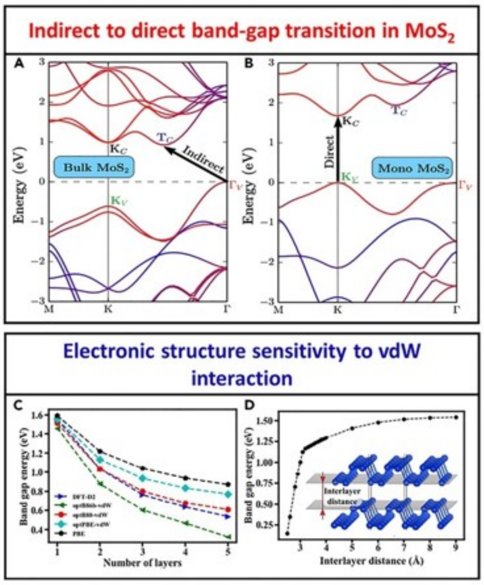

Figure 3. Thickness dependence of the electronic structure of 2D materials.

The accuracy of DFT calculations for electronic structure is strongly influenced by the choice of pseudopotential function. Selecting an appropriate pseudopotential can yield more accurate results. For example, in the semiconductor material RhTeCl, the choice of potential led to a significant discrepancy: the conventional PBE functional underestimated the band gap (1.21 eV), whereas the HSE06 functional provided a more accurate estimate of 2.12–2.24 eV [34]. Since the PBE functional tends to underestimate the band gap, we calculated the band structure using the hybrid screened functional HSE06, which is known to describe the exchange–correlation energy of electrons in solids more accurately (Figure 3). Role of van der Waals (vdW) interactions: (Figure 3A and Figure 3B) Atomically projected electronic band structure of MoS_2 in bulk (Figure 3A) and monolayer (Figure 3B) forms. The blue and red bands represent the S and Mo atomic projections, respectively. Figures 3A and Figure 3B are reproduced from [35]. (Figure 3C and Figure 3D) The HSE-calculated electronic band gap as a function of (Figure 3C) the number of layers, using different XC functionals for the internal expansion of bilayer phosphorene, and (Figure 3D) the interlayer spacing. The inset in (Figure 3D) shows the interlayer spacing in bilayer phosphorene. Figures 3C and Figure 3D are from [36].

3.1.2. Optical/Photonic properties

In addition to electronic properties, the optical and photonic properties of 2D materials play a crucial role in many applications, including optoelectronic devices (photodetectors, LEDs), energy systems (water splitting, catalysis), and optical coatings. Characteristic parameters such as optical absorption peaks, reflectivity, dielectric constant, refractive index, and optical conductivity have been extensively calculated using DFT. In the context of materials science and optics, the frequency-dependent Kramers–Kronig relations have emerged as a key tool for analyzing the optical response of materials under the influence of external photons. Specifically, the complex dielectric function is expressed as $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$, where $\varepsilon_1(\omega)$ represents the real part associated with energy storage, and $\varepsilon_2(\omega)$ represents the imaginary part characterizing energy dissipation [37]. Calculations of $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ using DFT help elucidate the optical mechanisms of materials. For example, studies on 2D $Ni_2P_2S_2$ and $Ni_2P_2Se_2$ have demonstrated potential applications in optical coatings, waveguides, and photonic devices due to their stable dielectric behavior [37]. Similarly, DFT calculations for boron nitride, carbon nitride, boron carbide, and the ternary boron–carbon–nitride (BCN) system reveal significant modifications of optical properties upon doping, particularly with varying nitrogen content [38]. These results confirm that DFT is a powerful tool for predicting and guiding the design of 2D materials for next-generation photonic applications.

3.1.3. Material defects and environmental interactions

Defects in 2D materials play a key role in tailoring their electronic, optical, and chemical properties, thereby affecting the performance of nanoscale devices. Common defects include point defects (vacancies, interstitials, and dopants) and extended defects (dislocations and grain boundaries). Defect formation can occur naturally at thermodynamic equilibrium, such as thermally induced point defects, or result in more complex structures like lattice dislocations and grain boundaries. Some defects also arise from the finite dimensions of the crystal, such as edges and surfaces. Additionally, defects can be intentionally introduced through electron or ion irradiation, or via chemical treatments. Theoretical calculations based on DFT are frequently employed to investigate the formation, stability, and properties of these defects. Defects in 2D materials not only influence their fundamental properties but also enable numerous potential applications in electronics, catalysis, and photonics. In nanoelectronics, vacancies in MoS_2 have been shown to create trap states within the band gap, affecting electron transport and the stability of thin-channel transistors [39, 40]. In graphene, doping with nitrogen (N) or boron (B) can tune conductivity, open a band gap, and improve performance in field-effect transistors (FETs) [41]. In catalysis, sulfur vacancies in MoS_2 serve as efficient active sites for the hydrogen evolution reaction (HER), enhancing catalytic activity compared to the defect-free structure [42]. Defects are also important in photonics: in hBN, nitrogen vacancies and complex defect centers can generate single-photon emitters, which are highly promising for quantum computing and optical communication applications [43]. Consequently, the design and controlled engineering of defects has become a critical strategy for developing 2D materials for next-generation electronic and optoelectronic devices.

3.2. Molecular dynamics: Practical applications

MD is one of the primary tools used to study the evolution of 2D materials at the atomic scale. MD is a powerful computational method that enables the simulation of atomic motion over time based on interatomic potentials. In the field of 2D materials, MD has proven to play a crucial role in predicting and analyzing mechanical and thermal properties, defect dynamics, as well as interlayer interactions in complex 2D systems.

3.2.1. Synthesis techniques

MD simulations are an important tool in the study of 2D materials, particularly for characterizing synthesis techniques and structural evolution at the atomic level. Through MD, researchers can observe the self-assembly of atoms, nucleation, 2D layer growth, as well as the effects of temperature, pressure, and catalysts on the final structure. Chemical vapor deposition (CVD) is a widely used synthesis technique for fabricating high-quality, large-area single- or multilayer graphene. However, due to limited atomic-level understanding, many challenges have hindered its development. With the advancement of MD, the growth mechanisms and reaction pathways of carbon-based precursors have been thoroughly elucidated. For example, Meng et al. [44] studied the effects of carbon concentration and temperature on graphene growth kinetics on Ni(111) surfaces using elemental carbon precursors, thereby determining an optimal defect-annealing temperature of 1000 K. Similarly, Chen et al. [45] investigated the CVD pathway of CH_4 decomposition and the subsequent evolution from carbon segments to graphene. Furthermore, MD has been combined with Atomic Layer Deposition (ALD) technology to simulate the synthesis of 2D materials with atomic precision. ALD enables the creation of uniform thin layers with controlled thickness through cycles of adsorption and removal of precursors on the material surface [46]. MD can simulate each of these steps in detail, including precursor adsorption, surface chemical reactions, and the temporal growth of the thin layer. For instance, MD simulations of boron nitride (BN) thin-film growth using BCl_3 and NH_3 on Si(100) surfaces [47] revealed the initial growth mechanisms of BN and its evolution at different temperatures (750 K, 1000 K, 1250 K, 1750 K, and 2000 K), thereby identifying suitable conditions to promote film formation and growth.

3.2.2. Mechanical properties studies

The mechanical properties of 2D materials [48] are of particular interest in industrial applications, such as protective coatings [49] and diffusion barriers in electronic devices [50].

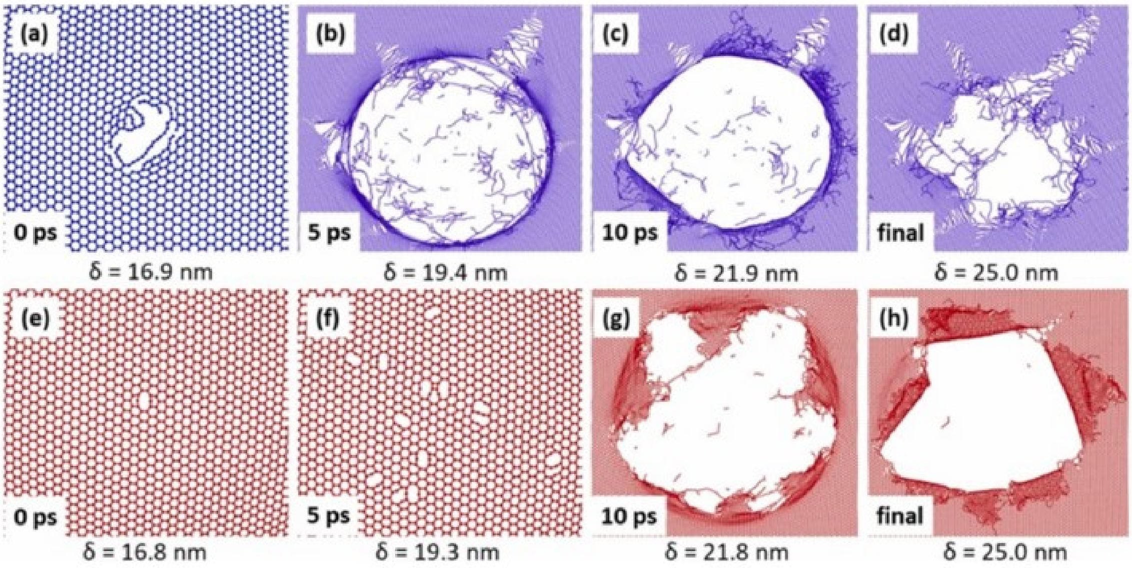

Figure 4. Monolayers of graphene (top) and hBN (bottom) at different time intervals during nanoindentation simulations [52].

These properties can be quantified using various parameters [51], including Young's modulus (Y), flexural strength (D), and fracture strain (ϵ). As discussed in previous sections, these quantities can be effectively estimated using MD simulations. MD allows scientists to calculate the mechanical characteristics of 2D materials with high accuracy, including elastic modulus, tensile strength, ductility, and elastic limit for materials such as graphene, MoS_2, WS_2, and phosphorene. Graphene, in particular, has been extensively studied due to its exceptional mechanical strength. For example, MD simulations have calculated the flexural strength of graphene to be approximately 1.2–1.3 eV [51,52], in good agreement with the experimental value of 1.17 eV [53]. Similarly, single-layer hBN has attracted attention because of its unique mechanical properties [54], especially its stability at higher temperatures compared to graphene. MD simulations estimated the flexural strength of hBN to be 1.13 ± 0.02 eV, which closely matches the experimental value of 0.95 eV. The failure strain was calculated as 15%, in agreement with the experimental value of 12.5 ± 3% [55]. In a recent study, Patra et al. [53] examined the fracture behavior of graphene and hBN nanosheets over different time scales. In graphene, C atoms form chain-like structures after the C–C bonds break (Figures 4a–4d), contributing to the exceptional strength of the nanosheets. In the case of a monolayer hBN, fracture initiates at point defects, which grow over time until the film completely fractures (Figures 4e–4h).

3.2.3. Surface interactions and redox

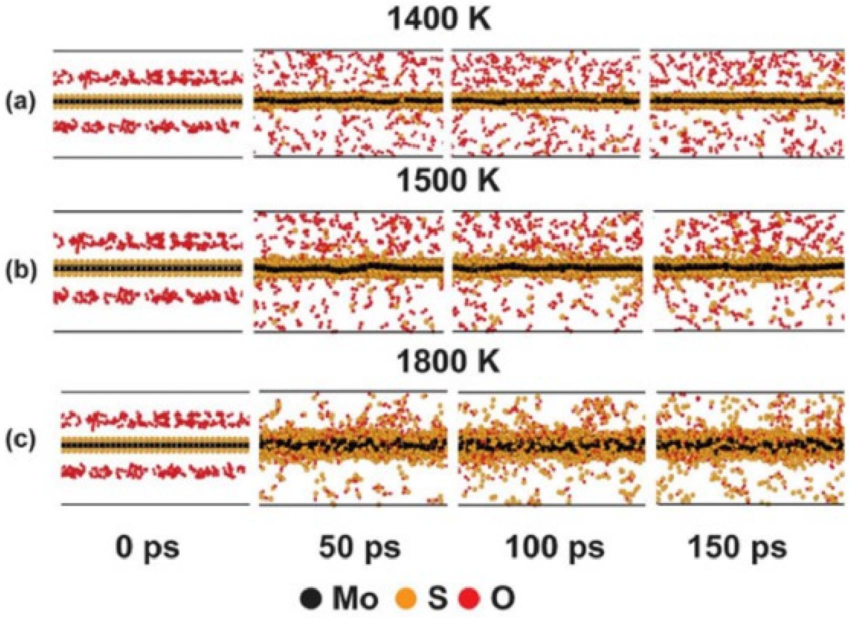

Figure 5. RMD snapshots during MoS_2 oxidation at (a) 1400 K, 1500 K (b), and 1800 K (c) at different time stages. The black, yellow, and red spheres represent molybdenum, sulfur, and oxygen atoms, respectively [56].

MD has become a powerful tool for studying the oxidation mechanisms of 2D materials, owing to its ability to simulate atomic dynamics and surface chemistry in real time. In 2D materials such as graphene, MoS_2, hBN, and phosphorene, oxidation typically begins with the adsorption and dissociation of O_2 molecules on the surface, which subsequently form oxygen clusters or generate oxidation defects. MD, particularly when using reactive force fields such as ReaxFF, can directly simulate the formation and breaking of chemical bonds during the process, enabling the observation of progression from the initial stage (adsorption and diffusion) to the later stage (stable oxide formation or structural degradation) on the pico to nanosecond timescale. For example, researchers have characterized the natural oxidation of MoS_2 thin films in an O_2 environment, revealing a three-step mechanism: adsorption of O_2 molecules, dissociation of O_2 into O atoms that bond with S, and the formation of SO_2 species that desorb, leaving surface defects that lead to structural degradation and corrosion [56,57] (Figure 5). In addition to elucidating oxidation mechanisms, MD can predict the influence of environmental factors on the process, such as temperature, oxygen pressure, and the presence of water or dissolved ions. This is particularly important for practical applications, where 2D materials often operate in atmospheric or electrochemical solution environments. For instance, besides analyzing the oxidation mechanism of MoS_2 in O_2 environments, the authors also investigated the effect of temperature on oxidation behavior (Figure 6).

Similarly, Roghayyeh Lotfi and colleagues [58] studied the effects of different environments (dry air, wet air, H_2O_2) on the oxidation of the Ti_3C_2 MXene structure.

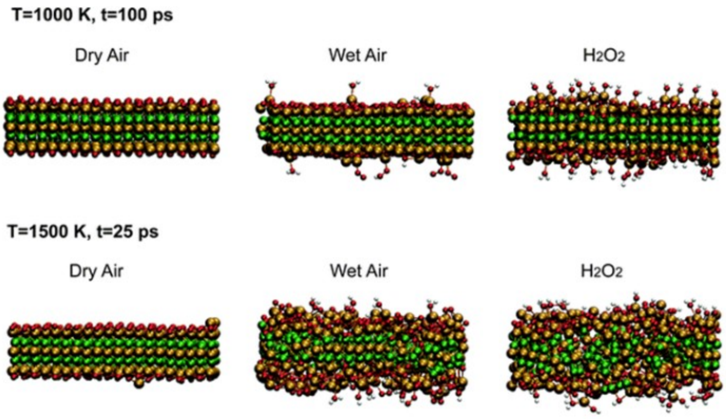

Figure 6. Comparison of MXene oxidation rates in three different environments (Ti: brown, C: green, O: red and H: white) [57].

3.2.4. Defects

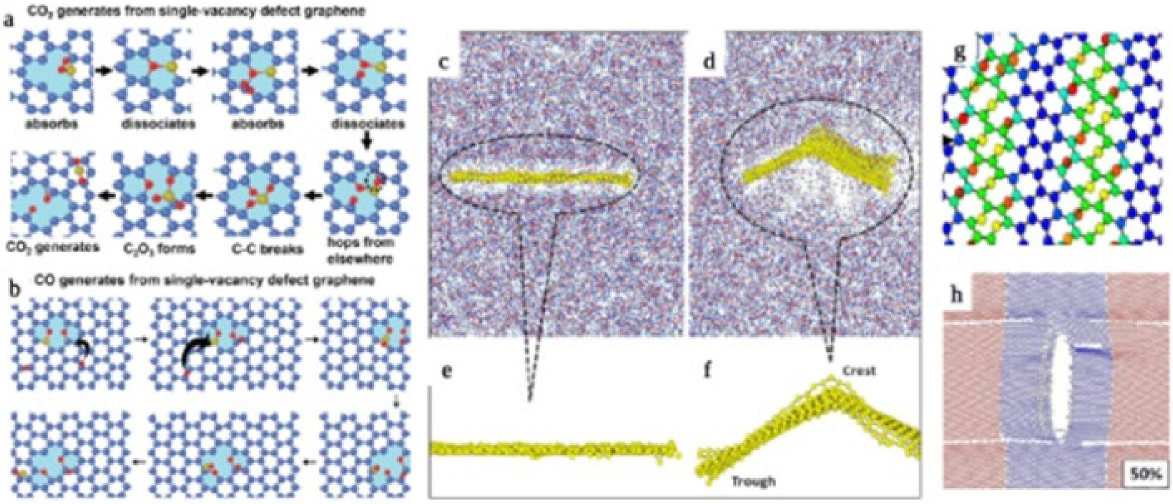

Figure 7. Four oxidation modes for defect containing graphene sheets. CO_2 (a) and CO (b) are the modes generated for a defect containing graphene sheet [58]; (c) and (d) are pristine and bicrystalline graphene in the graphene/polyethylene system; (e) and (f) are pristine and wrinkled isolated planar bicrystalline graphene [60]. Schematic illustration of the random distribution of epoxide (–O–) functional groups at GBs of bicrystalline polycrystalline graphene in sandwich structure (g) and with damaged morphology with 50% epoxide coverage for 21.8° ZZ bicrystalline graphene(h). Taken from [62].

The behavior of defects in materials is critical and can be effectively studied using computational methods. Using DFT, one can calculate the probability of defect formation at the atomic scale through defect formation energies or energy barriers for defect migration or diffusion. MD, on the other hand, provides a clear view of the mechanisms underlying the occurrence of point defects, dislocations, and grain boundaries, as well as their impact on material properties [58]. For example, Zheng et al. [59] investigated defect-promoted oxygen adsorption and desorption of gasification products (CO, CO_2) on graphene. As shown in Figures 7a and Figures 7b, uncoordinated C surface atoms facilitate the functionalization of the surface with oxygen by weakening the O=O bond. The adsorption of excess O atoms further induces the dissociation of CO_2 or CO through the formation of epoxy groups, increasing the size of the defect. Xu et al. [60] studied the mechanical properties of graphene oxide (GO) with grain boundaries (GBs) and demonstrated that GBs stimulate the formation of defect clusters, providing pathways for defect propagation. This leads to a noticeable decrease in tensile strength, which may be exacerbated by bonding between defects and high oxygen content functional groups at the GBs. Verma et al. [61] examined the interfacial properties of graphene/polyethylene (PE) nanoparticles using MD and found that bicrystalline graphene containing GBs outperformed pristine graphene in enhancing the tensile strength, shear strength, and adhesive strength of the reinforced PE nanoparticles, the results are shown in Figure 7c-7h. To address the advantages and limitations of DFT and MD potentials, we provide a systematic comparison, focusing on the technical strengths and weaknesses of these methods for 2D materials:

For DFT:

-Recognition and Limitations: Local density approximation (LDA) and generalized gradient approximation (GGA), such as PBE, often underestimate the band gap and have difficulty accurately describing van der Waals (vdW) interactions, which are critical in layered 2D materials.

-Comparative Analysis of Higher-Level Methods: Hybrid Functionals: Hybrid functionals significantly improve band gap predictions for 2D semiconductors. For example, PBE predicts 1.21 eV while HSE06 predicts 2.12–2.24 eV for RhTeCl. HSE06 represents a good compromise between computational cost and accuracy for electronic properties.

-GW Approximation: GW, combined with the Bethe–Salpeter Equation (BSE) for optical properties, is considered the gold standard for calculating band gaps and excitons, although it incurs very high computational costs.

-vdW Corrections: Including vdW corrections (vdW-DFT, DFT-D2, DFT-D3) is essential for accurately modeling multilayer 2D materials.

For MD Interaction Potentials:

-Comparative Analysis: Key potentials include Tersoff, ReaxFF, and machine learning-based potentials.

-Tersoff/Stillinger–Weber: Strengths: Computationally efficient for simple C/Si systems, e.g., calculating the mechanical properties of graphene or h-BN. Weaknesses: Cannot model chemical reactions or bond formation/breaking.

-ReaxFF: Strengths: Capable of simulating complex chemical processes, including oxidation, reduction, and surface reactions. Limitations: Accuracy depends strongly on parameterization and is more computationally expensive than classical potentials.

-Machine Learning Potentials (ML Potentials/GAP/DeePMD): These provide an optimized solution, combining DFT-level accuracy with MD-level computational efficiency.

3.2.5. Limitations and future directions

In this paper, we provide an overview of recent atomistic simulation studies on the properties of 2D materials, with particular emphasis on first-principles calculations and MD simulations. DFT and Molecular Dynamics are powerful tools for simulating material properties and gaining insight into the mechanisms underlying material behavior. They provide crucial information on how materials are organized and formed at the atomic and molecular levels. Although DFT and MD have proven essential in the study of 2D materials, several limitations remain. MD simulations are typically restricted to systems containing a few thousand to a few million atoms and timescales ranging from pico- to nanoseconds, whereas real-world phenomena such as crack propagation, long-term oxidation, or self-assembly of heterostructures occur on much larger spatial and temporal scales. Additionally, the accuracy of traditional force fields, such as Lennard–Jones, Tersoff, or Stillinger–Weber, is limited in describing complex chemical interactions, particularly oxidation, reduction, or doping processes. Reactive force fields (ReaxFF) have improved this situation, but parameter tuning still requires significant effort and computational resources [32]. Similarly, DFT with standard exchange correlation approximations (GGA, LDA) often underestimates the band gap and struggles to describe systems with weak van der Waals interactions or complex electron dynamics. Advanced methods, such as DFT+U, hybrid functionals (HSE06), or GW, provide more accurate results but at much higher computational cost [25, 63]. Moreover, most current simulations are performed under vacuum or idealized conditions, which do not fully reflect realistic environments such as ionic solutions, aqueous media, or mixed gases [64]. The scope of use, benefits and limitations of different types of potential energy functions in material simulation are summarized in Table 1.

Table 1. The capabilities, strengths and limitations of different calculation methods.

Method	**Properties**	**Strengths**	**Limitations**
DFT (LDA/GGA)	Electronic structure, band gap, mechanics, optics.	Quantum mechanical foundation, precise calculation of basic structure.	Underestimation of band gap. High computational cost for large systems (> several hundred atoms).
DFT (Hybrid/GW)	Band gap, Exciton, precise electronic structure.	High accuracy, overcomes the band gap problem of GGA/LDA.	The computational cost is very high, limited to very small systems (< 100 atoms).
MD (Classic - Tersoff/LJ)	Mechanics, thermodynamics, physical dynamics	Simulate large systems (millions of atoms) and long times (ns).	Cannot describe chemical reactions. Accuracy depends on interaction potential.
MD (Reaction - ReaxFF)	Reaction Kinetics, Oxidation/Reduction, Defects	Describe the breaking/forming of chemical bonds accurately.	Requires complex parameter tuning. More expensive than classical MD.
ML-Potentials	Mechanics, Heat, Reactions, Defects at Large Scale.		DFT level accuracy with MD level computation speed. Large DFT dataset required for training

To overcome these limitations and expand the applications of DFT and MD, several future research directions have been proposed:

-Development of more accurate reactive force fields or the application of machine learning-based methods (ML-based force fields) will enable more efficient simulations of complex chemical processes, including oxidation, reduction, doping, and catalytic reactions on 2D materials [65].

-Multiscale modeling approaches that combine DFT, MD, and continuum or coarse-grained MD can help predict mechanical, thermal, electrical, and chemical properties of materials under realistic conditions.

-Extension to realistic environmental conditions, including temperature, pressure, ionic solutions, or mixed gases, will improve the evaluation of materials for applications such as sensors, batteries, and catalysis.

-Integration of artificial intelligence (AI) and machine learning (ML) with MD and DFT can help predict forces and material properties based on existing data, accelerate simulations, and scale up research [66].

These strategies are expected to accelerate the discovery of new 2D materials and complex heterostructures, thereby narrowing the gap between simulation and experiment and optimizing performance for high-tech applications.

Specific applications include:

-Generating accurate interaction potentials for 2D materials and simulating thermal transport or defect kinetics at large scales (millions of atoms) with DFT level accuracy, which classical MD cannot achieve.

-High throughput screening (HTS): Using DFT to screen thousands of candidate 2D materials from large databases, predicting new stable materials with desirable band gaps for electronic and photonic applications. HTS accelerates the 2D material discovery cycle.

-DFT–MD hybrid/multiscale methods: Hybrid approaches are emerging as an essential trend to overcome the size and timescale limitations of standalone DFT or MD.

-Ab initio MD (AIMD): Forces are computed directly from DFT during MD simulations. For example, AIMD can capture the exact chemical reaction mechanism in the initial oxidation of MoS_2, which ReaxFF may not describe accurately.

-MD/continuum approaches: MD simulations of atomic-level processes, such as crack propagation, can be transferred to continuum mechanics models to simulate larger-scale 2D materials, as discussed in the proposed research directions.

Funding: This work received no funding.

Data Availability Statement: The data that support the findings of this study are available from the corresponding authors upon reasonable request.

Competing interests: The authors declare that they have no competing interests.

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