

# Machine Learning-Assisted Performance Prediction and Design of MXene Materials

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**Abstract:** MXenes are not a single fixed material family, but a broad set of two-dimensional transition-metal carbides and nitrides. Their conductivity, hydrophilic surfaces, layered structure, and adjustable terminations explain why they are frequently studied for electrocatalysis, energy storage, and multifunctional devices. The same flexibility also makes their design difficult. Changing the metal element, carbide/nitride framework, surface group, defect state, interlayer environment, or heterointerface may alter the final property. Exhaustive trial-and-error experiments or one-by-one DFT calculations are therefore inefficient. In this setting, machine learning (ML) combined with density functional theory (DFT) offers a practical way to screen structures, estimate properties, and narrow the candidate space. Here, reported ML-assisted studies on MXene prediction and design are organized by target property and workflow. The electrocatalysis part covers adsorption free energies, overpotentials, catalytic activity, and complex active sites. The energy-storage part discusses capacity, voltage, capacitance, and electronic-structure descriptors. The later sections examine ML–DFT screening, graph neural networks, uncertainty quantification, active learning, and interpretability. The literature still shows several weak points: small curated datasets, inconsistent data standards, simplified treatment of mixed terminations and defects, and limited transfer across MXene systems. More realistic descriptors, standardized datasets, multi-target screening, interpretable models, and tighter experiment–ML–DFT feedback are needed.

**Keywords:** MXene; machine learning; density functional theory; electrocatalysis; electrochemical energy storage; high-throughput screening

## 1. Introduction

Energy research is being shaped by two practical pressures: reducing fossil-fuel dependence and storing intermittent renewable electricity. Wind and solar power have expanded quickly, but their output changes with weather and day-night cycles. This makes storage and conversion technologies central to low-carbon energy systems [1,2]. Better materials are needed not only for higher energy density, but also for faster transport, stable cycling, and efficient interfacial reactions.

Among the available technologies, electrochemical energy-storage and conversion systems, including lithium/sodium-ion batteries, supercapacitors, and electrocatalytic systems, are widely studied because they offer high conversion efficiency, rapid charge/discharge capability, and broad application potential [2–4]. The rapid growth of electric vehicles, renewable-energy utilization, and grid-scale storage has created stronger demand for electrode materials with higher energy density, faster ion/electron transport, and greater cycling stability [3,4]. These improvements ultimately depend on the coordinated optimization of intrinsic material structures and





interfacial properties, making the development of tunable high-performance electrode materials a core task in advancing electrochemical technologies [3–5].

Two-dimensional nanomaterials have become a major focus in energy-materials research because they offer high specific surface area, tunable electronic structures, and abundant surface active sites. MXenes are an emerging family of two-dimensional transition-metal carbides and nitrides. Since Naguib et al. first prepared  $\text{Ti}_3\text{C}_2$  two-dimensional nanocrystals by selectively etching  $\text{Ti}_3\text{AlC}_2$  [6], MXenes have attracted extensive interest. Subsequent studies expanded MXenes into a broad family with diverse compositions and structural forms and clarified their derivation from MAX phases, as well as the tunability of surface terminations, conductivity, and wettability [7]. Because MXenes combine rich compositional possibilities, adjustable surface terminations, and favorable interfacial chemistry, they show promise in energy storage, electrocatalysis, electromagnetic shielding, and multifunctional devices [3,8]. In storage and catalysis in particular, their metallic conductivity, hydrophilicity, and tunable interfacial structures give them distinct advantages for high-rate charge storage and multielectron transfer reactions [3,4,8]. Recent experimental work also illustrates the role of interfacial and electrode-structure engineering in MXene energy storage. Thalji et al. constructed a binder-free Ni–Fe sulfide@ $\text{Ti}_3\text{C}_2\text{T}_x$  hierarchical electrode by combining a conductive MXene scaffold with redox-active Ni–Fe sulfide. The electrode delivered a specific capacity of  $1693 \text{ C g}^{-1}$  at  $1 \text{ A g}^{-1}$  and retained 98.5% of its capacity after 15,000 cycles [9].

Despite this promise, MXene design and performance optimization remain challenging. MXenes have complex compositions and rich surface-termination chemistry; different combinations of transition metals, layer configurations, and terminal groups can strongly change their electronic structures and electrochemical behavior [3,7,8]. Interlayer-spacing regulation, defect distributions, and electrode-electrolyte interfacial interactions further increase the complexity of performance modulation [3,8]. For a material system controlled by multiple coupled factors, conventional optimization based on experience or one-factor-at-a-time trial and error often cannot deliver systematic performance improvement.

Theoretical calculations, especially density functional theory (DFT), have been central to understanding the electronic structures, adsorption behavior, and reaction mechanisms of MXenes. For example, studies of surface-termination stability, electrical conductivity, and hydrogen evolution reaction (HER) activity have shown that surface terminations and local electronic structures strongly affect the adsorption free energy of hydrogen intermediates ( $\text{H}^*$ ) and thus determine HER catalytic potential [4]. However, as the candidate space expands, screening every structure solely through first-principles calculations becomes limited by computational cost and time. When transition-metal combinations, surface-termination patterns, and single-atom doping are all considered, the number of candidate structures grows rapidly, making one-by-one DFT calculations inefficient and expensive. At the same time, open materials databases and high-throughput platforms represented by the Materials Project have provided a foundation for accumulating, sharing, and retrieving materials data, creating conditions for more efficient screening methods [10].

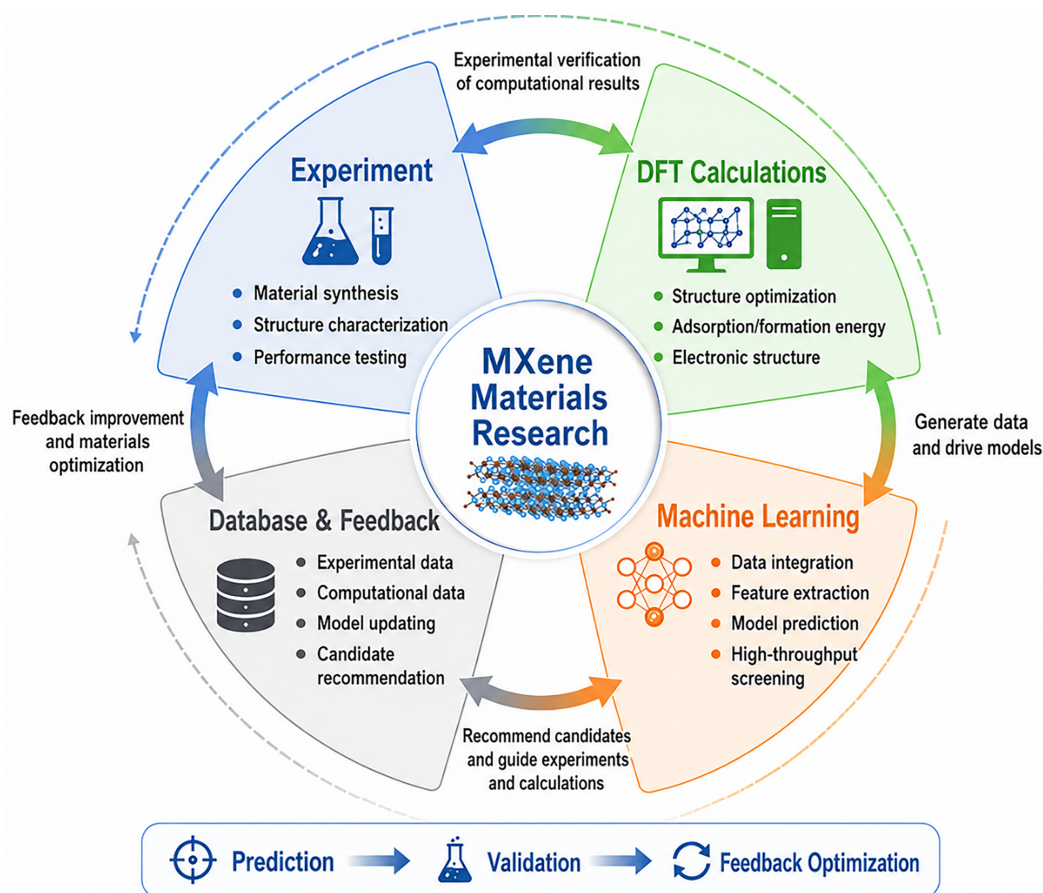
Open materials databases also make data-driven modeling more realistic. During the past decade, machine learning has moved from a supporting statistical tool to a regular part of materials discovery and performance optimization [11]. Data-driven materials science now links databases, high-throughput calculations, and artificial intelligence (AI) with conventional experimental and theoretical work [11]. Similar data-driven strategies are also being explored in other compositionally complex materials. For example, Al Zoubi et al. discussed ML-assisted studies of high-entropy multi-principal-element nanoparticles, in which compositional and structural information is used to relate phase formation and material properties. Their review also highlights the importance of data quality and experimental validation in ML-assisted materials design [12]. In catalysis, ML is often used for property prediction, descriptor selection, and catalyst screening, and it increasingly connects experimental observations with theoretical calculations [13]. For MXenes, this is especially useful because composition and interface chemistry are difficult to search manually. ML models can estimate adsorption energy, voltage, capacity, and related descriptors at relatively low cost, rank candidate structures, and point to structural variables that control performance [11,13].

However, although machine learning is advancing quickly in materials research, many specific materials systems still face limited data scale, inconsistent data sources, and weak model generalization [11,14]. The candidate-structure space may be vast, but the high cost of DFT calculations often restricts available high-quality datasets to only tens or hundreds of samples, creating a typical small-data regime. Related reviews have noted that many materials machine-learning tasks remain in this small-data stage, where data quality, data management, and modeling strategies suited to limited samples are decisive challenges [14]. This issue is especially pronounced for MXenes because the available data often depend on costly experiments or DFT calculations, and different studies use different structural settings, computational conditions, and target properties. Thus, building models with strong accuracy, generalization, and physical interpretability under limited-data conditions is now a central problem in ML-assisted MXene design [11,14].

As research has expanded from pristine MXenes to single-atom sites, heterostructures, and complex local active centers, materials design has also shifted from single-property prediction toward the joint optimization of stability, activity, and structural complexity. Studies of single-atom catalysis show that isolated metal atoms can improve atom utilization while providing tunable local coordination environments, opening new routes for catalytic-site design [15]. In MXene systems, this means that machine learning is no longer limited to predicting a single material property; it is increasingly being used for complex-structure screening, multi-objective optimization, and mechanism-oriented descriptor discovery [13,15].

Several recent reviews have discussed machine learning, artificial intelligence, and computational methods in MXene research from different perspectives. Gouveia et al. focused on first-principles calculations and ML for interpreting and predicting MXene structures and properties [16]. Irvani et al. provided a broader AI-oriented overview covering MXene synthesis and multiple application areas [17]. Saju et al. focused on MXene supercapacitors and ML-assisted performance prediction [18], whereas Dananjaya et al. discussed MXene composites, 3D/4D printing, and AI/ML integration [19]. Task-specific reviews have also discussed ML-assisted theoretical screening of HER electrocatalysts [20]. These reviews provide useful background, but they are mainly organized around computational methods, application areas, or specific device classes. Direct comparison across studies of the full workflow—from data source and material representation to model selection, validation, and materials screening—is less common. In addition, issues such as DFT-derived label errors, idealized surface models, model transferability, and experimental validation are not always discussed systematically across different MXene studies.

To address these gaps, this review is organized by prediction target and methodological workflow. We compare ML-assisted MXene studies in electrocatalysis, energy storage, electronic-property prediction, and high-throughput screening, with particular attention to ML–DFT integration, descriptors and structural representations, validation strategies, and model interpretability. We also examine the shift from single-property prediction toward multi-objective screening and materials design, and discuss how DFT error propagation, realistic surface chemistry, model transferability, and experimental validation affect prediction reliability. The aim is therefore not only to summarize reported ML applications, but also to compare the strengths and limitations of different workflows for MXene materials discovery. Figure 1 summarizes the links among experiments, DFT calculations, ML prediction, and validation.



**Figure 1.** Schematic illustration of the synergistic integration of experiments, DFT calculations, and machine learning in MXene materials research.

In this workflow, DFT provides training data and descriptors, ML screens a larger candidate space, and experiments test selected predictions. Lin et al. provide a representative MXene example [21]. They combined DFT calculations with ML screening to evaluate a large space of MXene-supported single-atom catalysts, identified an important descriptor through feature analysis, and experimentally tested selected candidates. The predicted  $\text{Mo}_2\text{CO}_2\text{-Zr}$  catalyst showed a Faradaic efficiency of 31.7% and an  $\text{NH}_3$  production rate of  $2.8 \mu\text{g h}^{-1} \text{mgcat}^{-1}$ . However, this workflow is not yet a fully closed loop because the experimental results were used mainly for validation and were not automatically returned to retrain the model or select candidates for the next screening cycle.

## 2. Research Progress in Machine Learning for MXene-Based Electrocatalytic Applications

This section focuses on how machine learning is being applied to MXene-based electrocatalysis. The discussion follows three linked topics: adsorption-free-energy prediction, overpotential and activity prediction, and the design of complex active sites. The aim is not only to list reported models, but also to show how ML is changing MXene electrocatalyst screening from empirical selection toward descriptor-guided design.

As two-dimensional materials databases expand and high-throughput calculations mature, machine learning is now an effective way to reduce the cost of large-scale screening. In MXene systems, rich compositional combinations and diverse surface terminations make the relationships among composition, termination, active sites, adsorption energies, overpotentials, and other properties highly nonlinear. Traditional trial-and-error experiments are inefficient for optimization, while large-scale DFT screening remains time- and resource-intensive. Machine learning may therefore accelerate the prediction of adsorption energies, reaction intermediate energies, overpotentials, and stability, enabling more efficient candidate screening [22,23].

MXenes provide metallic conductivity, adjustable surface terminations, and abundant surface sites, making them attractive candidates for several electrocatalytic reactions, including the hydrogen evolution reaction (HER), oxygen reduction reaction (ORR), oxygen evolution reaction (OER), and  $\text{CO}_2$  reduction reaction ( $\text{CO}_2\text{RR}$ ). In the ML literature, three tasks appear most often: predicting adsorption-related descriptors, estimating overpotential or overall activity, and screening more complicated sites such as single atoms, Janus surfaces, and heterostructures. These tasks are discussed below.

### 2.1. Prediction of Adsorption Free Energies and Reaction Intermediate Energies

In MXene-based electrocatalytic systems, reaction activity is largely determined by the ability of the catalyst surface to adsorb and activate key reaction intermediates. Because MXenes possess tunable transition-metal layer compositions, abundant surface termination groups, and diverse local active sites, their interfacial electronic structures are highly sensitive to composition, termination, and site selection, which in turn strongly affects the adsorption strength of reaction intermediates [22]. According to the Sabatier principle, an ideal catalyst should interact with key intermediates at an appropriate strength: overly strong adsorption may hinder subsequent desorption or conversion steps, whereas overly weak adsorption makes effective activation difficult. Accordingly, adsorption energies and their free-energy-corrected forms, such as adsorption free energies ( $\Delta G_{\text{ads}}$  or  $\Delta G_{\text{H}^*}$ ), are widely regarded as core descriptors linking the local electronic structure of MXenes with catalytic performance [24]. They also provide a key entry point for applying machine learning to MXene electrocatalyst screening and performance prediction.

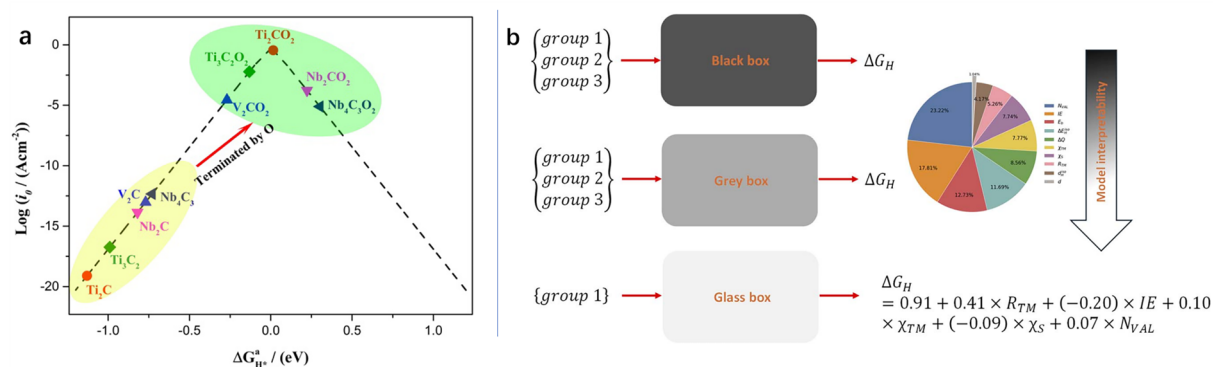
In existing machine-learning studies on MXene electrocatalysis, the prediction of adsorption free energies, represented by the hydrogen adsorption free energy ( $\Delta G_{\text{H}^*}$ ) in the hydrogen evolution reaction (HER), is one of the earliest and most typical applications [25,26]. Focusing on  $\Delta G_{\text{H}^*}$  as a classical descriptor, researchers have constructed MXene datasets covering different metal compositions, surface terminations, and site environments based on high-throughput DFT calculations, and have used machine learning models to rapidly screen candidate catalysts with moderate  $\text{H}^*$  adsorption strength [25,26]. Related studies have further extended HER activity prediction from pristine MXenes to non-metal-doped systems, showing that doping-induced local electronic structure reconstruction can significantly regulate  $\text{H}^*$  adsorption behavior [27]. This strategy has subsequently been extended to more complex reaction processes, such as key intermediate adsorption in  $\text{CO}_2$  activation [28] and the prediction of adsorption energies and related energetic quantities in the water–gas shift reaction [29]. These studies indicate that the role of machine learning in MXene systems is not limited to the prediction of a single  $\Delta G_{\text{H}^*}$  descriptor, but can be extended to adsorption free energy prediction in different catalytic reactions [30].

Most adsorption-energy models are trained on first-principles data. A typical study builds MXene surfaces with different metal compositions, terminations, and adsorption sites, calculates adsorption energies, and then applies zero-point-energy and entropy corrections to obtain  $\Delta G_{\text{ads}}$  or  $\Delta G_{\text{H}^*}$  [26–30]. These values are used as regression targets or activity descriptors. Because each DFT calculation is expensive, datasets often contain only tens to hundreds of structures. In that small-data regime, random forest [31], gradient boosting [32], support vector

regression, and kernel ridge regression often behave more robustly than deep neural networks [14]. Some studies also learn electronic information, such as the density of states directly [33].

Descriptor engineering is an important factor affecting the accuracy of adsorption energy prediction. For MXene systems, commonly used features can be grouped into three categories: intrinsic elemental properties, such as electronegativity, d-electron count, and atomic radius; structural parameters, such as coordination environment, bond length, adsorption site, and termination coverage; and electronic-structure indicators, such as work function, Fermi level, d-band center, and Bader charge. Among them, the d-band center theory provides an important physical framework for understanding adsorption behavior [22]. However, in multi-terminated MXenes or heterostructures, termination-induced charge redistribution and interfacial polarization may weaken simple linear correlations based on a single descriptor. Accordingly, recent studies tend to combine elemental, structural, and electronic features rather than relying on a single descriptor to evaluate adsorption behavior.

Interpretability is now a particularly useful part of adsorption-energy modeling [28]. Feature-importance ranking, Shapley additive explanations (SHAP) analysis, and partial-dependence plots help identify how electron transfer ability, local coordination, and surface termination affect  $\Delta G_{\text{ads}}$ . These tools are not a substitute for electronic-structure analysis, but they make the model output easier to connect with chemistry. For instance, a model may indicate that electronegativity differences, d-electron configuration, or charge redistribution around an active site are more influential than a simple composition label. Such information can guide the next round of DFT calculations or experiments instead of leaving the model as a black box. Figure 2a shows a volcano-type relationship between the HER exchange current density and hydrogen adsorption free energy ( $\Delta G_{\text{H}^*}$ ) for different MXene systems, illustrating the link between  $\text{H}^*$  adsorption strength and catalytic activity. Figure 2b shows an interpretable machine learning framework that transforms the traditional “black-box” model into a more transparent “glass-box” model.



**Figure 2.** Schematic illustration of adsorption free energy descriptors and interpretable machine learning modeling for MXenes. **(a)** Volcano-type relationship between exchange current density and hydrogen adsorption free energy ( $\Delta G_{\text{H}^*}$ ) in the MXene-catalyzed hydrogen evolution reaction. Reprinted with permission from ref. [4]. Copyright 2017 American Chemical Society. **(b)** HER activity prediction for MXene-based single-atom catalysts [34].

Adsorption free energy prediction is more than a numerical regression problem. It links electronic structure, surface adsorption, and catalytic activity in MXene catalyst design. After  $\Delta G_{\text{H}^*}$  or related descriptors are predicted, candidate materials can be ranked quickly, and structures with adsorption strengths close to the optimal range can be selected for additional DFT or experimental validation. The same workflow can also be extended to  $\text{CO}_2$  activation, water-gas shift reactions, and other processes involving multiple intermediates [35]. The limitation is clear as well: a single adsorption descriptor cannot fully describe reaction kinetics, active-site durability, or electrolyte effects. For this reason, adsorption-energy models should be read as an entry point rather than a complete activity assessment.

Adsorption free energy prediction remains one of the most useful starting points for ML in MXene electrocatalysis. Practical activity, however, also depends on overpotential, reaction pathways, site stability, mass transfer, and the real surface environment [36]. The next step is therefore to connect adsorption descriptors with broader activity indicators.

## 2.2. Prediction of Overpotential and Catalytic Activity

The intermediate adsorption free energy alone is not enough to evaluate actual electrocatalytic performance. More complete indicators include theoretical overpotential ( $\eta$ ), exchange current density, and limiting potential

(U<sub>L</sub>) [37,38]. ML studies on MXene electrocatalysis have therefore extended from  $\Delta G_{H^*}$  prediction to multistep activity estimation, especially for ORR and OER.

For ORR and OER, activity depends on the free-energy changes of several adsorbed intermediates, including OH\*, O\*, and OOH\* [37]. The computational hydrogen electrode model [23] converts these step energies into theoretical overpotentials, which can then be linked to catalyst composition and local structure. This is a harder learning problem than HER descriptor prediction because errors in several intermediate energies can accumulate in the final activity ranking.

From the perspective of research development, early machine learning studies on MXene electrocatalysis mainly focused on the prediction of  $\Delta G_{H^*}$  in HER [25], building on earlier studies linking exchange current density with catalyst activity [39]. Earlier studies showed that surface termination regulation could improve the HER activity of certain MXenes. Subsequently, machine learning models were used to expand DFT-based high-throughput screening [26], enabling rapid ranking and selection of candidate catalysts in a larger materials space [25–27]. In comparison, multi-intermediate reactions such as ORR and OER better demonstrate the importance of overall activity prediction, because these reactions require simultaneous consideration of multiple intermediate free energy changes, theoretical overpotentials, and bifunctional catalytic activity.

Currently, machine learning studies on ORR/OER bifunctional activity in MXene systems mainly involve design strategies based on heterostructures, Janus structures, and single-atom sites. Chen et al. studied 78 M–N<sub>4</sub>–Gr/MXene heterostructures and combined DFT calculations with a random forest model to predict ORR/OER overpotentials [40]. They screened Ni–N<sub>4</sub>–Gr/Nb<sub>2</sub>C, Ni–N<sub>4</sub>–Gr/V<sub>2</sub>C, Ru–N<sub>4</sub>–Gr/Nb<sub>2</sub>C, and Co–N<sub>4</sub>–Gr/V<sub>2</sub>C as candidate systems with excellent monofunctional or bifunctional activity, and identified charge transfer at the active center and the d-band center as important descriptors affecting catalytic performance [40]. Bai et al. further expanded the research scope to 153 MN<sub>4</sub>–Gra/M<sub>2</sub>NO heterostructures and constructed ORR/OER overpotential prediction models using gradient boosting regression, symbolic regression, and SHAP analysis. They found that CoN<sub>4</sub>–Gra/Ti<sub>2</sub>NO exhibited low ORR and OER overpotentials, indicating the distinct roles of the MXene side and the MN<sub>4</sub>–Gra side in bifunctional catalysis [41]. Similarly, Ma et al. developed an ORR/OER overpotential prediction model for Pt-doped dual-transition-metal Janus-MXene single-atom catalysts and screened Pt-VO–MnTiCO<sub>2</sub> and Pt-VO–PdTiCO<sub>2</sub> as low-overpotential candidates. Their results showed that OH\* adsorption, binding energy, and the d-band center of the Pt site are important factors affecting bifunctional activity [42].

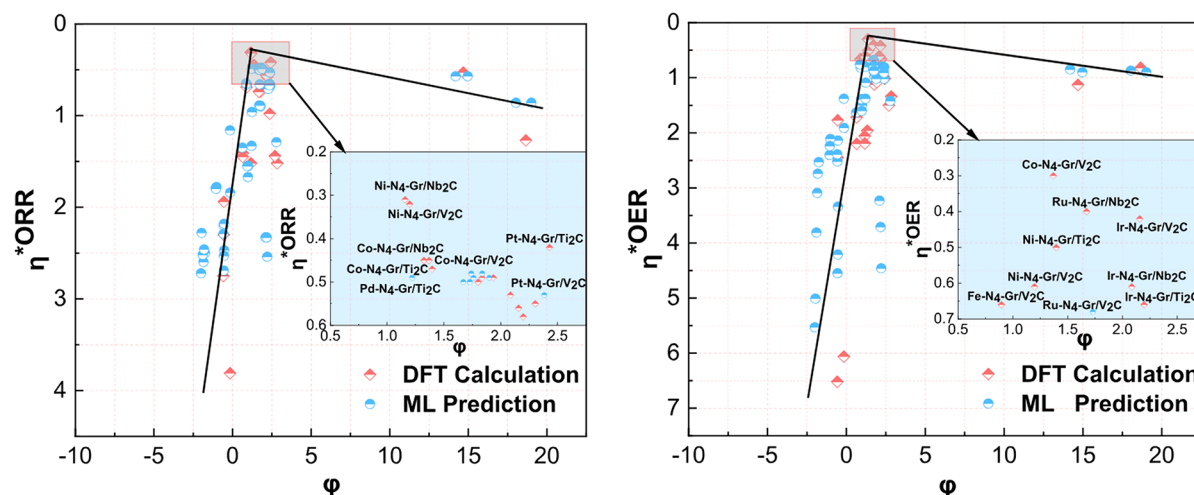
Beyond overpotential prediction for a single reaction system, machine learning has also been applied to the screening of bifunctional and even multifunctional catalysts. Anand et al. combined DFT calculations with machine learning to systematically screen large-scale single-atom-doped MXene combinations. They found that Ni-, Cu-, and Fe-doped systems showed the best performance for OER, ORR, and HER, respectively, and further proposed bifunctional and trifunctional candidate systems [43] for water splitting and metal–air batteries [44]. This study indicates that, when the research target expands from a single electrocatalytic reaction to the joint evaluation of multiple reactions, machine learning may not only be used for overpotential prediction, but also for comparing catalytic activity across different reactions and prioritizing candidate materials.

ML-assisted MXene electrocatalysis has also begun to extend to CO<sub>2</sub>RR. Wang et al. combined first-principles calculations with machine learning to study oxygen-vacancy- and transition-metal-doped M<sub>2</sub>CO<sub>2</sub> (M = V, Nb, and Ta) MXenes. Nb-doped Ta<sub>2</sub>CO<sub>2</sub> with dual oxygen vacancies was identified as a promising catalyst for CH<sub>4</sub> formation, with a limiting potential of –0.31 V. Feature analysis further identified the CO<sub>2</sub> adsorption Gibbs free energy and the transition-metal valence-electron count as important descriptors of CO<sub>2</sub>RR activity [45].

For HER,  $\Delta G_{H^*}$  close to 0 eV is a compact and useful descriptor. ORR and OER do not offer the same simplicity. They involve multiple intermediates, electron-transfer steps, and scaling relations, so the model has to connect local electronic structure with several adsorption energies and an overpotential target. In bifunctional screening, the compromise is even sharper: a candidate must satisfy ORR and OER requirements while remaining stable. That is why descriptor choice and multi-target evaluation matter more here than in a simple single-output regression task. As shown in Figure 3, the ORR and OER overpotentials show a typical volcano-type trend with the descriptor  $\phi$ , and high-activity catalytic systems with low overpotentials are distributed within a specific range of  $\phi$ . The DFT calculation and machine-learning prediction results are highly consistent, suggesting that reasonable physical descriptors can guide the model to identify high-activity regions and greatly improve the efficiency of catalyst screening and ranking.

Compared with single adsorption-energy prediction, overpotential prediction is closer to a practical activity assessment. The central issue is whether the chosen descriptors describe local electronic structure and the energetics of the key reaction steps. When they are too simplified, the model may rank candidates well inside the training set but fail on new surface structures.





**Figure 3.** Relationship between the intrinsic catalytic activity descriptor  $\phi$  and the theoretical ORR/OER overpotentials in MXene-based M–N<sub>4</sub>–Gr/MXene heterostructure catalysts. Red markers represent DFT-calculated results, blue circles represent machine-learning-predicted results, and the inset highlights the low-overpotential candidate region. Reprinted with permission from ref. [40]. Copyright 2023 American Chemical Society.

The broader use of ML for overpotential and activity prediction is valuable, but the present models still have narrow boundaries. ORR/OER datasets are usually small because each surface and intermediate configuration requires DFT work. Surface termination disorder, solvent effects, reconstruction of active sites, and electrolyte conditions [16] are also simplified in many datasets. A model may therefore rank ideal structures convincingly while giving weak guidance for experimental catalysts. More reliable activity prediction will require reaction-pathway information, stability constraints, uncertainty estimates, and validation outside the training family. Compared with HER and ORR/OER, however, ML-assisted studies of MXene CO<sub>2</sub>RR remain relatively limited, indicating that this direction is still at an earlier stage of data-driven development.

### 2.3. Machine-Learning-Based Design of Single-Atom and Heterostructured Catalysts

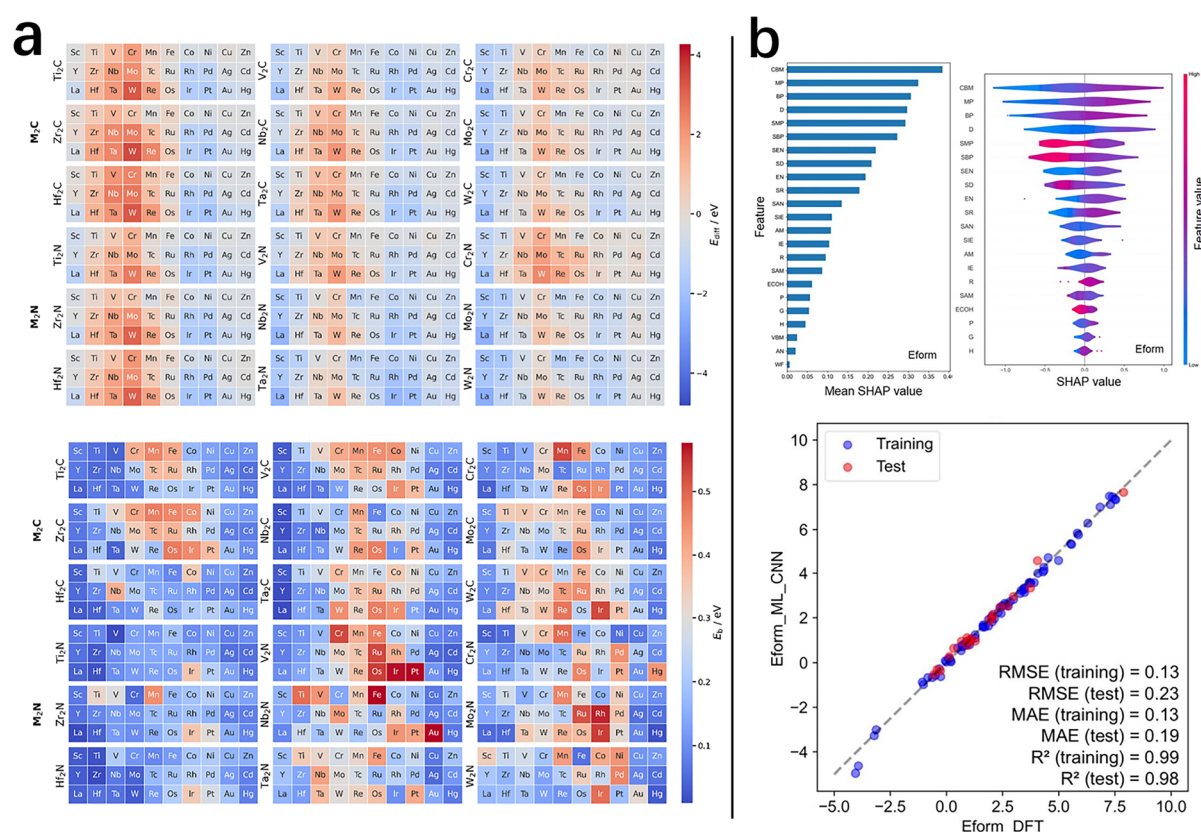
Composition control and termination tuning alone often cannot fully break adsorption-energy scaling relations [24]. For that reason, recent work has moved toward local active-site design, including single-atom catalysts (SACs), Janus MXenes, and heterostructures [15,40]. These structures create isolated metal centers, asymmetric electric fields, or interfacial coupling, each of which can reshape adsorption behavior [24]. They also multiply the number of possible structures.

Among these structural strategies, SAC@MXene systems are currently among the most representative research objects [15,34,46]. Their advantage lies not only in the highly dispersed active sites provided by isolated metal atoms, but also in the fact that the interaction between single atoms and the substrate can modify the local electronic structure, thereby potentially tuning the scaling relationships among different intermediate adsorption energies. Previous studies have shown that surface terminations and local defects are critical for the stable anchoring of single atoms [47,48]. This also indicates that, in single-atom design, the first issue to address is not catalytic activity itself, but whether the single atom can remain stable on the MXene surface [46,49]. Only when stability is ensured does further optimization and utilization of the local electronic structure become meaningful.

For SAC@MXene systems, stability is usually checked before activity. A common first screen compares the adsorption energy of a metal atom with its cohesive energy [49]; if aggregation is favored, the single-atom site is unlikely to be stable. DFT studies have also examined diffusion barriers, vacancy anchoring, and metal-support interactions [50]. ML models can learn from these quantities and quickly estimate which metal/support combinations are worth further testing. This is important because an active single atom is not useful if it migrates, clusters, or detaches under operating conditions.

Figure 4 illustrates the basic idea of machine learning-assisted stability evaluation and activity screening for SAC@MXene systems. At the computational screening level (Figure 4a), data-driven models can be used to predict the adsorption energies and diffusion barriers of different transition-metal single atoms on various MXene supports, and heat maps can be constructed accordingly to help identify candidate anchoring sites with strong adsorption and high diffusion barriers. As shown in Figure 4b, a convolutional neural network (CNN) model combined with SHAP feature analysis can be used to predict the formation energies of functionalized MXene single-atom catalysts. The model achieves a high coefficient of determination ( $R^2$ ) value on the test set, indicating

that it can reproduce DFT trends well. Meanwhile, SHAP analysis can identify the major structural features affecting formation energy, providing a reference for stability screening and subsequent activity optimization.



**Figure 4.** Schematic illustration of machine learning-assisted stability and activity co-design for MXene single-atom catalysts. (a) Diffusion barrier and binding energy maps of single metal atoms on MXene supports. Reproduced from ref. [49] under the terms of the CC BY-NC-ND 4.0 license. Copyright 2025 The Author(s). (b) SHAP feature importance and CNN-DFT prediction results for formation energy prediction of functionalized MXene single-atom catalysts. Reprinted with permission from ref. [46]. Copyright 2025 Royal Society of Chemistry.

After the preliminary stability issue is addressed, machine learning further enters the stage of activity evaluation and interpretable optimization [34]. For reactions such as HER, where catalytic performance is closely related to the adsorption of key intermediates, as well as ORR, OER, and CO<sub>2</sub>RR, which involve multiple intermediates, catalytic performance is usually affected by intermediate adsorption strength, electron transfer, and local coordination environment. Accordingly, activity modeling of SAC@MXene systems cannot remain at the level of a single descriptor, but needs to further identify local electronic-structure and coordination-environment factors closely related to activity. Based on DFT databases of MXene-based single-atom catalysts, previous studies have developed HER activity prediction models that rely only on simple features and do not require additional DFT post-processing. Building on this, interpretable models with explicit analytical expressions have gradually been developed [34]. These studies show that machine learning may not only shorten the screening cycle of candidate materials, but also extract physically meaningful activity-controlling factors, providing a more direct basis for early-stage experimental screening.

Beyond HER, machine learning applications in SAC@MXene systems have also begun to extend to more complex small-molecule activation scenarios. For example, in CO<sub>2</sub> activation, when transition-metal single atoms are supported on Mo<sub>2</sub>CO<sub>x</sub> and Ti<sub>2</sub>CO<sub>x</sub> surfaces [51], the metal-MXene interface affects CO<sub>2</sub> adsorption configurations, charge transfer pathways, and C–O bond cleavage barriers [50]. Related studies have further used machine learning models to predict adsorption energies and transition-state-related energies, indicating that the role of machine learning in complex single-atom systems is beginning to shift from the prediction of stable adsorption-state properties toward energy modeling closer to the reaction mechanism [50,51]. Compared with studies that focus only on final activity values, this type of work emphasizes the connection among interfacial charge transfer, key descriptors, and reaction mechanisms, thereby providing more specific mechanistic guidance for single-atom site design.

In addition to single-atom systems, Janus MXenes and heterostructures further expand the structural design space of MXenes. Because Janus structures have asymmetric terminations on the two surfaces, they can introduce built-in electric fields and asymmetric charge distributions within the material, thereby modifying the electronic environment of surface adsorption sites. Similarly, forming heterostructures between MXenes and other two-dimensional materials [41] can create new active regions through interfacial charge transfer, band alignment, and local strain effects. Notably, these studies can be regarded as complementary to the single-atom design route. Their focus is often more related to overall activity or bifunctional overpotential prediction, rather than single-atom stability and local site design itself [40–43]. Even so, these works still demonstrate that the core value of complex structural engineering lies in constructing suitable reaction environments, rather than passively screening the original MXene surface. Descriptor-based models can use elemental properties, coordination environments, vacancy information, charge descriptors, and adsorption energies. Graph-based models can represent the local environment more directly [33,52,53].

The design of single-atom, Janus, and heterostructured MXenes marks a shift from general property optimization to local active-site engineering. This direction requires fast screening, but it also needs physically meaningful descriptors. Accordingly, high predicted activity or a low theoretical overpotential should be treated as a screening signal, rather than as direct evidence that a catalyst is synthesizable or stable under operating conditions. For future work, the most useful models will be those that evaluate stability, activity, synthesizability, and interfacial structure together [46,54], rather than treating these factors as separate afterthoughts.

Comparison of the reported electrocatalytic studies shows that no single ML algorithm is optimal for all tasks. Chen et al. compared five regression models for ORR/OER overpotential prediction and found that random forest regression performed best, with root mean square error (RMSE) values of 0.10 and 0.23 V and  $R^2$  values of 0.92 and 0.80 for ORR and OER, respectively [40]. Bai et al. obtained the best predictive performance using gradient boosting regression, with test-set  $R^2$  values of 0.95 and 0.84 for ORR and OER, while symbolic regression gave lower accuracy but produced explicit analytical expressions that are easier to interpret [41]. These results show that tree-based ensemble models are effective at capturing nonlinear relationships in small-to-medium tabular datasets, but their performance still depends on descriptor quality and the chemical space covered by the training data. Simpler or symbolic models may give slightly lower accuracy but offer clearer physical interpretation. For example, Chowdhury et al. reported mean absolute error (MAE) values of about 0.13–0.14 eV for more complex ensemble models, whereas a simpler interpretable model achieved an MAE of about 0.17 eV using only readily available non-DFT features [34]. Therefore, model selection should depend on whether the main goal is predictive accuracy, interpretability, or rapid prescreening. Metrics such as  $R^2$ , RMSE, and MAE should also not be compared directly across studies without considering differences in dataset size, target definition, feature construction, and validation strategy.

### 3. Research Progress in Machine Learning for MXene-Based Energy-Storage Applications

In energy-storage studies, MXenes are attractive because their composition, layered structure, and O/OH/F terminations can all be tuned. These variables affect ion intercalation, charge storage, and interfacial reactions, and thus influence capacity, voltage, rate capability, and cycling stability. The challenge is that they rarely act alone. Surface chemistry, interlayer spacing, defects, flake size, and electrolyte environment may change at the same time. ML is valuable in this part of the field because it can relate such coupled variables to performance data and reduce the amount of blind screening [3,18,55].

Against this background, the following discussion considers three groups of ML applications in MXene energy storage: prediction of capacity, voltage, and capacitance; modeling of electronic-structure descriptors; and analysis of multiscale structural features such as terminations, defects, and interlayer environments.

#### 3.1. Prediction of Capacity, Specific Capacitance, and Operating Voltage

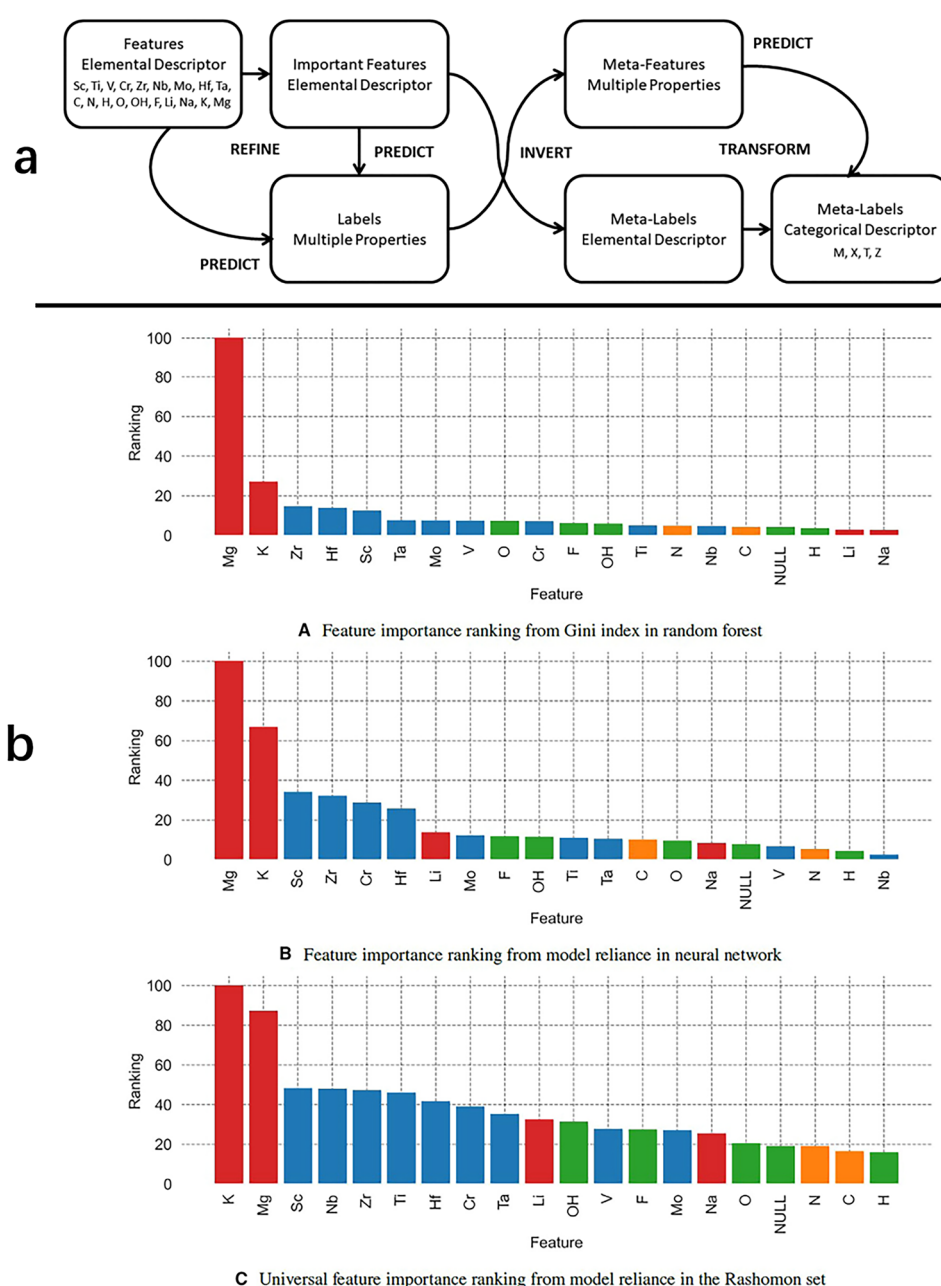
In energy storage research, capacity, voltage, and capacitance are important indicators for evaluating electrode materials. They reflect the energy storage capability, output potential characteristics, and charge storage ability of a material, respectively, and together determine its practical application potential. Because the composition, surface terminations, intercalated ion species, and interlayer structures of MXenes are highly tunable, their related properties are often jointly affected by multiple factors.

For battery-type energy storage materials, specific capacity and operating voltage are two of the most critical performance parameters. The former mainly depends on the number of reversibly intercalated ions, material composition, and charge transfer ability during intercalation, whereas the latter is closely related to the free energy change before and after ion intercalation. Previous first-principles-based global screening studies have shown that

different intercalated ions, transition-metal species, and surface terminations can significantly affect the capacity and voltage of MXenes. Among them,  $\text{Li}^+$  and  $\text{Mg}^{2+}$  usually lead to higher specific capacities than  $\text{Na}^+$  and  $\text{K}^+$ , while O-terminated and light-transition-metal systems often show better capacity and voltage performance [55]. These results indicate that MXene energy storage performance is jointly controlled by multiple structural and compositional factors, providing a basis for subsequent machine learning modeling of specific capacity and voltage.

Figure 5 uses battery-type MXenes to illustrate how multi-target ML and inverse design are usually organized. In the workflow, elemental descriptors are used to predict several targets at the same time, including voltage, theoretical capacity, and induced charge. The inverse-design step then searches for compositions that satisfy more than one requirement. The feature-importance analysis in Figure 5b shows why the model makes particular selections. Rather than only reporting a predicted capacity or voltage, the workflow links the prediction back to variables such as transition-metal identity, surface chemistry, and electronic structure.

Figure 5 also shows a useful shift in battery-type MXene research. The model is not asked to predict capacity alone; it combines performance prediction, stability assessment, electronic-structure classification, and composition search. This is closer to the real electrode-design problem. A material with high theoretical capacity is still unattractive if its voltage is unsuitable, its ion adsorption is unstable, or its structure changes too much during cycling. Multi-target models handle these trade-offs more explicitly than isolated capacity predictors [56].



**Figure 5.** Schematic illustration of machine learning-assisted multi-target prediction and key feature identification for battery-type MXene energy storage materials. (a) Multi-target machine learning and inverse design workflow for

MXene energy storage materials. Adapted with permission from ref. [56]. Copyright 2022 American Chemical Society. (b) Feature importance ranking results based on random forest, neural networks, and the Rashomon set [57].

Different from battery-type ion intercalation storage, supercapacitors usually involve both electric double-layer capacitance and pseudocapacitance. The former mainly originates from interfacial charge separation, whereas the latter arises from fast surface redox reactions. Accordingly, the modeling target is no longer limited to ion intercalation thermodynamics, but involves multiple factors such as surface active sites, charge density distribution, electronic conductivity, and ion adsorption ability. Classical studies have shown that MXenes can exhibit pronounced pseudocapacitive charge storage behavior, and that their high-rate electrochemical performance is closely related to the accessibility of ions to active sites in the electrode structure. For example, Lukatskaya et al. found that, by constructing electrode structures more favorable for ion transport,  $\text{Ti}_3\text{C}_2\text{T}_x$ -based MXenes could maintain high specific capacitance even at high scan rates, while hydrogel-type electrodes could achieve very high volumetric capacitance [58]. This indicates that, for MXene supercapacitors, capacitance behavior cannot be simply attributed to a single adsorption process, but requires simultaneous consideration of surface redox reactions, electron/ion transport, and electrode structure design.

For the screening of MXene pseudocapacitive materials, Wang et al. conducted a structured study based on a dataset of 600 MXenes. The dataset covered  $\text{M}_2\text{XT}_2$  ( $\text{T} = \text{bare}, \text{O}, \text{S}$ ) and doped systems, all obtained from individual DFT calculations to ensure consistency of the training data. In terms of modeling method, the authors used sure independence screening and sparsifying operator (SISSO) to extract analytical descriptors for pseudocapacitance [59] and found that the key factors governing pseudocapacitive behavior differ under different termination conditions. For bare surfaces, ion adsorption strength and the density of states approximately 1.0 eV above the Fermi level play major roles. For surface-functionalized systems, factors such as electronegativity and heat capacity become more important [60]. The significance of this work lies in the fact that it not only enables rapid screening of pseudocapacitive materials, but also helps establish clearer structure–performance relationships under different termination conditions.

In addition to material-level screening of ideal MXenes, machine learning has also begun to enter performance prediction scenarios closer to practical devices. For example, in aluminum-ion batteries, Li et al. established a machine learning model for MXene cathode materials based on experimental data, which was used to predict battery state and initial discharge capacity. After correction with a small amount of  $\text{Ti}_2\text{C}$  data, the model successfully predicted the capacity and cycling performance of a new  $\text{Ti}_2\text{C}$  cathode [61]. This indicates that machine learning may not only screen theoretical materials spaces, but also combine limited experimental data to estimate the performance of new electrode materials in specific battery systems [61].

For supercapacitor composite electrodes, Shariq et al. used multiple linear regression, support vector regression, random forest, and artificial neural network models to predict in a structured way the specific capacitance, electrical conductivity, and sheet resistance of MXene/graphene nanosheet composite electrodes. The results showed that the artificial neural network performed best among these models and identified 20 wt% graphene nanosheets as the optimal composite ratio [62]. This work suggests that, when the research target is extended from ideal single-phase MXenes to realistic composite electrodes, machine learning may still effectively identify favorable composite schemes under the influence of multiple parameters, thereby improving the efficiency of materials design.

In addition, machine learning studies on supercapacitors also provide useful methodological references. Zhu et al. constructed a dataset based on hundreds of published papers and used an artificial neural network to predict the capacitance of carbon-based supercapacitors. Specific surface area, pore size, ID/IG ratio, nitrogen doping level, and voltage window were selected as input features. The results showed that artificial neural network (ANN) models outperformed linear regression and Lasso models [63]. Although this study was not focused on MXenes, it demonstrates that, in the absence of a unified large-scale database, constructing training datasets through literature data mining and combining them with machine learning for multi-factor performance modeling is a feasible route in supercapacitor research. This strategy also provides a useful reference for capacitance prediction in MXene systems.

Currently, machine learning studies on supercapacitors are gradually extending from initial performance prediction to long-term service-related indicators such as cycling stability. Although such studies are not limited to MXene systems, their methodological value is still relevant to MXene energy storage research. For example, one study integrated data from more than 400 published papers to establish a machine learning model for cycling stability and found that electrode type, material dimensionality, and testing conditions are important factors affecting capacitance retention [64]. This suggests that future machine learning modeling of MXene electrodes



should not remain limited to capacity or specific capacitance, but should further incorporate indicators closer to device applications, such as cycling life, rate capability, and practical testing conditions.

Taken together, ML studies on MXene energy storage have moved from isolated predictions of capacity, voltage, or capacitance toward joint modeling of several performance indicators. However, theoretical capacity or capacitance alone does not determine practical electrode performance. Electrode thickness and mass loading affect ion-transport distance and the accessibility of active material, while porosity and conductive-network formation influence both ion diffusion and electron transport [62,65]. Binder content can change electrode conductivity, mechanical integrity, and the fraction of electrochemically inactive mass [66]. Electrolyte accessibility and electrolyte choice further affect ion transport, interfacial reactions, and the usable electrochemical window [18]. Cycling protocol, current density, and other testing conditions can also change the measured performance and long-term stability [64]. Therefore, materials ranked highly by idealized theoretical capacity or capacitance may not retain the same ranking under practical electrode conditions. These factors should be considered when ML predictions are compared with experiments or used for device-oriented screening.

### 3.2. Modeling of Electronic-Structure-Related Properties

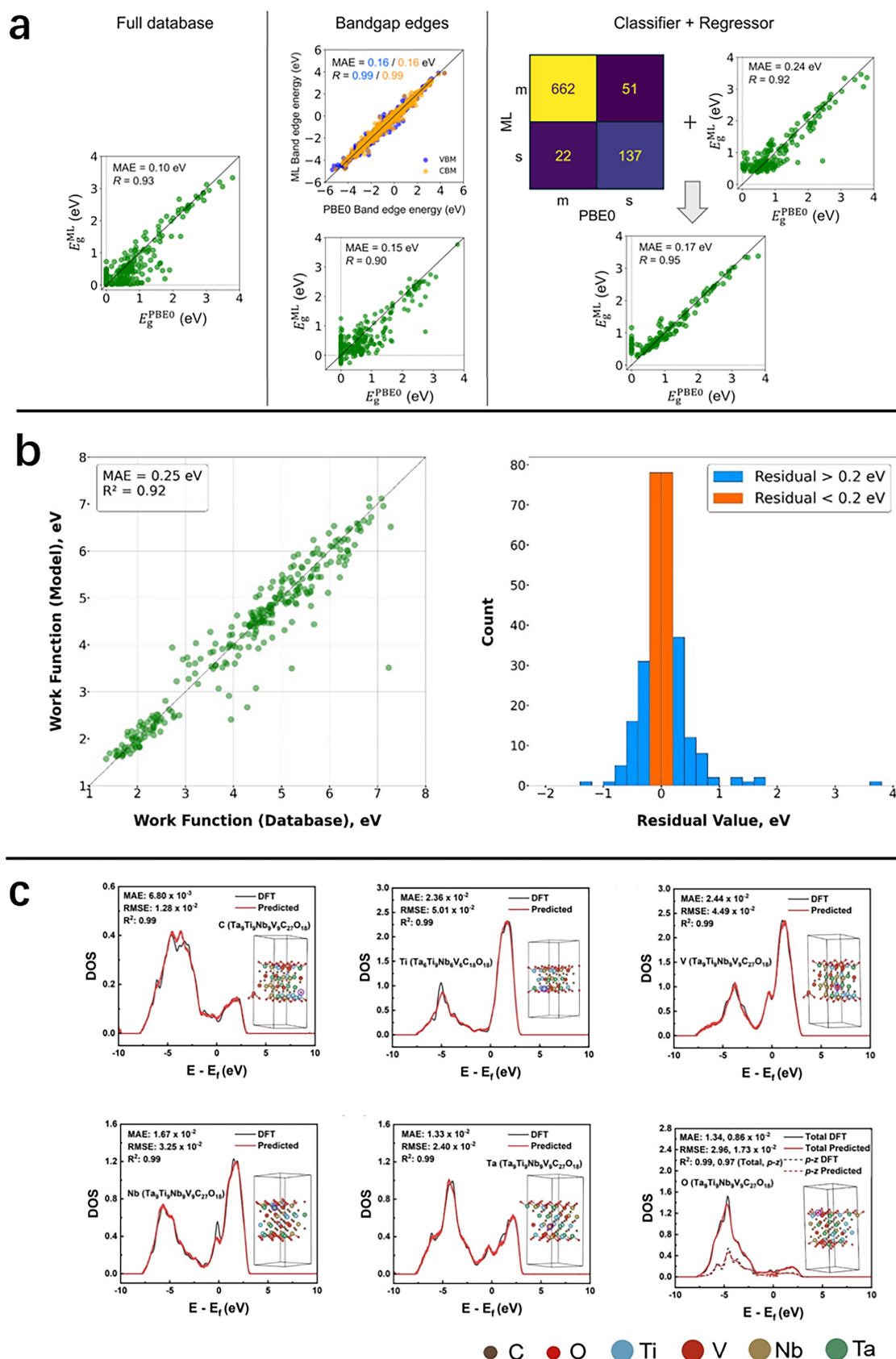
For MXene systems, electronic-structure parameters such as band gap, Fermi level, density of states (DOS), work function, and Bader charge not only reflect the intrinsic electrical conductivity and surface chemical activity of the material, but also further affect ion adsorption, interfacial charge transfer, and the thermodynamics of energy storage reactions. Accordingly, compared with directly predicting macroscopic properties only from composition or geometry, electronic-structure descriptors can help establish physically meaningful structure–performance relationships and provide a mechanistic framework for energy storage materials design. Previous systematic studies based on hybrid density functional theory have shown that the electronic properties of functionalized  $\text{Ti}_{n+1}\text{X}_n$  ( $\text{X} = \text{C}, \text{N}$ ) MXenes are highly sensitive to surface termination type and layer thickness. Different terminations can significantly change their metallicity, semiconducting character, and density of states near the Fermi level, with  $\text{Ti}_2\text{CO}_2$  predicted as one representative semiconducting MXene [67]. This indicates that, for MXene energy storage systems, electronic-structure parameters are not merely computational outputs, but important bases for understanding differences in conductivity, interfacial reactivity, and energy storage performance.

ML is now being used to predict electronic-structure parameters of MXenes directly, which makes it possible to build faster models for two-dimensional materials. Crystal graph convolutional neural networks (CGCNNs), for example, showed that material properties can be learned from graph representations of crystal structures [52]. Descriptor-based models such as those implemented in Magpie also demonstrated that composition and simple structural information can support property prediction in inorganic materials [68]. For functionalized MXenes, Rajan et al. used compositional and structural descriptors to predict band gaps and then screen semiconductor candidates [69]. Mishra et al. extended a similar idea to band-edge positioning [70,71]. Roy et al. further modeled MXene work functions using ML approaches [72].

To more clearly show the hierarchy of machine learning modeling for electronic structures, Figure 6 selects three representative prediction tasks: band gaps/band edges, work functions, and density of states. These tasks correspond to different levels of electronic-structure information, including electronic energy-level positions, interfacial charge transfer ability, and the full distribution of electronic states. Specifically, Figure 6a shows the classifier–regressor workflow used in the MXgap tool for band gap prediction of functionalized MXenes. This method first classifies MXenes as metallic or semiconducting, then performs band gap regression for semiconducting systems, and further supports screening related to band-edge positions and energy-level alignment. The results show that the model achieves an accuracy of 92% in metal/semiconductor classification and a mean absolute error of 0.17 eV in band gap prediction, indicating that machine learning may rapidly evaluate the electronic-structure characteristics of large-scale MXene candidate structures at relatively low computational cost.

Furthermore, for the work function, an important parameter affecting interfacial charge transfer and energy-level matching, Figure 6b shows the prediction results and residual distribution of machine learning models for MXene work functions. Roy et al. constructed a model based on MXene work function data from the Computational 2D Materials Database (C2DB), and the neural network model achieved a mean absolute error of 0.25 eV on the test set. Feature importance analysis further showed that properties such as the electronegativity of surface termination atoms strongly affect the work function. This indicates that machine learning may not only rapidly predict work functions, but also help identify key chemical factors regulating interfacial electronic properties.





**Figure 6.** Schematic illustration of machine learning-assisted MXene electronic-structure prediction and performance correlation. (a) Metal/semiconductor classification, band gap regression, and band-edge screening workflow in the MXgap tool. Adapted from ref. [73] under the terms of the CC BY 4.0 license. (b) MXene work function prediction results and residual distribution. Adapted from ref. [72] under the terms of the CC BY 4.0 license. (c) Comparison between graph neural network-predicted MXene density of states and DFT results. Adapted with permission from ref. [33]. Copyright 2024 Wiley-VCH GmbH.

To extend from single energy-level parameters to the full electronic-state distribution, Figure 6c compares the MXene density of states predicted by a graph neural network with DFT results. Related studies used a CGCNN model to predict the DOS of MXenes with complex compositions and further estimated Li adsorption energies based on the predicted DOS. This shows that DOS spectra can also be used as machine learning modeling targets [33] and can further support ion adsorption and energy storage performance prediction. Compared with predicting scalar properties such as band gap or work function alone, DOS prediction provides richer electronic-structure information and helps establish a continuous modeling pathway from atomic structure to electronic-state distribution and then to energy storage performance.

Figure 6 shows how electronic-structure quantities can move from being final DFT outputs to becoming intermediate variables in a design workflow. Band gap, Fermi level, density of states, band-edge position, work function, Bader charge, and d-band center can all act as descriptors for later performance models. For example, work function is related to interfacial charge transfer, and the density of states near the Fermi level is relevant to conductivity and catalytic or storage activity [74]. Once these quantities are predicted rapidly, they can be used to prescreen materials before detailed DFT calculations. The approach is useful, but it should be used carefully: electronic descriptors are sensitive to functional choice, surface termination, and structural relaxation, so inconsistent training data can easily weaken model transferability.

Electronic-structure modeling must also be paired with stability prediction. A favorable band structure or high theoretical capacity does not guarantee that an MXene can be synthesized or remain stable during operation. Quantities such as energy above the convex hull ( $E_{\text{hull}}$ ), formation energy, decomposition energy, phonon stability, and diffusion barriers help define this boundary. In high-throughput workflows, these stability descriptors are often used as filters before candidate materials are discussed as realistic electrodes [54,75–77].

The connection between electronic-structure descriptors and storage behavior is pushing MXene research from empirical tuning toward mechanism-guided design. Existing work shows that band gaps, band edges, work functions, density of states, and charge descriptors can be predicted and then used in downstream screening. In this setting, ML does two jobs at once: it accelerates calculation, and it helps identify which electronic variables are most relevant to the target performance.

Several practical barriers still remain. High-quality electronic-structure data are expensive, and public datasets are not yet large enough to cover the full range of MXene compositions, terminations, defects, and interlayer environments. Different studies may also use different exchange-correlation functionals, structural models, convergence criteria, and surface assumptions. These choices affect band gaps, work functions, and DOS features, so mixed datasets can introduce hidden bias. Even with a consistent computational protocol, DFT approximations, especially those related to the exchange-correlation functional, can introduce systematic errors into the calculated target properties [16]. When these DFT results are used as training labels, the ML model may inherit the same errors. A low prediction error against DFT data therefore shows mainly that the model reproduces the computational reference, rather than that it will achieve the same accuracy for experimental materials. This gap can become larger when real MXenes contain mixed terminations, defects, interlayer species, or other structural features that are not represented in the training data. Future studies should therefore report computational settings clearly, test model transferability beyond random data splits, and validate important candidates by independent DFT calculations or experiments [14].

In short, electronic-structure modeling helps MXene energy-storage research move beyond empirical trial-and-error. When combined with stability prediction and performance screening, it can support more mechanism-oriented design. The next challenge is to make these models robust for realistic surfaces, where mixed terminations, defects, intercalated ions, and disorder are common rather than exceptional.

### 3.3. Multiscale Structural Features and Their Effects on Energy Storage Performance

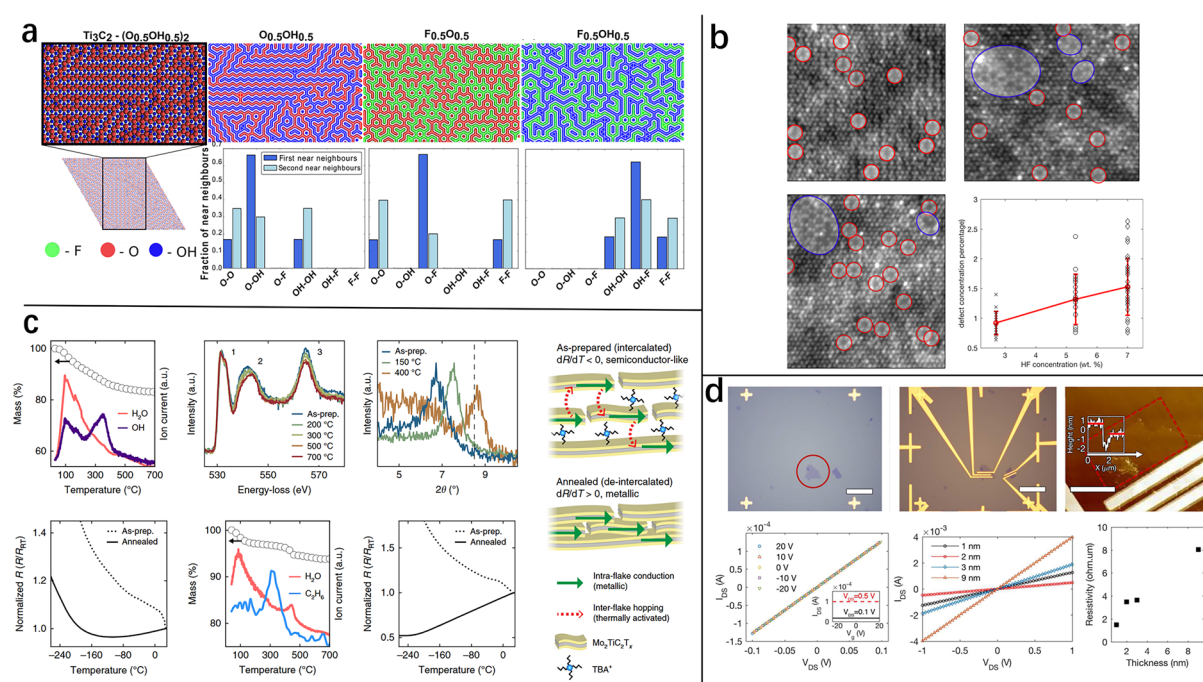
In energy storage systems, the electrochemical performance of MXene materials is not determined by a single structural factor, but is jointly affected by multiple factors, including interlayer spacing, surface terminations, defect distribution, intercalated ion species, and multiscale morphology [3,78–80]. Unlike electrocatalytic studies, which often focus on local active sites, MXene energy storage behavior involves a broader set of structural factors: different structural parameters often constrain one another and jointly influence ion diffusion, charge transfer, structural stability, and cycling life. Accordingly, identifying dominant factors from structural information and establishing interpretable structure–performance relationships have become important entry points for applying machine learning to MXene energy storage research.

Surface terminations strongly affect MXene structure and interfacial behavior [81]. Many simplified models treat -O, -OH, and -F as separate ideal variables, but real samples often contain mixed terminations. Ibragimova et

al. used multiscale thermodynamic simulations to show that O, OH, and F groups on  $\text{Ti}_3\text{C}_2\text{T}_x$  can form non-random distributions, and that neighboring functional groups influence local stability [78]. Hart et al. further showed that termination and intercalation regulate MXene electronic properties [80]. These results remind us that a single termination label is often too crude for realistic structure-property modeling.

Vibrational and spectroscopic studies give a similar message. Hu et al. compared bare  $\text{Ti}_3\text{C}_2$  with O-, F-, and OH-terminated  $\text{Ti}_3\text{C}_2\text{T}_2$  and showed that terminal atoms change lattice vibrations by modifying the valence-electron distribution of surface Ti atoms [82]. Sarycheva and Gogotsi emphasized that Raman spectra of  $\text{Ti}_3\text{C}_2\text{T}_x$  are influenced by terminations, intercalants, stacking, and defects [83]. Later *in situ* and ML-potential studies also connected termination chemistry and lattice dynamics with Raman or phonon features [84–86]. For ML models, these observations are useful because they connect measurable spectra with structural variables that are otherwise difficult to encode.

Figure 7 collects these multiscale factors in a single picture. Mixed O/OH/F terminations, vacancies, interlayer species, and flake thickness all affect the structural state of MXenes and the transport paths available to ions or electrons. This point is important for energy-storage modeling: the structure used in a DFT cell is often cleaner than the material tested in an electrode. A useful ML descriptor set should therefore include both atomic-level features and experimentally accessible morphology or processing information.



**Figure 7.** Schematic illustration of the effects of multiscale structural factors on the structural states and transport behavior of MXenes. (a) Spatial distribution and nearest-neighbor relationships of O, OH, and F mixed terminations on  $\text{Ti}_3\text{C}_2$  surfaces, reflecting the complexity of surface termination composition and arrangement. Adapted from ref. [78] under the terms of the CC BY license. (b) Atomic-scale structures of Ti vacancies and vacancy clusters in monolayer  $\text{Ti}_3\text{C}_2\text{T}_x$ , together with statistical results showing the dependence of defect concentration on etching conditions. Adapted with permission from ref. [79]. Copyright 2016 American Chemical Society. (c) Effects of annealing-induced de-intercalation on the resistance and transport behavior of MXene films. Adapted from ref. [80] under the terms of the CC BY 4.0 license. (d) Thickness-dependent electrical transport measurements of monolayer and few-layer  $\text{Ti}_3\text{C}_2\text{T}_x$  flake devices. Adapted with permission from ref. [79]. Copyright 2016 American Chemical Society.

The practical question is not how to optimize one structural parameter in isolation, but how to treat terminations, defects, intercalation, morphology, and local disorder together. This is where ML is useful. It can extract patterns from datasets that contain many coupled variables and then relate those patterns to transport, stability, and storage performance. Even so, the model inputs must reflect real MXene structures. A model trained only on ideal crystals may miss important effects caused by mixed terminations, vacancies, interlayer species, and structural disorder in experimentally prepared MXenes [78–80,87]. These features can change local coordination, charge distribution, adsorption behavior, and transport pathways. As a result, a model trained mainly on ideal structures may lose accuracy when applied to real surfaces outside its training distribution. Future descriptors should therefore include termination composition and arrangement, vacancy and defect information, interlayer

species, and local structural disorder. Graph-based or ensemble representations may be useful when these features cannot be described adequately by simple composition-based descriptors [87].

Building on this, Fang et al. further combined graph neural networks with Monte Carlo sampling to model ensemble properties of  $\text{Ti}_3\text{C}_2\text{T}_{2-x}$  systems containing O/F terminations and termination vacancies. They showed that electrical conductivity is sensitive to the local chemical environment and surface termination distribution. F terminations introduce both charge scattering and electron-filling effects, while termination vacancies further enhance scattering and reduce conductivity. In contrast, the optical response is more strongly related to the global composition of surface terminations [87]. This result is particularly informative for energy storage systems because it shows that structure–performance relationships in real materials cannot always be described by a single ideal configuration, but often need to be understood within a finite-temperature and disorder-ensemble-averaged framework. Accordingly, energy storage performance analysis should gradually move from an “ideal single-configuration” perspective toward “multi-configuration-based statistical screening”.

As research objects extend from ideal crystals to real surfaces and complex microscopic morphologies, the extraction of multiscale structural features is now another key issue in structure–performance modeling. Conventional statistical parameters, such as average roughness and root-mean-square roughness, usually reflect only the average surface fluctuation or local fluctuation amplitude, and are insufficient for fully describing structural differences across different length scales in surface morphology. Aglikov et al. introduced topological data analysis into the study of layer-by-layer assembled systems containing MXene components. By converting atomic force microscopy (AFM) data into persistence diagrams, they extracted roughness features at different length scales and structural differences along different directions that are difficult to capture using traditional statistical indicators, and combined these features with machine learning to identify structural parameters [88]. Although this work was not directly focused on the electrochemical performance of MXene energy storage electrodes, its methodology is informative. Machine learning may be used not only for performance prediction, but also for complex structural description, key information extraction, and simplified representation, thereby providing model input features for building higher-quality structure–performance relationships.

In practical MXene energy storage materials, multiple structural factors usually act simultaneously, and their effects often show strong correlations and nonlinear characteristics. The role of machine learning in such problems is to compare the relative contributions of different structural parameters to capacity, conductivity, rate capability, or cycling stability from multivariable data through feature importance analysis, SHAP values, or partial dependence plots. For example, changes in interlayer spacing can affect ion intercalation and transport, but beyond a certain range, structural stability may become the dominant factor. A moderate concentration of vacancy defects may improve ion diffusion and rate capability, whereas excessive defect concentration may damage cycling life. Mixed terminations can simultaneously change surface hydrophilicity, ion adsorption, and electronic transport. Compared with simple single-variable empirical judgment, data-driven methods are more suitable for describing such non-monotonic relationships and multifactor effects, thereby providing a basis for structural engineering optimization [60,87,88].

Recent studies have begun to combine machine learning analysis with physical models, shifting the study of structure–performance relationships from simple correlation analysis toward further verification of physical causes. For example, feature importance rankings obtained from machine learning may be combined with charge transfer analysis, vibrational mode analysis, and local electronic-structure features to screen physically meaningful key variables. Meanwhile, methods with analytical expression capability may help condense empirical patterns from complex data into more compact and interpretable structure–performance relationships [16,59,89]. Although this direction is still developing in MXene energy storage systems, its significance is clear: the goal of machine learning should not be limited to improving prediction accuracy, but should also serve the establishment of verifiable and transferable mechanistic understanding frameworks [14,16,60,87].

For experimental optimization, data-driven structure-performance analysis can connect synthesis conditions, characterization results, and measured electrochemical behavior. It helps evaluate candidate structures quickly and narrow the search space. It can also build a chain from preparation conditions to structural states and then to performance outcomes. This is useful only when the input data are recorded carefully; otherwise, the model may learn differences in testing protocol rather than real material effects.

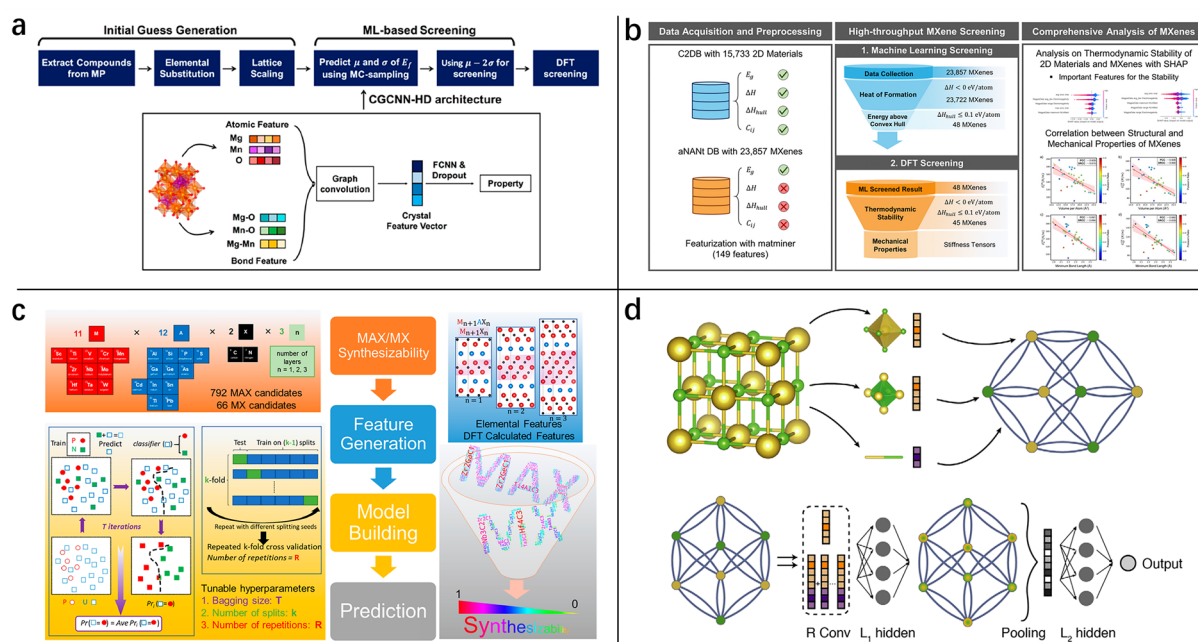
Real MXene energy-storage behavior is difficult to explain with a single structural descriptor. Surface terminations, defect states, interlayer spacing, flake morphology, and electrode architecture all contribute, and their effects are often coupled. ML provides a useful way to analyze these multilevel variables, but it should be paired with characterization and physical interpretation. Otherwise, the model may identify correlations that are statistically strong but chemically weak.

#### 4. ML–DFT Framework for High-Throughput Screening

Currently, the application of machine learning in MXene research has expanded from single-property prediction to large-scale candidate structure screening. The ML–DFT screening framework, which combines machine learning with first-principles calculations, can first use models to pre-screen large numbers of candidate structures and then use DFT to re-evaluate selected candidates. In this way, property prediction, stability evaluation, and candidate material screening can be integrated into a unified workflow [16,75].

A typical workflow starts by generating candidate structures and descriptors, then training a model on existing DFT or experimental data. The model is used to predict properties for a larger candidate pool. Promising or uncertain candidates are checked by DFT, and the new results can be added back to the dataset [90].

Figure 8 summarizes the practical modules often used in ML–DFT screening: ML prescreening, DFT re-evaluation, stability screening, synthesizability prediction, and crystal-graph representation. The figure should be read as a flexible toolkit rather than a fixed pipeline. Figure 8a shows an uncertainty-quantified ML–DFT screening workflow, in which a modified CGCNN model first narrows the candidate space and DFT calculations are then used for verification. Figure 8b illustrates ML-based screening of MXene chemical spaces using energetic and mechanical-property criteria. Figure 8c shows how positive-unlabeled learning can evaluate the synthesizability of MAX phases and MXenes when reliable negative samples are limited. Figure 8d presents the basic idea of crystal graph convolutional neural networks, where crystal structures are converted into graph representations for property prediction.



**Figure 8.** Representative methods in ML–DFT high-throughput screening and their applications in MXene materials discovery. **(a)** Uncertainty-quantified hybrid ML–DFT high-throughput screening workflow. Adapted with permission from ref. [90]. Copyright 2020 American Chemical Society. **(b)** Stability and mechanical property screening workflow for large-scale MXene chemical spaces. Adapted with permission from ref. [76]. Copyright 2024 Royal Society of Chemistry. **(c)** Positive-unlabeled learning framework for predicting the synthesizability of MAX phases and MXenes. Adapted with permission from ref. [54]. Copyright 2019 American Chemical Society. **(d)** Structural representation and property prediction process in crystal graph convolutional neural networks. Adapted with permission from ref. [52]. Copyright 2018 American Physical Society.

These screening strategies serve different purposes. Descriptor-based models are suitable for small to medium-sized datasets when meaningful compositional, structural, or electronic features can be defined. They are efficient and relatively easy to interpret, but their performance depends strongly on descriptor quality and may decrease when complex local environments are poorly represented [14,91]. Graph-based models such as CGCNN learn directly from atomic connectivity and local structural environments, making them useful for chemically and structurally diverse candidate spaces. However, they usually require more training data, so descriptor-based models may still be preferable for very small datasets [52,92]. Active learning is useful when new DFT calculations or experiments are costly because it selects informative or uncertain candidates for labeling and updates the model



iteratively. Its performance, however, depends on the acquisition strategy and the reliability of uncertainty estimates [14,90]. Automated machine learning (AutoML) can automate data preprocessing, model selection, and hyperparameter optimization, which is useful when many conventional models and parameter settings need to be compared. However, it cannot compensate for poor input representations or an inappropriate search space [91,93]. Therefore, the screening strategy should be selected according to dataset size, structural complexity, labeling cost, and the required level of validation.

To provide a direct comparison of representative ML-assisted MXene studies, Table 1 summarizes the MXene system, dataset size and source, descriptors or material representations, ML algorithms, prediction targets, validation strategies, and key outcomes. Table 1 also shows clear differences in dataset scale and validation practice among application areas. Electrocatalytic studies commonly use relatively small DFT-derived datasets, whereas some electronic-property and materials-screening studies use larger databases or candidate spaces. Reported  $R^2$ , MAE, and RMSE values should therefore be interpreted together with dataset size, chemical-space coverage, and validation strategy rather than compared directly across studies.

High prediction accuracy alone does not guarantee successful materials discovery. In the above workflow, target performance must be checked together with stability and synthesizability [94]. If the model searches only for high activity or high capacity, it may favor hypothetical structures that are unstable, mechanically weak, or difficult to prepare. This problem is especially visible for MXenes, where many proposed compositions look promising in property prediction but may fail precursor, termination, or stability constraints. Screening should therefore include formation energy, decomposition tendency, mechanical robustness, surface stability, and synthesis feasibility.

Crystal-structure-aware models such as CGCNN are attractive because they encode local atomic environments directly. For MXenes with mixed metals, defects, and surface groups, this representation can capture bonds and coordination environments more naturally than a hand-built descriptor table. The advantage is not automatic. When datasets are small or structural labels are inconsistent, a simpler model with clearer descriptors may generalize better. Model choice should be tied to data size, target property, and the structural diversity of the candidate pool [92].

Notably, MXene high-throughput screening does not always require complete crystal structure inputs or deep learning models. In many practical studies, structural model generation, feature engineering, and model selection still play important roles. For example, in a study on the metallophilicity of ordered five-atomic-layer MXenes, researchers generated large-scale metal adsorption systems using a high-throughput automated workflow, and combined structural descriptors, feature engineering, and AutoML model selection to systematically evaluate metal–MXene interactions [91]. This type of work shows that, for specific tasks, automated workflows, reasonable feature construction, and model search strategies can also form effective screening workflows, rather than relying on a single model type.

Model validation should match the intended use of the model. Random train–test splitting is useful for evaluating interpolation performance, but in small MXene datasets, closely related compositions or structures may appear in both subsets. A high test score therefore does not necessarily demonstrate transferability to unseen chemical or structural spaces [14,16]. K-fold cross-validation reduces the dependence on a single data split and provides a more stable estimate of internal model performance. More demanding tests, such as leave-one-metal, leave-one-substrate, or unseen-termination validation, can better evaluate transferability beyond the training domain [25,34,72]. External validation using independently generated DFT or experimental data provides a stronger test of generalization [14,16]. Therefore, studies intended for materials screening should distinguish internal predictive accuracy from transferability beyond the training distribution and, when possible, combine internal validation with independent external validation.

In addition to models themselves, databases and open-source toolchains are also important data and software foundations for implementing ML–DFT high-throughput screening. Databases such as the Materials Project, Open Quantum Materials Database (OQMD), and C2DB provide large-scale structural and property data, which can be used as data sources for model training, model testing, and candidate structure generation [10,95,96]. At the implementation level, pymatgen is useful for crystal structure processing, phase diagram construction, thermodynamic stability analysis, and access to Materials Project data, while matminer is useful for materials data retrieval, feature extraction, and machine learning modeling [97,98]. For MXenes, whose structures contain many tunable factors and whose target properties are diverse, the combination of open databases and open-source toolchains [99] helps form a reproducible workflow of “data acquisition–feature extraction–model training–result validation”.



**Table 1.** Comparison of representative machine-learning studies on MXene property prediction, screening, and materials design.

| MXene System                                                                                  | Dataset Size                                                           | Data Source                               | Descriptors/<br>Representation                                                                                                | ML Algorithm                                        | Prediction Target                                                        | Validation<br>Strategy/Metric                                                                                                                                                          | Key Outcomes                                                                                                                                                                                | Reference |
|-----------------------------------------------------------------------------------------------|------------------------------------------------------------------------|-------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------|--------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| <b>Electrocatalysis</b>                                                                       |                                                                        |                                           |                                                                                                                               |                                                     |                                                                          |                                                                                                                                                                                        |                                                                                                                                                                                             |           |
| Bare and S-terminated $M_{n+1}X_n$ MXenes                                                     | 132 DFT-labeled cases + 167 additional candidates screened (299 total) | DFT                                       | Simple elemental/structural descriptors; termination and atomic properties                                                    | Elman ANN; KRR; SVR; RFR                            | $\Delta G_{H^*}$                                                         | 100 repeated 75/25 splits; RFR test RMSE = $0.27 \pm 0.07$ eV; leave-one-chemical-group-out RMSE $\approx 0.35$ eV                                                                     | Eight candidates were initially identified; $Os_2B$ and S-terminated $Sc_{n+1}N_n$ remained active across higher H coverages.                                                               | [25]      |
| Single-atom catalysts supported on bare $M_2C$ MXenes                                         | 208 DFT-derived SAC samples                                            | New DFT dataset generated in the study    | 10 core tabulated/structural/SAC features, expanded to 16; final glass-box model used simple non-DFT features                 | LR; Ridge; LASSO; RF; ET; DT; GB; AdaBoost; XGBoost | $\Delta G_{H^*}$                                                         | 15% fixed external test set + 10-fold CV on the remaining 85%; leave-one-metal/support tests; complex models MAE $\approx 0.13 - 0.14$ eV; final interpretable model $\approx 0.17$ eV | A simple analytical model reached about 0.17 eV error using readily available features and was proposed for first-order screening of bare- $M_2C$ SACs.                                     | [34]      |
| M– $N_4$ –Gr/MXene heterostructures                                                           | 78 systems (28 DFT-labeled + 50 ML-predicted)                          | DFT                                       | 12 atomic, electronic, and local-environment features, including charge-transfer and d-band descriptors                       | GBR; RFR; GPR; KNR; SVR                             | ORR/OER overpotential                                                    | 3:1 train/test split + 4-fold CV; RFR $R^2 = 0.92/0.80$ and RMSE = $0.10/0.23$ V for ORR/OER; selected predictions rechecked by DFT                                                    | RFR performed best among the tested models and was used to screen Ni-, Ru-, and Co-based ORR/OER candidates.                                                                                | [40]      |
| MN <sub>4</sub> –Gra/ $M_2NO$ heterostructures                                                | 153 systems (19 DFT-labeled + 134 ML-predicted)                        | DFT                                       | Atomic intrinsic and local-environment features; feature-importance and SHAP analysis                                         | GBR; RFR; SVR; symbolic regression                  | ORR/OER overpotential                                                    | 90/10 split + DFT recheck; GBR test $R^2 = 0.95/0.84$ for ORR/OER                                                                                                                      | GBR gave the best predictive performance, while symbolic regression provided explicit relations for interpretation.                                                                         | [41]      |
| Pure and vacancy-containing MXenes                                                            | 114 samples (60 pure + 54 defective)                                   | Published DFT data + new DFT calculations | 18 physicochemical/electronic descriptors; $\epsilon_d$ , $\chi_M$ , and metal valence-electron count among the main features | MLR; DTR; RFR                                       | CO <sub>2</sub> adsorption energy, C–O length, O–C–O angle, Bader charge | 80/20 split with model tuning/CV; RFR test MAE for CO <sub>2</sub> adsorption energy = $0.42 \pm 0.06$ eV                                                                              | RFR identified d-band center, surface-metal electronegativity, and metal valence-electron count as important descriptors for CO <sub>2</sub> activation.                                    | [28]      |
| TM/A <sub>2</sub> -Ta <sub>2</sub> CO <sub>2</sub> with dual O vacancies and single-TM doping | 14 ML samples                                                          | First-principles calculations             | 15 intrinsic descriptors; LASSO retained 8, with $\Delta G(CO_2)$ and TM valence-electron count ranked highest                | GBR; ENR; KRR; RFR; XGBR; SVR; DTR                  | CO <sub>2</sub> RR limiting potential to CH <sub>4</sub>                 | Held-out testing only because $n = 14$ ; the paper reports GBR $R^2 = 0.999$ and RMSE = $0.010$ V. The very small dataset limits assessment of generalization.                         | Nb/A <sub>2</sub> -Ta <sub>2</sub> CO <sub>2</sub> gave $U_L = -0.31$ V for CH <sub>4</sub> formation; ML ranked $\Delta G(CO_2)$ and TM valence-electron count as the leading descriptors. | [45]      |

Table 1. Cont.

| MXene System                                                   | Dataset Size                                                                          | Data Source                                                 | Descriptors/<br>Representation                                                                            | ML Algorithm                                         | Prediction Target                                                                      | Validation<br>Strategy/Metric                                                                                                                                             | Key Outcomes                                                                                                                                                    | Reference |
|----------------------------------------------------------------|---------------------------------------------------------------------------------------|-------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------|------------------------------------------------------|----------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| <b>Electrocatalysis</b>                                        |                                                                                       |                                                             |                                                                                                           |                                                      |                                                                                        |                                                                                                                                                                           |                                                                                                                                                                 |           |
| MXene-supported single-atom catalysts                          | 3146 candidates screened; 228–281 DFT-labeled samples for each prediction target      | DFT labels + experimental validation of selected MXene-SACs | 18 structural/electronic descriptors; feature analysis yielded $\Delta E$                                 | Extra Trees                                          | NRR elementary-step $\Delta G$ values and $\Delta G_{H^*}$                             | 75/25 split; $R^2 \approx 0.71 - 0.76$ ; 10 synthesized MXene-SACs were experimentally tested                                                                             | ML narrowed a 3146-structure space and experiment tested 10 MXene-SACs; $Mo_2CO_2$ -Zr reached FE = 31.7% and an $NH_3$ rate of $2.8 \mu g h^{-1} mgcat^{-1}$ . | [21]      |
| <b>Energy storage</b>                                          |                                                                                       |                                                             |                                                                                                           |                                                      |                                                                                        |                                                                                                                                                                           |                                                                                                                                                                 |           |
| Li/Na/K/Mg-intercalated MXenes with H/O/OH/F/bare terminations | 360 DFT compounds                                                                     | Published DFT dataset                                       | 20-D elemental and 4-D categorical encodings; reduced after preprocessing                                 | Multi-target random forest regression/classification | Voltage, theoretical capacity, induced charge; inverse prediction of MXene composition | 80/20 train/test split with cross-validation; the 16-feature forward multi-target model gave MAE = 0.0257 and MSE = 0.0025 on normalized targets                          | The inverse model proposed $Li_2M_2C$ and $Mg_2M_2C$ ( $M = Sc, Ti, Cr$ ) for further study based on capacity, voltage, and induced charge.                     | [56]      |
| $M_2XT_2$ (bare/O/S) and doped MXenes                          | ~600 DFT candidates screened; 200 samples used in five SISSO subsets (21/73/17/17/72) | DFT calculations generated in the study                     | Ion binding, DOS near $E_F$ , work function, electronegativity, and related elemental/electronic features | SISSO                                                | Pseudocapacitance                                                                      | 500 repeated random 4:1 train/test splits; test error evaluated for the SISSO expressions                                                                                 | Separate analytical pseudocapacitance formulas were obtained for five MXene groups, with different controlling features across the groups.                      | [60]      |
| MXenes for anchoring Al–S battery intermediates                | ~600 DFT-labeled adsorption cases; ~5930 configurations screened                      | DFT                                                         | 105 initial descriptors; SelectKBest/ANOVA feature selection                                              | LS; PLS; Ridge; KRR; GBR; DTR; XGBR; RFR             | Adsorption energy/anchoring effect                                                     | Repeated 10-fold CV + LOOCV; XGBR test MAE $\approx 0.24$ eV                                                                                                              | The workflow identified 42 candidates with suitable anchoring, and O/F terminations were frequently favorable.                                                  | [100]     |
| $Ti_3C_2T_x$ /graphene-nanoplatelet composite electrodes       | 5 electrode compositions measured under multiple experimental conditions              | Experimental measurements                                   | GNP wt.%, potential window, scan rate, and electrode/operating variables                                  | MLR; SVR; RF; ANN                                    | Specific capacitance, sheet resistance, conductivity, cyclic retention                 | Experimental datasets were split 80/20; ANN performed best overall, with $R^2 \approx 0.79 - 0.95$ across specific-capacitance, sheet-resistance, and conductivity models | MG-80 delivered $226.6 F g^{-1}$ at $5 mV s^{-1}$ and retained 84.2% after 5000 cycles; ANN was then used to extrapolate cycling retention to 10,000 cycles.    | [62]      |

Table 1. Cont.

| MXene System                                                                                                                                                                         | Dataset Size                                                                                 | Data Source                                                                               | Descriptors/<br>Representation                                                                                      | ML Algorithm                                                                                         | Prediction Target                                                                           | Validation<br>Strategy/Metric                                                                                                                                                                       | Key Outcomes                                                                                                                                                                                | Reference |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| <b>Electronic properties &amp; materials screening</b>                                                                                                                               |                                                                                              |                                                                                           |                                                                                                                     |                                                                                                      |                                                                                             |                                                                                                                                                                                                     |                                                                                                                                                                                             |           |
| Diverse terminated MXenes; La-based MXenes used for a screening example                                                                                                              | 4356 PBE0-labeled structures + 396 La-based structures screened                              | PBE0 hybrid-DFT database + PBE0 rechecks                                                  | Periodic-table, structural/stacking/site, and electronic features                                                   | Classifier–regressor pipeline (GBC + RFR)                                                            | Metal/semiconductor or classification and band gap                                          | Internal test evaluation; classification accuracy = 92% and band-gap MAE = 0.17 eV; screened La-MXenes were rechecked with PBE0                                                                     | ML selected 14 La-based candidates for further checking; six satisfied the required water-splitting band alignment after PBE0 evaluation. The MXgap tool was released.                      | [73]      |
| M <sub>2</sub> X/M <sub>3</sub> X <sub>2</sub> /M <sub>4</sub> X <sub>3</sub> MXenes with O/F/OH/bare terminations; extension to Br/Cl/S/N/NH                                        | 275 C2DB samples + 40 new DFT samples; 315 after augmentation                                | C2DB + 40 new DFT calculations + Ti <sub>3</sub> C <sub>2</sub> experimental measurements | 15-feature model with reduced 10/8/5-feature versions; termination-related chemical descriptors were most important | Linear models; RF; NN; symbolic transformer                                                          | Work function                                                                               | 5-fold CV; 15-feature NN test MAE = 0.25 eV on the original set; transfer to 40 unseen-termination MXenes gave test MAE = 0.76 eV; retraining an 8-feature NN on 315 samples reduced MAE to 0.28 eV | The study showed strong termination dependence of work function and a clear loss of accuracy on unseen terminations; adding targeted DFT data improved transferability.                     | [72]      |
| Single-M MXenes and their MAX precursors                                                                                                                                             | 66 MXene candidates (10 known positive + 56 unlabeled); 792 MAX candidates                   | Experimental synthesis labels + elemental and DFT-derived data                            | Elemental plus structural, thermodynamic, and electronic features; PCA/feature selection                            | PU learning; transductive bagging with decision-tree base classifier; RESVM comparison               | Synthesizability score                                                                      | 10-fold CV/TPR evaluation on known positives; thermodynamic, elastic, and phase-stability checks plus comparison with experimental evidence                                                         | The model predicted 18 MXenes and 111 MAX phases as synthesizable and identified 20 high-ranking MAX/MXene precursor–product pairs.                                                         | [54]      |
| Broad stoichiometric and non-stoichiometric MXene chemical space                                                                                                                     | 15,733 C2DB materials for training + 23,857 MXenes in the aNANt database screened            | C2DB training labels + aNANt target database + DFT validation                             | 149 composition-based features generated with matminer                                                              | RF; LGBM; ET; DT; KNN for $\Delta H$ ; RF/LGBM/CatBoost ensemble voting for $\Delta H_{\text{hull}}$ | Thermodynamic stability ( $\Delta H$ , $\Delta H_{\text{hull}}$ ) and mechanical properties | 5-fold CV; ET for $\Delta H$ : $R^2 = 0.943$ , MAE = 0.103 eV atom <sup>-1</sup> , RMSE = 0.164 eV atom <sup>-1</sup> ; 45 final candidates were checked by DFT                                     | 48 ML-screened candidates; 45 DFT-confirmed, including 23 newly identified stable MXenes; mechanical robustness further evaluated.                                                          | [76]      |
| Termination-disordered Ti <sub>3</sub> C <sub>2</sub> O <sub>2-x</sub> F <sub>x</sub> and vacancy-containing Ti <sub>3</sub> C <sub>2</sub> O <sub>2-x-y</sub> F <sub>x</sub> MXenes | 1000 fully terminated O/F configurations + 2000 additional vacancy-containing configurations | High-throughput DFT + Wannier-based optical/transport calculations                        | Equivariant GNN; vacancy-aware persistent-homology features and virtual nodes for partially terminated structures   | Equivariant multi-task GNN + Monte Carlo                                                             | Energy, optical conductivity, electrical conductivity, ensemble properties                  | For the vacancy-containing dataset, $R^2 = 0.99/0.87/0.98$ and MAPE = 0.02%/3.48%/6.88% for energy/optical/electrical targets                                                                       | Monte Carlo sampling captured order–disorder effects; electrical conductivity was sensitive to local disorder, while optical conductivity mainly reflected overall termination composition. | [87]      |

Feature-importance analysis provides a global ranking of influential descriptors, but the result may depend on the fitted model and can be difficult to interpret when variables are correlated [101]. SHAP analysis provides feature contributions for individual predictions and can also be summarized globally, although correlated inputs may complicate feature attribution [89]. Partial-dependence plots show the average relationship between selected features and model outputs, but they can become difficult to interpret when multiple variables or interaction effects are involved. These methods are therefore complementary rather than interchangeable and should be combined with physical analysis when drawing mechanistic conclusions. These tools are useful because they turn a ranked list of candidates into design rules that can be checked by DFT, spectroscopy, or experiment.

Furthermore, the ML–DFT high-throughput screening framework also reflects the transition of materials design from experience-driven selection toward a process supported by databases, model prediction, and validation feedback. In this process, AutoML can reduce the dependence of model selection and hyperparameter tuning on researcher experience, thereby improving the efficiency and reproducibility of model construction. Positive-unlabeled learning is suitable for scenarios lacking complete negative labels and can help evaluate the potential synthesizability of candidate structures [102]. Although these methods are not exclusive to MXene systems, they are relatively compatible with common challenges in MXene research, such as small datasets, high-dimensional combinatorial spaces, and the scarcity of positive examples. Accordingly, they provide useful methodological references.

At the same time, ML–DFT high-throughput screening for MXenes is not developing in isolation, but is connected with methodological advances in computational catalysis and materials informatics [103]. Machine learning studies in heterogeneous catalysis have shown that dataset construction, descriptor selection, model training, high-throughput screening, and result interpretation [104] are important factors affecting the efficiency of catalyst design [13]. For MXene systems, the particular challenge lies in the simultaneous involvement of two-dimensional structures, surface terminations, defect states, and multiple application targets such as electrocatalysis and energy storage. Accordingly, it is especially necessary to combine databases, machine learning models, and first-principles calculations to form screening workflows that can simultaneously handle property prediction, stability evaluation, and candidate validation.

ML–DFT high-throughput screening is helping MXene research move from one-property prediction toward candidate discovery workflows. It also connects data collection, model prediction, candidate ranking, validation, and model updating. The main challenge is reliability: the screening result is only as strong as the dataset, structural representation, uncertainty estimate, and validation strategy behind it.

## 5. Extended Applications of Machine Learning in Non-Electrochemical MXene Research

ML appears most often in MXene electrocatalysis and energy-storage studies, but similar ideas are now being tested in mechanics, thermal transport, sensing, environmental remediation, and photocatalysis [105–117]. These fields use different targets and data sources, so a model built for adsorption energy cannot simply be transferred to, for example, a sensing signal or a membrane-flux task. The shared problem is still recognizable: MXenes have many adjustable structural variables, while experiments and calculations provide incomplete but useful observations.

In mechanical property research, machine learning has been used to predict the elastic modulus, strength, and compression behavior of MXenes and their composites. For MXene materials, the mechanical response depends not only on the transition-metal and C/N frameworks, but also on surface terminations, local bonding environments, and the stability of layered structures. Machine learning models can establish structure–mechanical property relationships based on high-throughput calculations or experimental data, and feature importance analysis can further identify structural or compositional features closely related to mechanical performance [105]. For MXene-based aerogels and composites, machine learning may also be used to establish relationships between component ratios, pore structural features, compressive modulus, and recovery behavior, providing guidance for optimizing composite ratios and pore structures [106]. Accordingly, in this direction, machine learning mainly contributes to rapid mechanical property prediction, candidate structure screening, and identification of key features affecting mechanical response.

In addition to mechanical properties, machine learning has also begun to be used in thermal and photoresponse-related studies of MXenes [107]. In thermal transport processes, surface terminations, asymmetric structures, and lattice anharmonicity can affect phonon propagation and lattice thermal conductivity. Machine learning potentials can simulate finite-temperature structural evolution and can be used to analyze thermal conductivity, phonon spectra, and anharmonic behavior [85]. In addition, machine learning has been applied to the design of MXene aerogels for thermal management and the structural optimization of solar absorbers [108,109]. These studies show that, in non-electrochemical scenarios, machine learning may be used not only to predict single

physical quantities, but also to analyze multivariable relationships among structural parameters, experimental conditions, and engineering performance.

ML is also useful for characterization signal analysis and multiscale structural information extraction. MXenes contain surface terminations, defects, interlayer stacking, and morphology variations, so signals from Raman spectra, microscopy, spectroscopy, or sensing arrays are often difficult to interpret by eye. Data-driven models can classify patterns, extract hidden features, and connect them with structural or performance differences. This role is different from property prediction, but it is equally relevant for understanding real MXene samples.

Environmental remediation and separation processes are also important non-electrochemical application directions for MXenes. Owing to their tunable interlayer channels and abundant surface functional groups, MXenes can be used in membrane separation, adsorption removal, and pollutant treatment. Recently, machine learning has been used for the structural design and global optimization of desalination MXene membranes. By establishing relationships between membrane structural parameters, water flux, and ion rejection, machine learning may help screen candidate membrane structures with favorable separation performance [110]. Similarly, in adsorption materials research, machine learning may help analyze experimental variables affecting dye removal efficiency in composite materials and predict adsorption performance [111]. These studies show that the role of machine learning in MXene environmental applications mainly lies in screening complex experimental variables, predicting performance, and optimizing structural parameters.

At the device level, MXene-ML work has expanded to intelligent sensing, biodetection, and healthcare-related applications [118]. MXenes are suitable for these platforms because of their conductivity, surface chemistry, and interfacial tunability. The data, however, are different from DFT property tables. Sensing signals are often multichannel, noisy, and affected by device fabrication or sample conditions. ML methods such as pattern recognition, feature extraction, and nonlinear classification are therefore used to separate target responses from background variation and interference [112–116].

In photocatalytic applications, machine learning and artificial intelligence methods have also begun to be used for performance prediction and candidate screening of MXene-based materials. Photocatalytic processes involve multiple factors, including light absorption, band positions, carrier separation, surface reaction sites, and reaction conditions. Accordingly, relying only on empirical judgment is insufficient for systematically comparing the effects of different MXene compositions and composite structures. Related reviews indicate that artificial intelligence methods are useful for data organization, performance prediction, reaction condition optimization, and candidate system screening in MXene-based photocatalytic materials [117]. Although this direction is still at an early stage, it shows that machine learning may also support multivariable performance analysis and material combination screening in non-electrochemical MXene applications.

To summarize these non-electrochemical applications more clearly, Table 2 compares representative studies in terms of the ML task, input data type, typical models or methods, current evidence and limitations, and representative references. The maturity of ML applications across these fields is not uniform. Mechanical-property studies include both high-throughput computational screening with interpretable descriptor discovery and experimental-data-based prediction [105,106], while sensing and biodetection studies have already incorporated multichannel experimental signals and real-sample validation [113–115]. Thermal, structural-characterization, and environmental applications use different approaches, including machine-learning potentials, image- or spectrum-based analysis, and optimization-assisted prediction, but most studies remain focused on specific materials or tasks [85,86,88,107,110,111]. The optical and photonic studies discussed here are largely simulation-driven [109], whereas MXene-specific ML studies in photocatalysis remain comparatively limited [117]. Neuromorphic work represents a distinct direction, in which MXene-based devices participate directly in learning or computing rather than serving only as materials whose properties are predicted by ML [119]. Overall, compared with electrocatalysis and energy storage, the main limitations of these non-electrochemical applications lie less in the availability of ML algorithms than in the lack of reusable datasets, standardized input representations, cross-system validation, and integrated prediction–validation–design workflows.

Compared with property prediction and sensing recognition, neuromorphic information processing places more emphasis on the dynamic response behavior of MXene-based devices. Some flexible MXene-based devices can exhibit synapse-like response characteristics during ion migration, adsorption, and desorption, making them useful for simulating information storage, adaptive learning, and pattern recognition processes [119]. In such studies, the role of machine learning is no longer limited to predicting material properties. Instead, it is combined with device output signals to identify dynamic response patterns and process complex signals. This indicates that machine learning research on MXenes is extending from material parameter prediction to device behavior analysis.



**Table 2.** Comparison of machine-learning tasks, input data, representative models/methods, and evidence across non-electrochemical MXene applications.

| Application Area                     | ML Task                                                                                                                                        | Input Data Type                                                                                                                                                                                             | Typical Models/Methods                                                                                                 | Evidence and Main Limitation                                                                                                                                                                                                                                | Representative References |
|--------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------|
| Mechanical properties                | Prediction of tensile stiffness and strength; prediction of compressive modulus; identification of key mechanical descriptors                  | High-throughput DFT mechanical-property data for 157 MXenes; literature-derived experimental composition and structural variables for Ti <sub>3</sub> C <sub>2</sub> -based aerogels                        | SISSO; ANN; SVM; RF                                                                                                    | High-throughput DFT/SISSO and small experimental-data models have both been reported. Current experimental datasets are small, and cross-system validation remains limited.                                                                                 | [105,106]                 |
| Thermal/thermophysical properties    | Finite-temperature phonon and lattice-thermal-conductivity modeling; surrogate prediction of dynamic viscosity                                 | First-principles MD energies, forces, and stresses for Mo <sub>2</sub> TiC <sub>2</sub> -related MXenes; experimental temperature, MXene concentration, and viscosity data for MXene–soybean-oil nanofluids | Moment tensor potential (MTP) + MD; Bayesian-optimized LSTM; MLP                                                       | ML potentials and experimental surrogate models have both been demonstrated, but each study is limited to a narrow MXene system and target property.                                                                                                        | [85,107]                  |
| Optical/photonic devices             | Surrogate prediction and geometry optimization of solar-absorber performance                                                                   | COMSOL-generated geometric parameters and spectral absorptance for a MXene/tungsten absorber design                                                                                                         | Neural-network regression (NNR/ANN)                                                                                    | The representative study is simulation-based and tied to one absorber architecture; independent experimental validation of the ML surrogate remains limited.                                                                                                | [109]                     |
| Structural characterization          | Finite-temperature/disorder-aware Raman simulation; AFM roughness analysis and bilayer-number recognition in LbL samples containing PEI/MXene  | DFT/MD configurations, force and Raman-related data for Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> ; AFM topography and TDA-derived multiscale roughness features from LbL polyelectrolyte samples       | ML force field + MD/RGDOS; TDA + supervised ML                                                                         | ML has been used to include disorder and temperature in Raman modeling and to classify multiscale AFM roughness. These workflows are specialized; the Aglikov study covers several LbL systems, only one of which contains MXene.                           | [86,88]                   |
| Environmental remediation/separation | Prediction and optimization of water flux and salt rejection; adsorption-capacity prediction and process-variable analysis                     | MD-derived membrane structural/operating variables; experimental adsorption variables such as m/v ratio, dosage, pH, dye concentration, and solution volume                                                 | RF; XGBoost; SHAP-assisted interpretation; PSO/GA optimization; bootstrap-assisted regression                          | Both simulation-driven optimization and experimental-data regression have been reported. Current models remain application-specific and have not demonstrated broad transfer across membrane or adsorbent families.                                         | [110,111]                 |
| Sensing/biodetection                 | Classification and quantitative analysis of gas, electrochemical, SERS, fluorescence, and colorimetric signals                                 | Experimental multichannel gas responses, volunteer breath samples, electrochemical/SERS spectra, smartphone RGB values, and real-sample measurements                                                        | ANN; SVM; RVM; pattern-recognition classifiers                                                                         | Multiple MXene sensors have been combined with ML and real-sample testing. Performance remains closely tied to device fabrication, sensing conditions, and the population represented in each dataset; cross-device transferability has rarely been tested. | [113–115]                 |
| Photocatalysis                       | AI/ML-assisted materials screening, performance prediction, process optimization, and decision-support concepts for MXene-based photocatalysis | Mixed computational and experimental photocatalytic descriptors discussed in review literature; limited MXene-specific primary ML datasets                                                                  | Supervised, unsupervised, reinforcement-learning, and deep-learning methods discussed mainly at review/framework level | MXene-specific primary ML studies remain limited. Much of the current evidence is methodological or review-based rather than based on standardized, reusable MXene-specific datasets and external validation.                                               | [117]                     |

## 6. Conclusions and Outlook

The combination of ML and first-principles calculations is now a practical strategy for MXene property prediction, structure screening, and candidate optimization. The reported targets already include adsorption free energy, overpotential, capacity, voltage, work function, thermal conductivity, and other quantities. Still, the field should be read with some caution. Many models are trained on small datasets, idealized structures, and narrowly defined application settings. These constraints limit how directly the predictions can guide experimental synthesis or device testing.

First, structural representation needs to move closer to real MXene material states. Many present models still use static descriptors such as composition, lattice parameters, termination type, and a few electronic-structure quantities. These inputs are useful, but they do not fully describe mixed terminations, defect disorder, interlayer intercalation, local reconstruction, or structural evolution during operation. Future models should combine graph representations, local coordination descriptors, electronic features, and morphology-related parameters. For energy storage, sensing, and environmental applications, variables such as interlayer spacing, pore structure, flake size, stacking state, and testing conditions should also be recorded.

Second, screening should move beyond single-property prediction. Many MXene studies still focus on one target, such as adsorption free energy, overpotential, capacity, or formation energy. Practical design is broader than that. Activity, stability, conductivity, synthesizability, cycling life, and cost often need to be considered together. For electrocatalysis, this means evaluating multistep reaction energetics, overpotential, and active-site stability rather than only one adsorption energy. For energy storage, theoretical capacity must be considered together with voltage, ion diffusion, structural stability, and cycling behavior.

Third, MXene datasets need better scale, quality, and comparability. The small-data problem is still common because experiments and DFT calculations are expensive. Different papers also use different structural models, computational settings, surface assumptions, and performance metrics, which makes data merging difficult. Future datasets should record composition, structure, computational details, experimental conditions, and target properties in a consistent way. Negative samples, unstable structures, and failed calculations should also be kept when possible, because they help models learn the boundary between promising and unrealistic candidates.

Fourth, ML should not remain a black-box ranking tool. For MXenes, whose surface chemistry and structure can be tuned in many ways, a candidate list alone gives limited guidance. SHAP analysis, feature-importance ranking [101], symbolic regression, physics-constrained models, and uncertainty quantification can help explain why a model makes a prediction. These explanations should then be checked against DFT electronic structures, spectroscopy, and experimental performance. This cross-checking is necessary if ML results are to become design rules rather than only numerical outputs.

Finally, the field needs a stronger feedback loop among experiments, calculations, and models. A common workflow still trains on existing data, predicts a candidate list, and validates only a few structures. The new results are not always returned to the training set in a planned way. Active learning and uncertainty sampling could make this process more efficient by choosing the next DFT calculations or experiments according to model uncertainty. Automated experiments and high-throughput characterization may eventually support such loops, but reproducible protocols and data standards must come first.

For MXene research, the main value of ML is not just saving DFT time. The more important contribution is pattern finding: extracting usable rules from complicated composition-structure-property data. If standardized datasets, realistic descriptors, multi-target optimization, interpretable models, and validation loops continue to improve, ML can become a more dependable tool for MXene design in electrocatalysis, energy storage, and multifunctional devices.

## Author Contributions

Q.L.: Conceptualization, Investigation, Visualization, Writing—original draft, Writing—review & editing; L.L.: Conceptualization, Supervision, Funding acquisition, Writing—review & editing; X.W.: Investigation, Writing—original draft, Writing—review; X.B.: Investigation, Writing—review & editing. All authors have read and agreed to the published version of the manuscript.

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### Institutional Review Board Statement

Not applicable.

### Informed Consent Statement

Not applicable.

### Data Availability Statement

This study is a review paper and does not generate new original data. All analyses are based on published literature, and relevant references have been adequately cited in the text.

### Conflicts of Interest

The authors declare no conflict of interest.

### Use of AI and AI-Assisted Technologies

During the preparation of this work, the authors used ChatGPT (OpenAI), DeepSeek, Gemini (Google), and Doubao (ByteDance), mainly for preliminary summarization and review of published literature, translation, and language editing to improve the clarity and readability of the manuscript.

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