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MXenes and artificial intelligence: fostering advancements in synthesis techniques and breakthroughs in applications

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This review explores the synergistic relationship between MXenes and artificial intelligence (AI), highlighting recent advancements in predicting and optimizing the properties, synthesis routes, and diverse applications of MXenes and their composites. MXenes possess fascinating characteristics that position them as promising candidates for a variety of technological applications, including energy storage, sensors/detectors, actuators, catalysis, and neuromorphic systems. The integration of AI methodologies provides a robust toolkit to tackle the complexities inherent in MXene research, facilitating property predictions and innovative applications. We discuss the challenges associated with the predictive capabilities for novel properties of MXenes and emphasize the necessity for sophisticated AI models to unravel the intricate relationships between structural features and material behaviors. Moreover, we examine the optimization of synthesis routes for MXenes through AI-driven approaches, underscoring the potential for streamlining and enhancing synthesis processes *via* data-driven insights. Furthermore, the role of AI is elucidated in enabling targeted applications of MXenes across multiple domains, illustrating the correlations between MXene properties and application performance. The synergistic integration of MXenes and AI marks the dawn of a new era in material design and innovation, with profound implications for advancing diverse technological frontiers.

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1. Introduction

In the realm of advanced materials, MXenes have emerged as fascinating two-dimensional (2D) phenomena, captivating the scientific community and holding the promise to transform industries (Fig. 1).[1] With their unique combination of extraordinary properties, MXenes have the potential to impact the newer developments in fields such as energy storage, (bio) electronics, catalysis, biomedicine, (bio)sensing, water treatment and soft robotics, among others.[2–5] Their exceptional electrical conductivity, combined with good mechanical strength, makes them suitable for flexible and wearable electronics.[6] MXenes are also renowned for their high thermal stability, which enables their integration into devices working under challenging temperature conditions.[7] Additionally, these materials exhibit exceptional electrochemical properties, making them ideal candidates for supercapacitors and batteries.[8] MXenes, encompassing carbides, nitrides, oxycarbides, and carbonitrides of early transition metals, like Ti, Nb, and Mo, stand out in the domain of 2D materials for various reasons.[9] These materials exhibit a broad spectrum of structures, ranging from 2 to 5 layers of early transition metal atoms (M elements) bonded by 1 to 4 layers of nonmetal atoms (X = C, N, O). This unique feature allows for the incorporation of multiple M metals in a single configuration, leading to ordered

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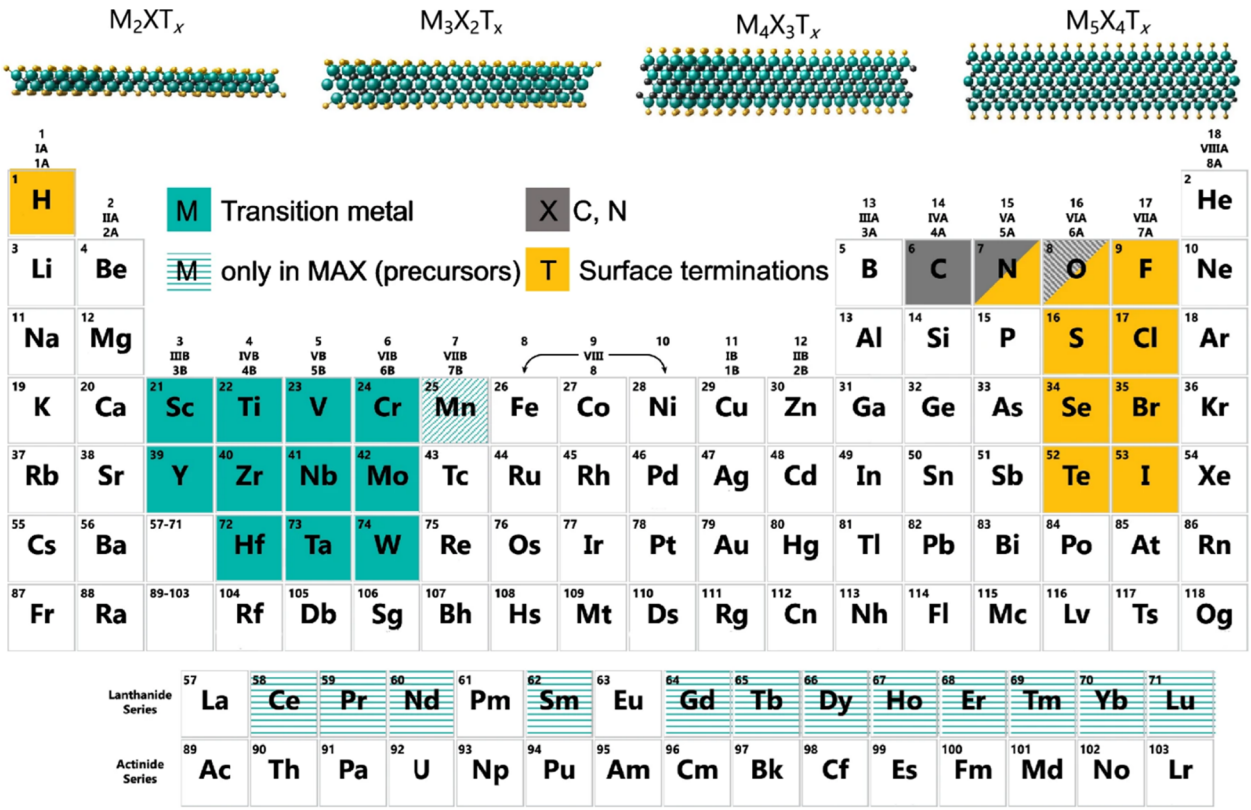

Fig. 1 The periodic table displays the elements employed in the synthesis of MXenes. Metals (M elements) are highlighted in green, nonmetals (X elements) in gray, and terminating elements (T) in dark yellow. Rare-earth elements, represented by striped backgrounds, may constitute components of in-plane ordered MAX structures. Elements with diagonal stripes are solely documented in MXene precursors (MAX phases). Oxygen is uniquely marked with gray diagonal stripes due to its involvement in the recently unveiled oxycarbide MXene. Reproduced with permission from ref. 1. Copyright 2022 Springer Nature.

in-plane and out-of-plane MXenes or random solid solutions. Noteworthy are the high-entropy MXenes, which can encompass 3 to 5 different metals. The hexagonal arrangement of MXenes mirrors a (111) slice of the bulk cubic carbide/nitride's cubic NaCl structure. Moreover, the surface terminations of MXenes exhibit a variety of elements such as chalcogens, oxygen, halogens, OH groups, and amines. Recent advancements have introduced antimony and phosphorus into this category, further expanding the versatility of MXenes in material science domain. The distinct characteristics and structural diversity of MXenes render them a fascinating area of exploration for researchers seeking novel materials with unique properties and innovative applications.[1,9]

Artificial intelligence (AI) technologies can be applied in the design and application of MXenes and their derivatives (Fig. 2). AI approaches, such as machine learning (ML) and deep learning (DL), can assist in the prediction and optimization of MXene synthesis parameters, allowing researchers to efficiently explore the synthesis conditions and maximize the yield and quality of ensued MXene-based materials.[10] In terms of applications, AI can aid in the characterization and understanding of MXenes through data analysis and modeling.[11] AI techniques are able to help analyze large datasets obtained from various characterization methods, such as electron microscopy and spectroscopy, to extract meaningful information and identify trends.[12] This can accelerate the discovery and design of new MXenes and their derivatives with desired properties for specific purposes, encompassing sensing, energy storage, catalysis, and electronics.[13]

AI techniques can aid in the development of accurate models that describe the behavior of MXenes in different environments and under varying conditions. These models can help predict and optimize the properties and performance of MXene-based materials, leading to improved device efficiency, durability, and functionality.[14] By leveraging AI algorithms for materials informatics, researchers are able to rapidly assess and predict the properties of a large number of MXene compositions and configurations (*e.g.*, electrochemical, thermophysical, electronic, and mechanical properties). This can significantly speed up the identification of promising MXene candidates for specific applications.[10,15,16] For instance, in one study, ML was employed to forecast the mechanical properties of MXene-based aerogels from a dataset comprising 540 potential inputs.[10] Another area where AI can contribute is in the process optimization of the synthesis and application domains of MXenes. AI algorithms help analyze experimental data and identify the optimal synthesis conditions, leading to improved efficiency and reproducibility in MXene synthesis. By learning from past experiments and adjusting parameters for subsequent syntheses, AI is capable of assisting researchers fine-tune

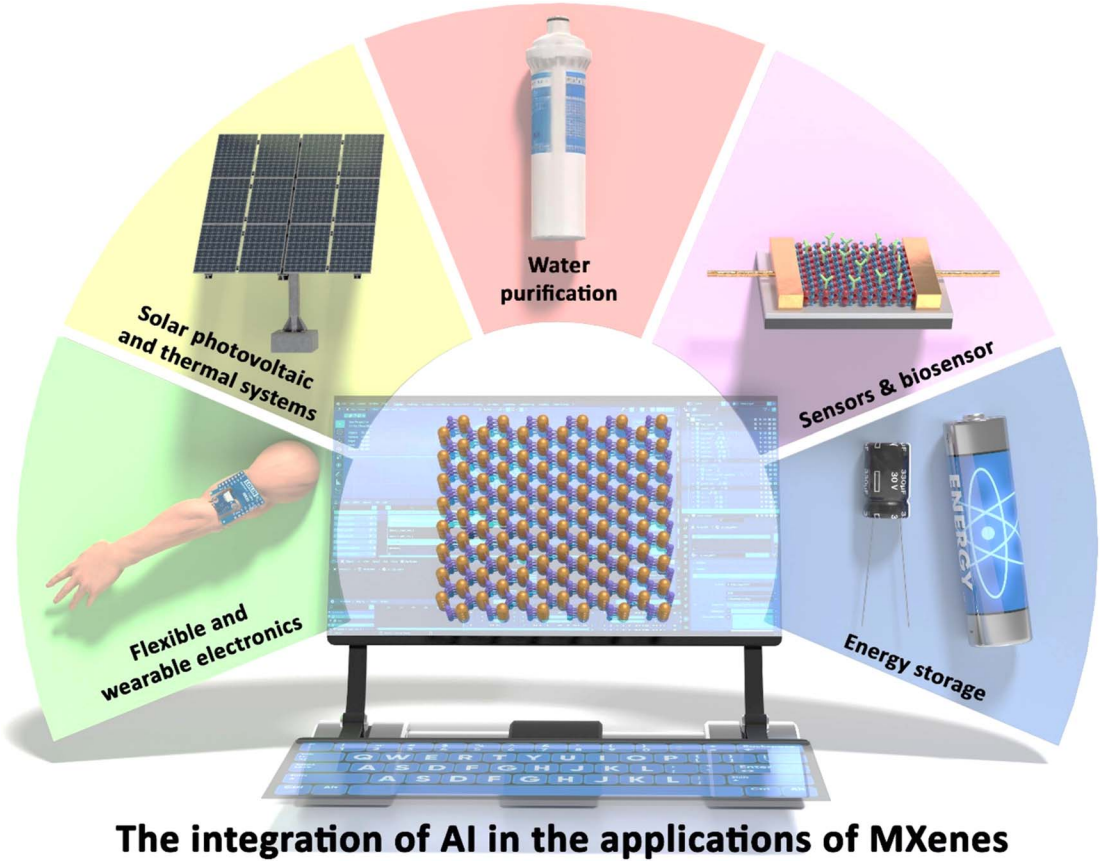

Fig. 2 The integration of AI in the applications of MXenes and their derivatives.

the synthesis process and achieve better control over MXene material properties.[17,18]

2. Recent advancements

AI techniques have ushered in a new era in the study of MXenes and their composites, offering innovative solutions to complex problems faced by chemists and physicists. Below, we delve into several specific AI methodologies and provide examples of their application in MXene research. ML stands at the forefront of AI applications in MXene systems. Researchers employ supervised and unsupervised learning techniques to analyze vast datasets of known materials. For instance, researchers can utilize a supervised ML model, like Random Forest (RF) or Support Vector Regression (SVR), to predict the stability and performance of various MXene compositions.[10,19] Multiple Linear Regression (MLR) is a statistical method used to model the relationship between a dependent variable and multiple independent variables by fitting a linear equation to the observed data. It is straightforward and interpretable, making it suitable for understanding the influence of various factors on a single outcome.[14] SVR is a type of ML model that uses support vector machines to perform regression tasks, focusing on finding a hyperplane that best fits the data while maintaining a margin of tolerance. This method is particularly effective in handling high-dimensional spaces and is robust to outliers.[20] RF is an ensemble learning technique that constructs multiple decision trees during training and outputs the average prediction for regression tasks, enhancing accuracy and controlling overfitting. Its ability to handle large datasets and provide feature importance makes it a popular choice for various applications.[10,19] Artificial Neural Networks (ANN) are computational models inspired by the human brain, consisting of interconnected nodes (neurons) that process information in layers. ANNs excel in capturing complex, non-linear relationships within data, making them highly effective for a wide range of regression and classification tasks.[21]

One of the most significant applications is AI-accelerated or AI-assisted *ab initio* simulations.[22] These techniques utilize AI algorithms to enhance the efficiency and accuracy of quantum mechanical calculations, allowing researchers to predict the electronic and structural properties of MXenes with unprecedented precision. By reducing computational time, AI enables the exploration of complex systems that would otherwise be infeasible. Notably, AI significantly contributes to molecular dynamics simulations, where it can optimize the simulation parameters and predict material behavior over time. For instance, ML potentials can be employed to model atomic interactions more accurately, resulting in more realistic simulations of MXene behavior under various conditions. This capability is crucial for understanding phenomena such as thermal stability and mechanical properties. In addition to

these applications, AI-assisted data mining and prediction from experimental data remain equally vital. By integrating AI methods, researchers can extract meaningful insights from vast datasets and identify correlations that might be overlooked through traditional analysis. This dual approach—combining theoretical simulations with AI-enhanced experimental data analysis—amplifies the potential to advance the understanding of MXenes and their applications in various fields.[10,19]

By training the model on existing MXene data, the algorithm can identify patterns and correlations that inform researchers about which combinations might yield the most promising results. Notably, DL has developed the way spectra are analyzed. Convolutional Neural Networks (CNNs) can process complex spectroscopic data, such as X-ray diffraction (XRD) patterns or Raman spectra, to classify different MXene phases. A practical example includes a study where researchers trained a CNN on a dataset of MXene spectra.[23] The model successfully identified specific MXene structures from raw spectral data, significantly reducing the time needed for manual interpretation and enhancing accuracy. Genetic Algorithms (GAs) mimic the process of natural selection to solve optimization problems. In the context of MXene synthesis, GAs can help researchers find optimal conditions such as temperature, time, and precursor concentrations.[24] For instance, a team of scientists might apply a GA to optimize the synthesis of a new MXene variant. By iteratively selecting the best-performing conditions and combining them, the GA can efficiently guide the experimental process toward achieving desired material properties. Natural Language Processing (NLP) is another AI technique gaining traction in materials science.[25] Researchers can use NLP algorithms to mine scientific literature for relevant information about MXenes, enabling them to stay updated on recent advancements and identify gaps in knowledge. For instance, an NLP tool can analyze thousands of research papers and extract key findings, trends, and experimental methods pertinent to MXenes.[25] This data can inform new research directions and foster collaboration among scientists. AI-based simulation and modeling tools can predict the behavior of MXenes under various conditions. For instance, Reinforcement Learning (RL) can optimize the design of MXene-based devices by simulating their performance in different scenarios.[26] A case study might involve using RL to fine-tune the parameters of a MXene supercapacitor. The algorithm learns from each simulation and gradually improves the device design to maximize energy density and charge–discharge rates.

2.1. AI and properties of MXenes

MXenes have emerged as key players in various applications like energy storage, catalysis, environmental solutions, nanoelectronics, among several others. While their exceptional electrical conductivity and electrochemical activity are well-recognized, their mechanical properties are equally vital across these applications, yet often overlooked by researchers.[15] One study focused on predicting the tensile stiffness and strength of 157 potential MXene structures and uncovered a diverse range of tensile stiffness values, spanning from 81.71 to 561.4 N m^{-1}.[15] Notably, 42 of the examined structures exhibited greater stiffness than both graphene and monolayers of transition metal dichalcogenides (TMDs). It was found that tensile strength is significantly affected by variables such as material thickness, the strength of the bonds, and the nature of surface terminations. Remarkably, surface terminations exhibited a remarkable impact on tensile stiffness, enhancing it by nearly 100%. Leveraging an interpretable ML method, the study formulated an analytical formula for tensile stiffness, incorporating efficient and easily interpretable descriptors for accurate predictions. The tensile strength was found to scale significantly with thickness and bond strength, with potential enhancements from surface terminations and bond strength variations. While most MXenes exhibited metallic properties, a few MXene semiconductors with moderate band gaps showcased superior mechanical properties relative to widely used monolayer semiconductor TMDs.[15] These findings demonstrated the promising potential of MXene semiconductors in advancing next-generation 2D nanoscale electronics, paving the way for innovative monolayer devices.

Different ML models, including MLR, SVR, RF, and ANN, have been created and contrasted to forecast specific capacitance, electrical conductivity, and sheet resistance for energy storage devices based on MXene/graphene nanoplatelets (Fig. 3).[14] The objective of these models was to analyze the influence of the weight percentage (wt%) of graphene nanoplatelets in MXene, the optimal potential window, and scan rates on the output characteristics. The datasets were derived from real-time output measurements obtained during experimental trials involving various weight ratios of graphene nanoplatelets in MXene. The ANN emerged as the top-performing model among those assessed, with MLR, SVR, and RF following suit. Both the experimental outcomes and those generated by the ANN underscored that the electrode incorporating 20 wt% graphene nanoplatelets in MXene (MG-80) displayed the highest specific capacitance, reaching 226.6 F g^{-1} at 5 mV s^{-1}, alongside remarkable long-term stability, preserving 84.2% capacity even after 5000 cycles. The ANN model accurately predicted the cyclic stability of the MG-80 electrode for up to 10 000 cycles, emphasizing the model's precision in the development of energy storage devices.[14]

The impact of synthesis parameters, encompassing temperature fluctuations from 303 to 343 K and nanofluid concentrations ranging from 0.1 to 0.4 wt%, was thoroughly examined on the thermophysical characteristics of MXene ionanofluids. The investigation focused on crucial properties like thermal conductivity, specific heat capacity, thermal stability, and viscosity. To delve into these properties, a Levenberg–Marquardt (LM)-based Artificial Neural Network (ANN) model and Response Surface Methodology (RSM) were deployed using experimental data.[21] Both the ANN and RSM strategies played pivotal roles in predicting the thermophysical behavior of MXene ionanofluids under optimized conditions. The ANN model was meticulously trained, tested, and validated with experimental data, showcasing high accuracy with R^2 values nearing 1 and a minimal prediction error of merely 2%. The LM-based back-propagation algorithm exhibited commendably low

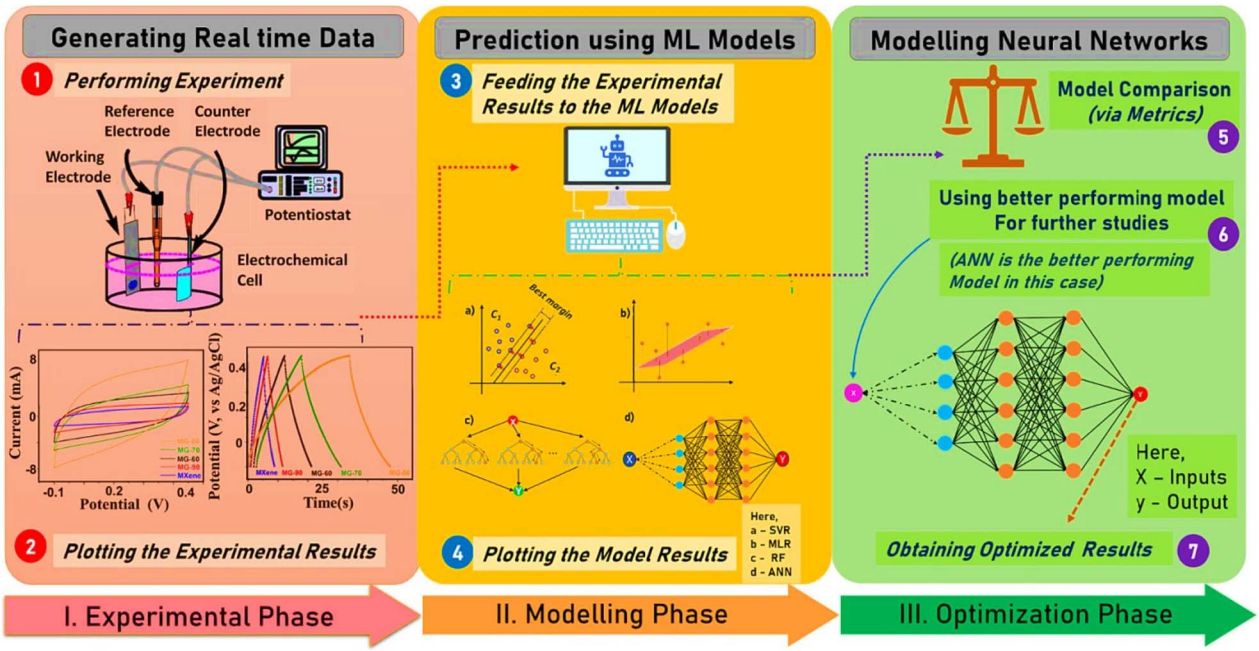

Fig. 3 A schematic representation of utilizing ML models to forecast electrochemical characteristics in supercapacitor electrodes with MXene and graphene nanoplatelets. Reproduced with permission from ref. 14. Copyright 2024 Elsevier.

error rates, ensuring the reliability of the predictions made. Meanwhile, RSM facilitated the establishment of relationships between input parameters and the thermophysical properties of MXene ionanofluids. By fine-tuning these parameters, MXene ionanofluids were tailored to showcase enhanced thermophysical properties, comprising a thermal conductivity of 0.776 W m^{-1} K^{-1}, a specific heat capacity of 2.5 J g^{-1} K^{-1}, thermal stability with a weight loss of 0.33931%, and a viscosity of 11.696 mPa s^{-1} at 343 K with a nanofluid concentration of 0.3 wt%. These optimized ionanofluids hold significant promise in boosting the efficiency of hybrid solar photovoltaic and thermal systems.[21]

He *et al.*[27] utilized ML methodologies and symbolic regression to explore material stabilities, with a specific focus on $A_{n+1}B_n$-type prototypical MXenes. Through the analysis of a limited dataset, various ML algorithms, including RF, K-Nearest Neighbors (KNN), Logistic Regression, Support Vector Machine (SVM), and Gaussian Naive Bayes (GaussianNB), were employed to assess the stabilities of MXenes. Among these algorithms, SVM offered the best accuracy to classify materials based on stability. Notably, symbolic regression was demonstrated as an effective approach for identifying relevant descriptors without labeling and formulating new descriptors that were linked to the stability of MXene materials.[27] This research underscores the effectiveness of ML and symbolic regression techniques in both material classification and stability description, showcasing their potential in material science research.

In terms of cytotoxicity of MXenes, studies have shown conflicting results.[28,29] Some research suggests that certain MXenes exhibit low cytotoxicity towards cells, making them promising candidates for biomedical applications. On the other hand, some studies have raised concerns about the potential cytotoxic effects of MXenes, especially at elevated concentrations. One of the critical factors influencing the cytotoxicity of MXenes is their surface chemistry. Functional groups on the surface of MXenes can interact with biological systems and impact cell viability. Additionally, the size and shape of MXene nanosheets play a role in determining their cytotoxic potential. *In vitro* assessments have been performed to analyze the cytotoxic effects of MXenes on different cell lines. These studies have shown that the cytotoxicity of MXenes can alter depending on the cell type, concentration, and exposure time. Furthermore, the mechanism of MXene-induced cytotoxicity is not fully understood and requires additional investigation.[30–33] A fraction of the rapidly expanding array of 2D materials undergo *in vitro* testing due to the time and cost involved in analysis.[34] ML techniques can be employed to extract fresh insights from existing biological datasets, offering guidance for experimental investigations. Marchwiany *et al.*[34] pinpointed the key surface-specific characteristics that potentially trigger cytotoxic reactions in 2D materials, particularly MXenes. Notably, the presence of transition metal oxides and lithium atoms on the surface were recognized as factors contributing to cytotoxicity. The developed ML model effectively forecasted toxicity levels for other untested MXenes, thus supplementing insights from traditional *in vitro* studies. This approach may reduce the necessity for extensive toxicological assessments and assist in mitigating setbacks in future biological applications.[34]

2.2. The integration of AI in the synthesis of MXenes

One of the commonly used methods to synthesize MXenes is the selective etching of MAX phases with hydrofluoric acid. The

process involves the removal of aluminum atoms from the MAX phase, followed by washing to obtain MXene flakes. By selecting different MAX phases and varying the delamination process, researchers can fabricate MXenes with tailored characteristics, opening up avenues for customization and optimization of material properties.[17,18,35] AI is able to play a vital role in accelerating the development of MXene-based composites and hybrid materials. AI algorithms are capable of predicting the compatibility and interactions between MXenes and other materials, thereby guiding the synthesis of MXene composites with optimized properties. This can lead to the development of MXene-based materials with enhanced mechanical strength, improved thermal stability, or tailored optical properties.

Frey and his team's studies open up exciting possibilities for the synthesis and exploration of advanced 2D materials with practical applications in various fields.[36] They delved into the realm of 2D materials using a cutting-edge positive-unlabeled (PU) ML framework. By leveraging elemental data and insights from extensive density functional theory calculations, they embarked on predicting the possibility of synthesizing proposed 2D materials. Their investigation centered around the MXene family, comprising 2D transition metal carbides, carbonitrides, and nitrides, in addition to their precursor materials known as MAX phases. Through the implementation of PU learning methodology, the researchers pinpointed 18 MXene compounds that exhibited high potential for synthesis. This meticulous analysis not only shed light on the promising MXenes but also extendible to their layered precursors. The study revealed 20 synthesizable MAX phases that could undergo chemical exfoliation to produce MXenes. Fig. 4 illustrates the computational framework and the PU learning algorithm.[36] PU learning emerged as a valuable tool in the realm of 2D material synthesis, offering a semi-supervised approach that tackles the complexities of understanding material creation. This method relied on utilizing positive data from experimentally synthesized materials while treating yet-to-be-synthesized materials as "unlabeled", presenting a unique framework for exploration. The initial phase of this exploration framework involved defining a comprehensive set of parameters, encompassing transition metal atoms, elements from the "A" group, and carbon or nitrogen atoms, among others. This meticulous process led to the identification of a substantial pool of potential candidates for single M MAX phases, which were further refined to 66 single M MXene candidates through a scrupulous selection process. To enhance computational efficiency, the researchers narrowed their focus to single M systems, excluding complex structures like solid solutions and ordered double transition metal configurations. This strategic decision aimed to prevent dataset imbalance and stabilize the PU learning models against overfitting the limited positive data available.

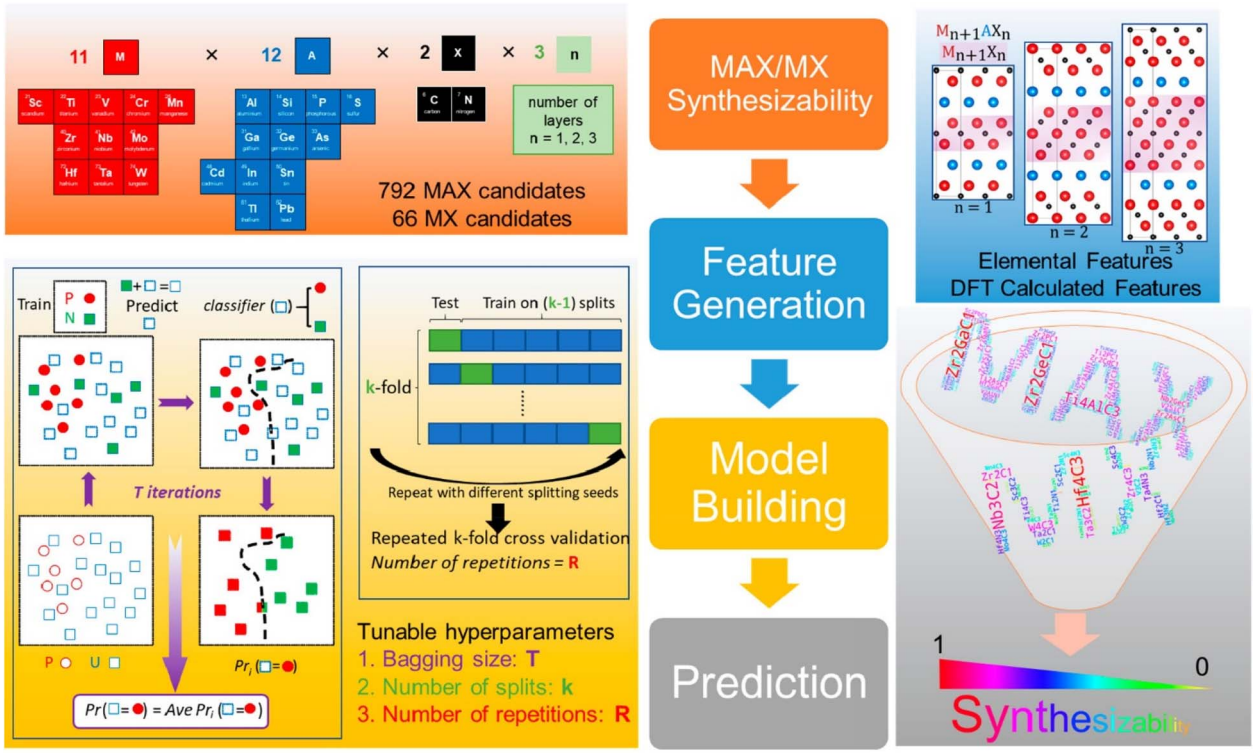

Fig. 4 The diagram illustrating the chemical exploration area and computational process involving PU learning is detailed below. The MAX/MXene exploration zone (top left) is outlined by all feasible combinations of M, A, and X atoms with $n = 1$, 2, or 3. Models showcasing the structure of the bulk MAX phase (top right) and its corresponding MXene variant, highlighted in pink. The representation of the PU learning procedure (bottom left) and its associated model parameters are described. Additionally, word clouds (bottom right) are utilized, where varying font sizes (large or small) and colors (red or orange) indicate the predicted synthesizability level of the specified compound. Reproduced with permission from ref. 36. Copyright 2019 American Chemical Society.

Each material candidate underwent thorough characterization, evaluating a multitude of structural, thermodynamic, electronic, and elemental properties. Leveraging density functional theory (DFT) calculations, the researchers optimized the structures and extracted vital parameters such as interlayer distances, bond lengths, and formation energies, among others, to generate a rich dataset of over 80 features for model development. This fastidious approach underscores the importance of feature selection in crafting robust models for 2D material synthesis.[36]

AI is able to aid in the discovery of novel MXene-based materials with tailored properties for specific uses. For instance, a unique approach was adopted to classify MXene chemical structures and anticipate various electrochemical properties.[37] Rethinking the design challenge could lead to the projection of MXene formulas based on specific battery performance metrics. This method combined multi-target regression and classification, highlighting key physicochemical traits crucial for battery advancements. The resultant inverse model proposed Li_2M_2C and Mg_2M_2C (where M = Sc, Ti, Cr) as promising candidates for focused investigation, given their advantageous gravimetric capacity, voltage, and induced charge characteristics.[37] Additionally, creating ultralight conductive aerogels with customized electrical and mechanical characteristics is crucial for a broad range of applications. Traditional methods involve time-consuming, iterative experiments spanning a broad parameter spectrum. To address this issue, a comprehensive workflow has been developed, merging

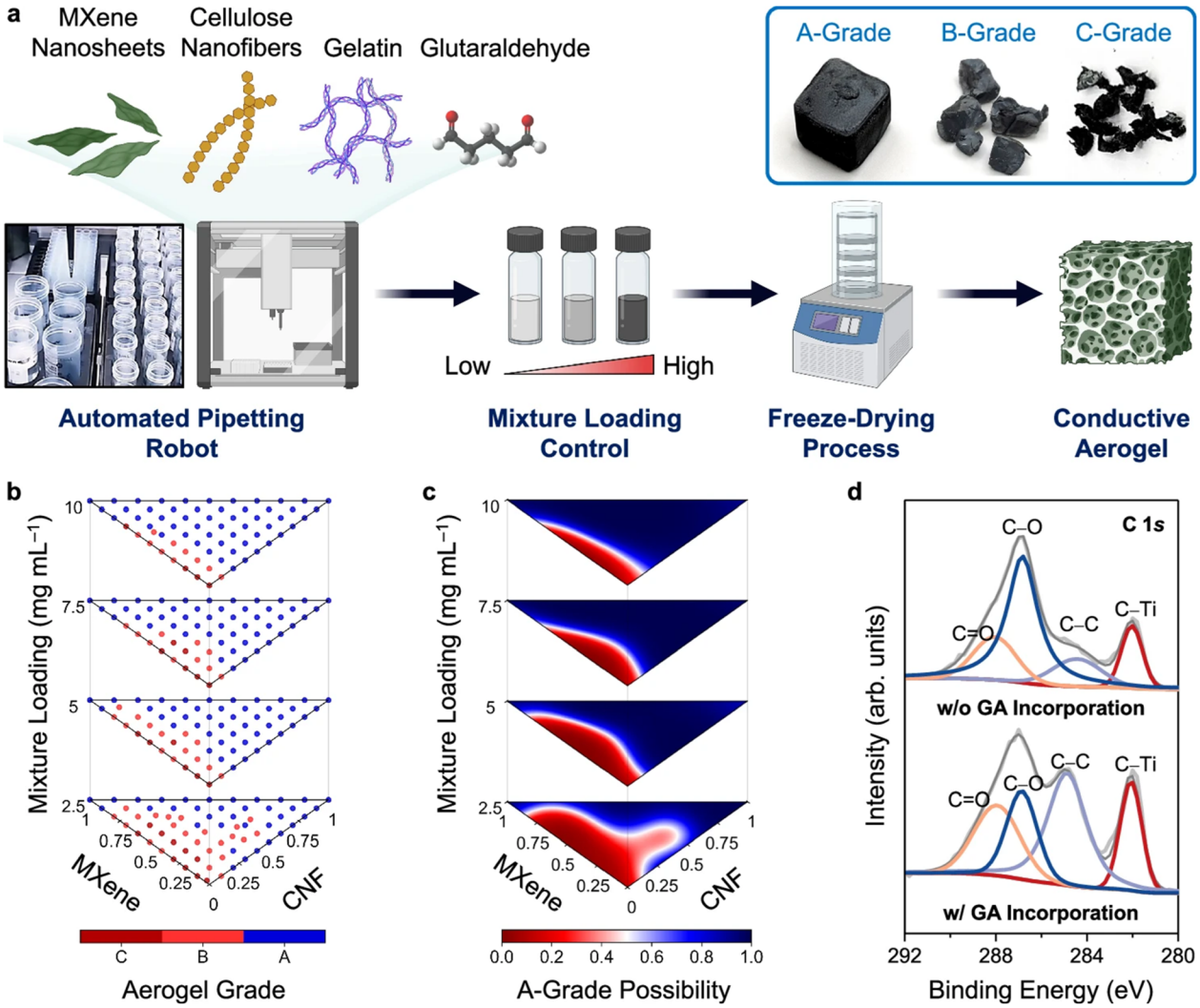

Fig. 5 (a) The diagram illustrates the production process of conductive aerogels expedited by an automated pipetting robot, namely the OT-2 robot. Four key components were integrated, encompassing MXene nanosheets, cellulose nanofibers (CNFs), gelatin, and glutaraldehyde (GA). By modifying the MXene/CNF/gelatin/GA ratios and mixture loadings (solid contents of aqueous mixtures), the mechanical and electrical characteristics of the conductive aerogels were regulated. (b) A total of 264 MXene/CNF/gelatin aerogels were generated, varying in quality based on their structural integrity and monolithic nature. (c) Four heat maps exhibit the potential to create top-tier A-grade conductive aerogels at specific MXene/CNF/gelatin ratios and mixture loadings. (d) Analysis of C 1s XPS spectra was conducted on two MXene/CNF aerogels (at an 80/20 ratio and 10 mg mL^{-1}), with and without the inclusion of GA. Reproduced from ref. 38. Copyright 2024 Springer Nature, under the terms of the Creative Commons CC BY license.

collaborative robotics with ML to expedite the design of conductive aerogels with adjustable properties.[38] An automated approach utilizing a pipetting robot was employed to generate 264 unique combinations of MXene ($Ti_3C_2T_x$), glutaraldehyde, gelatin, and cellulose at varying ratios and loadings (Fig. 5). Following freeze-drying, the structural integrity of the resulting aerogels was thoroughly evaluated to train a support vector machine classifier. Through 8 iterations of active learning, complemented by data augmentation, a total of 162 distinct conductive aerogels were synthesized and examined using robotics-driven platforms. This iterative process paved the way for the development of an artificial neural network prediction model, which played a dual role. Initially, the model accurately forecasted the physicochemical properties of the aerogels based on the synthesis parameters. Furthermore, it automated the design process, enabling the customization of aerogels to meet specific property requirements efficiently. By integrating model interpretation with finite element simulations, a robust correlation between aerogel density and compressive strength was established. The aerogels recommended by the predictive model exhibited notable conductivity, tailored strength, and resilience to pressure fluctuations. These characteristics enabled the consistent generation of Joule heating, making them ideal for applications requiring wearable thermal regulation. The innovative synthesis approach and predictive modeling techniques showcased in this study hold immense promise for advancing the development of functional materials with tailored properties for diverse applications.[38]

2.3. The integration of AI in the applications of MXenes

The exceptional properties of MXenes have sparked interest across several industries, propelling a wave of research into their applications. One of the most promising areas is energy storage, where MXenes have shown outstanding performance as anodes for lithium-ion batteries and materials for supercapacitors owing to their significant electrical conductivity and large surface area.[39–41] MXenes also exhibit impressive catalytic activity, rendering them potential candidates for appliances in water purification, chemical synthesis, and environmental remediation.[42–45] Furthermore, MXenes' excellent mechanical properties and optical transparency offer possibilities in flexible electronics, optoelectronics, and sensors.[46–50] Their diverse applications also extend to biomedical fields, with potential uses in biosensors, tissue engineering scaffolds, and drug delivery systems.[51–54] Additionally, the incorporation of MXenes in soft robotics presents a promising avenue for advancing the capabilities of flexible and adaptable robotic systems.[55]

2.3.1. Energy storage. MXenes and their composites have been widely designed for energy storage purposes, including supercapacitors and batteries, which are essential components of solar energy harvesting and storage systems.[56] Their high surface area, tunable electronic properties, and fast charge–discharge capabilities make MXenes promising candidates for improving the energy storage capacity and efficiency of solar-powered devices.[57–59] In addition to their electrical properties, MXenes exhibit excellent thermal conductivity, making them valuable for improving the thermal management of solar energy systems. By utilizing MXene-based materials as heat dissipation layers or thermal interface materials, solar panels can operate at lower temperatures, thereby increasing their efficiency and lifespan.[60] The exploration of MXenes as solar-absorbing materials represents a significant stride towards optimizing solar energy technologies. By leveraging advanced ML techniques and focusing on the unique properties of MXenes, researchers can unlock new avenues for efficient energy conversion, ultimately contributing to a more sustainable energy future. The ongoing investigations and developments in this field will undoubtedly yield exciting advancements, setting the stage for enhanced solar energy harvesting technologies. In a recent study, advanced ensemble ML techniques, including Matern 5/2 Gaussian Process Regression (GPR) and Quadratic SVR, were harnessed to predict the thermal conductivity, specific heat, and viscosity of novel ionic liquid-MXene hybrid nanofluids.[61] Through detailed laboratory experiments conducted across a range of temperatures and mass concentrations; significant insights were gleaned. The addition of 0.5 wt% of MXene nanomaterial to the pure aqueous ionic liquid (IL) solution led to a substantial enhancement in thermal conductivity, elevating it from 0.443 $W\ m^{-1}\ K^{-1}$ to 0.82 $W\ m^{-1}\ K^{-1}$ at 20 °C. Similarly, the specific heat capacity exhibited a notable increase, rising from 1.985 $J\ g^{-1}\ K^{-1}$ to 2.374 $J\ g^{-1}\ K^{-1}$ with the highest MXene loading, showcasing the remarkable thermal properties of the hybrid nanofluids. The data collected from experiments were split into training (70%) and testing (30%) sets to develop and assess the GPR and SVR models' predictive capabilities. Statistical metrics, including *R*-squared values and Root Mean Square Error (RMSE), were employed to evaluate the models' performance in predicting specific heat, viscosity, and thermal conductivity. Notably, the GPR models demonstrated superior performance across all statistical evaluations compared to the SVR models, with higher *R*-squared values and lower RMSE. The promising findings suggest that the investigated Ionic liquid-MXene hybrid nanofluids hold substantial potential as viable alternatives to water in specific solar energy applications. Leveraging the predictive power of advanced ML techniques can revolutionize the development and optimization of nanofluids for enhanced thermal properties, paving the way for sustainable energy solutions in various industries.[61]

The quest for efficient solar energy conversion is paramount in the field of renewable energy technologies. Central to this pursuit is the broadband absorption of the solar spectrum, a critical factor in solar cell technology. Despite significant advancements over the past decade, traditional materials and design methodologies continue to fall short of addressing realistic energy needs.[19] This is where MXenes emerge as a promising alternative, distinguished by their excellent spectral selectivity. By systematically investigating various MXenes-based metasurface absorbers (MMAs), researchers are able to unveil the potential of these materials in solar applications. One study detailed the construction of RF regression models tailored to different terminal groups of MMAs.[19] Through ML techniques, researchers could refine the entire process—from parameter selection to structural optimization—achieving an

impressive error margin of only 0.02%. This high degree of accuracy underscored the robustness of the approach. The simulation results revealed that the MMAO variant, specifically $Ti_3C_2O_2$, exhibited remarkable performance, absorbing 93.19% of the solar spectrum while emitting a mere 1.21% in the mid-infrared (MIR) band (5000–13000 nm). Such performance qualified it as a near-perfect solar absorber, highlighting the efficacy of MXenes when employed in conjunction with metasurfaces. The integration of MXenes with metasurfaces not only proved feasible but also effective in enhancing solar absorption capabilities. Furthermore, the incorporation of ML techniques enabled precise predictions regarding MMA structural parameters.[19] This innovative approach paves the way for a new paradigm in material selection and design methodologies for solar-thermal energy collection and manipulation.

Identifying crucial characteristics is vital in designing supercapacitor materials *via* the deployment of MXenes. In one study, a ML approach was applied to investigate the structure–property relationship based on a dataset of 600 MXenes, comprising M_2XT_2 (T = bare, O, S) and their doped variants (Fig. 6).[11] To ensure data accuracy, the properties of each MXene were individually computed using density functional theory. Subsequently, the SISSO technique was utilized to generate pseudocapacitance equations based on refined key characteristics linked to stability and electronic properties. It has been observed that on group-free surfaces, the strength of ion adsorption and the density of states within 1.0 eV above the Fermi level significantly influenced pseudocapacitance modulation. In the context of surface functionalization, parameters such as electronegativity and specific heat played pivotal roles in determining the levels of pseudocapacitance. Statistical analysis indicated that elements contributing to high pseudocapacitance were dispersed throughout various regions of the periodic table for group-free as well as O- and S-functionalized MXenes.[11] This correlation between structure and property offers theoretical insights for the statistical development of MXenes-based pseudocapacitive materials.

2.3.2. Sensors and detectors. By leveraging AI algorithms and predictive models, researchers can efficiently screen different compositions, structures, and functionalization of MXenes to identify ones with desired characteristics. This facilitate the discovery of MXenes with improved conductivity, enhanced electrochemical performance, or other properties important for targeted applications. In one study, a novel approach combining deep learning techniques with MXenes has been employed to create an MXene-based sound detector.[62] This detector showcased improved recognition capabilities and heightened sensitivity to pressure and vibrations, leading to the creation of a high-precision sound detection system. By rigorously training and testing the deep learning network model

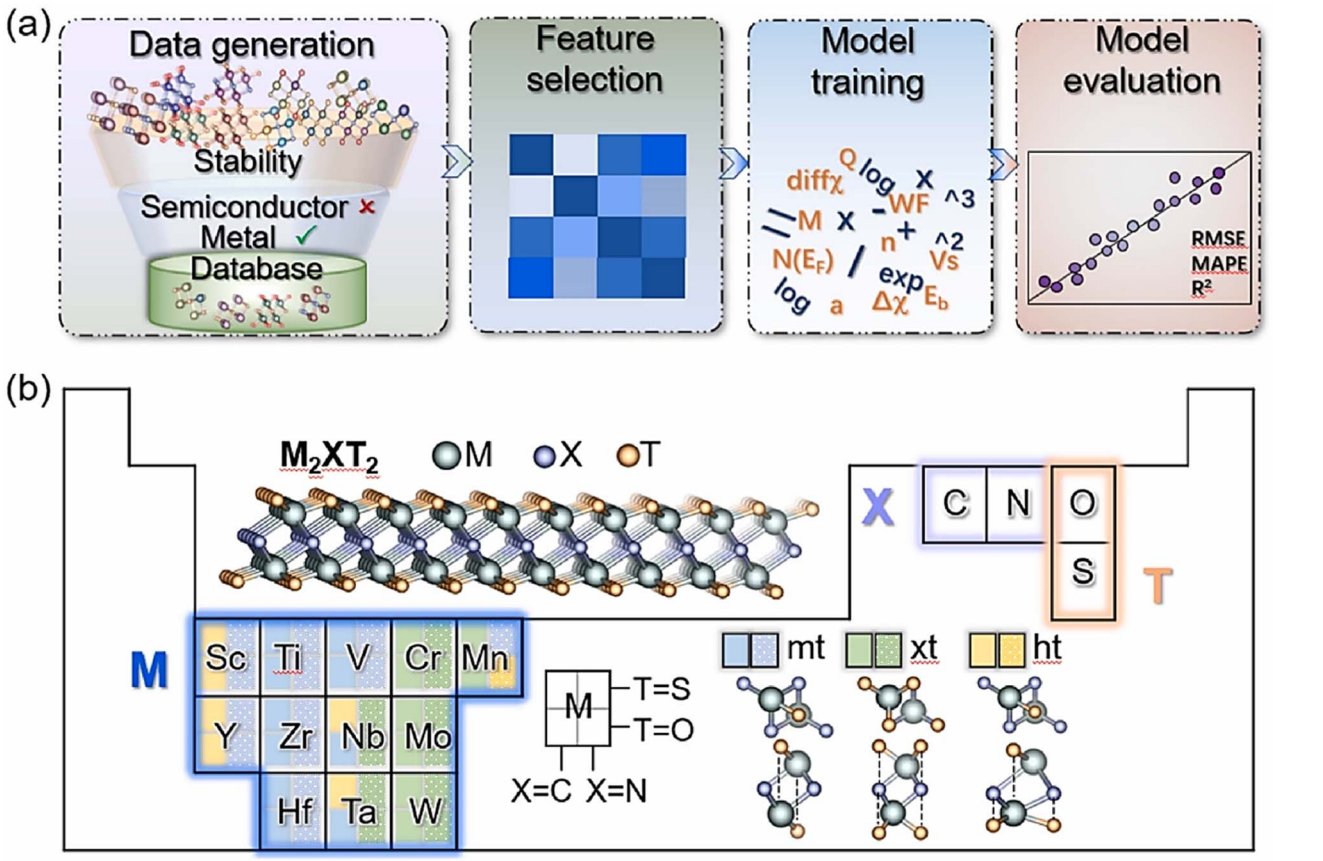

Fig. 6 (a) The process flow of ML is illustrated in the workflow diagram. (b) The distribution of elements and structures within M_2XT_2 (T = bare, O, S). Reproduced with permission from ref. 11. Copyright 2023 Elsevier.

with data gathered from the MXene-based sound detector, successful identification of both long and short vowels in human speech was accomplished.[62] This advancement paves the way for the rapid integration of artificial throat devices in biomedical applications and offers practical implementations in voice command systems, motion tracking technologies, and various other fields. In another study, artificial eardrums utilizing an acoustic sensor based on MXene ($Ti_3C_2T_x$) were developed to replicate the human eardrum's function for voice detection and recognition.[63] Integrating MXene with sizeable interlayer spacing and micro-pyramid polydimethylsiloxane arrays enabled a dual-stage enhancement of pressure and acoustic detection capabilities. This MXene-based artificial eardrum exhibited exceptional sensitivity, and boasted a remarkably low detection threshold of 0.1 Pa. Capitalizing on the outstanding sensitivity of the MXene eardrum, a ML algorithm achieved real-time voice classification with high precision. By categorizing 280 voice signals into seven distinct groups, the training set and test set produced accuracy rates of 96.4% and 95%, respectively.[63] The results highlight the MXene artificial intelligent eardrum's substantial capability for use in wearable acoustical healthcare devices.

The rapid evolution of AI is propelling the progress of flexible electronic materials. Despite this, challenges such as low mechanical properties, rigid signal transmission, and insensitive signal output have impeded the advancement of these materials as sensors. In one study, a novel approach was introduced by developing a super-stretchable MXene composite conductive hydrogel capable of withstanding tensile strains exceeding 1800%.[64] The ensuing hydrogel served as a flexible wearable sensor for real-time detection of human motion signals. Remarkable sensitivity was achieved, enabling the sensor to accurately capture diverse human movements, including joint bending, vocalization, swallowing, and pulse detection. Notably, the MXene composite hydrogel exhibited rapid resilience post-unloading reverse compressive stress, promptly generating a specific current response in the micro-pressure region without leaving any residual traces. This thixotropic sensor displayed swift responsiveness to bidirectional stress, offering significant potential in applications related to human motion detection and secure national defense information encryption.[64] Thus, the integration of MXenes in the development of flexible sensors marks a significant advancement with broad implications across various fields, including healthcare, technology, and defense.

An ultra-stretchable high-conductivity organohydrogel based on MXene (M–OH) was developed for human health monitoring and ML-assisted object recognition (Fig. 7).[65] A new material, created by immersing a hydrogel containing MXene ($Ti_3C_2T_x$), lithium salt (LS), poly(acrylamide) (PAM), and poly(vinyl alcohol) (PVA) in a glycerol–water mixture, has emerged as a game-changer in the realm of wearable technology. Termed M–OH, this innovative material boasts exceptional stretchability, capable of elongating up to an impressive 2000%, coupled with a noteworthy conductivity of 4.5 S m^{-1}. The remarkable properties of the M–OH material stem from the robust interaction between MXene and the dual-network structure of the PVA/PAM hydrogel, as well as the synergistic effects between MXene and LS. Leveraging these unique characteristics, the material was harnessed to create a wearable sensor that enables highly sensitive monitoring of human health, boasting a detection limit as low as 12 Pa. Furthermore, through the integration of pressure mapping image recognition technology, an 8 × 8 pixelated sensing array based on M–OH demonstrated exceptional performance in accurately identifying various objects, achieving an impressive accuracy rate of 97.54%. This feat was supported by a deep learning neural network (DNN), showcasing the material's potential in object recognition tasks. The research underscores the exceptional performance of the ultra-stretchable and highly conductive M–OH material in health monitoring and object recognition applications. This breakthrough opens up a myriad of possibilities for its utilization in AI, human–machine interfaces, and personal healthcare, heralding a new era of innovation in wearable technology.[65]

The intricate process of vision involves a fascinating transformation: light converts into color-based signals, which then morph into images for the brain to process. In this captivating realm, MXene emerges as a groundbreaking material with favorable energy band alignment. It plays a pivotal role in a perovskite-type photodetector array, specifically designed for image detection.[66,67] Ren *et al.*[68] took a bold step forward by developing laser-printed MXene/perovskite/MXene image sensors, paving the way for enhanced photodetection capabilities. The advancement of large-scale image sensor arrays, specifically those featuring a MXene/perovskite/MXene structure, marks a significant leap in photodetector technology. By employing top-down techniques such as spin-coating and laser-scribing, they successfully processed these materials into sub-millimeter photodetector arrays. This innovative approach not only allowed for large-scale production but also paved the way for further downsizing of device dimensions. The alignment of energy levels within these materials, combined with resonance enhancement, facilitated efficient charge transfer and detection, particularly in the near-infrared region. Remarkably, these sensors exhibited an impressive responsivity of 84.77 A W^{-1}, showcasing their capability to detect weak signals. Additionally, they achieved a specific detectivity of 3.22×10^{12} Jones, indicating their sensitivity and effectiveness. Moreover, a linear dynamic range (LDR) reaching 82 dB across a broadband wavelength spectrum—from visible light to near-infrared—underscored their versatility and performance. Notably, the device demonstrated exceptional image-capture capability under near-infrared illumination. This characteristic is particularly crucial for applications in various fields, including medical imaging and environmental monitoring. The tunability and compatibility of these devices with complementary metal-oxide-semiconductors (CMOS) technology hold promise for developing low-cost, high-performance, and large-format photodetector arrays.[68] This combination of advantages positions MXene/perovskite-based sensors as a formidable contender in the field of advanced imaging technologies, potentially revolutionizing how we capture and process images in the future.

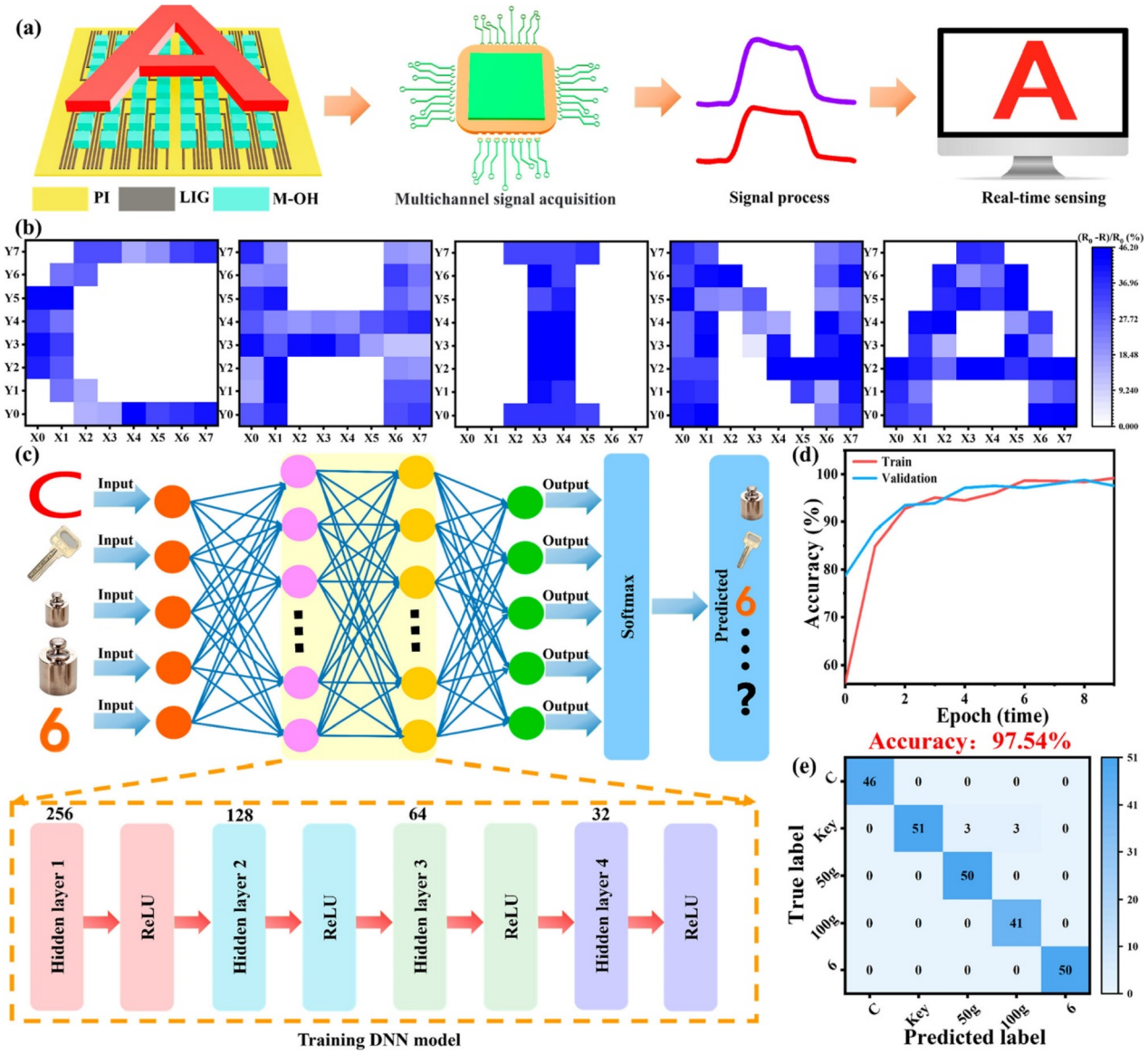

Fig. 7 Pressure mapping and object recognition by a multi-pixelated sensing array utilizing M–OH are explored. (a) The signal recording system is depicted in a schematic diagram. (b) Relative resistance variations from acrylic sheets with letters "C", "H", "I", "N" and "A" shapes pressing on the 8 × 8 pixelated sensor array are illustrated in a pressure mapping setup. (c) The object recognition process involves a DNN-based ML approach, showcasing a detailed framework for the proposed DNN. (d) The correlation between recognition accuracy and the number of epochs is analyzed. (e) Results of the DNN-based ML are presented in a confusion matrix, depicting the recognition outcomes for the five different objects. Reproduced with permission from ref. 65. Copyright 2023 American Chemical Society.

2.3.3. Actuators. The creation of actuators designed to simulate artificial reflexes is vital for enhancing the functionality of bionic robots and neural prosthetics.[69,70] These actuators enhance an organism's perception of stimuli such as heat, electrical properties, and light.[71–73] AI-trained agents facilitate the conversion of various signals into physical responses, achieving specific reflex actions. MXene-based actuators show considerable potential across various fields, including artificial prosthetics, service robotics, human–machine interfaces, and smart city applications.[55] In artificial prosthetics, there is a vision for integrating tactile, temperature, and humidity sensors, along with connections to artificial muscles. This integration aims to improve user experience and responsiveness. In the realm of service robotics, the utilization of intelligent sensors and actuators can significantly enhance machine vision and sensing speed, leading to more human-like interactions. Moreover, human–machine interfaces are expected to be pivotal in the evolution of consumer electronics.[72,74,75]

Recent advancements have led to the fabrication of various MXene-based actuators.[50,72,76–79] For instance, MXene/cellulose/polystyrene sulfonic acid composite membranes served as soft, intelligent actuators with multiple functionalities, including humidity-responsive actions, energy generation based on humidity, and self-powered sensing capabilities

integrated into AI devices, alongside real-time motion tracking.[76] These actuators operated through asymmetric expansion in response to moisture concentration differences, converting humidity into mechanical force. This mechanism allowed for proton diffusion in a designated direction, generating high power density electricity in an open voltage circuit.[76] Additionally, a novel MXene/cellulose bilayer heterostructure was introduced, which could respond to near-infrared light.[80] This structure mimicked the natural mechanisms of palisade mesophyll, expanding and contracting similarly to how leaves respond to water absorption. The MXene/cellulose mixture was employed to create artificial membranes, enabling the conversion of light into heat energy for thermal actuation. The development of this flexible sensor incorporated a biocompatible nanofiber skeleton, resembling the vascular structure of a leaf. The MXene-based composite, in conjunction with cellulose, activated the stratum corneum, while polycarbonate functions as an epidermis to facilitate hygroscopic actuation. This configuration allowed the sensor to respond dynamically to humidity changes, showcasing properties of contraction and expansion akin to a touch-me-not flower. To address potential deformation from continuous use, the actuator's design incorporated polymers to maintain structural integrity, preventing interlayer space reduction. Notably, the MXene layer remains stable throughout this process. The actuator demonstrated responsiveness to small quantities of water and near-infrared radiation, enhancing its applicability in advanced machinery. Its contraction under increased light intensity resulted from volume mismatches between the MXene/cellulose flexible fiber and the polycarbonate membrane.[80] Additionally, programmable behaviors were developed in a narrow rectangular area, allowing for manipulation of MXene/cellulose patterns into various configurations. These MXene-based actuators exhibited periodic bending and recovery under infrared light, mimicking natural movements, such as the folding of a box or the blooming of flowers. Performance metrics revealed an energy density of 0.74 W kg^{-1} and a power density of 0.92 W kg^{-1}, indicating their potential for applications like information encryption in displays activated by infrared light and intelligent switches for nightlights.[80] This innovative technology opens new avenues for enhancing brain-machine interface systems, further bridging the gap between human capabilities and robotic functionality.

2.3.4. Catalysis. ML algorithms excel in identifying key descriptors that significantly impact catalytic efficiency. In the context of MXenes, features such as binding energies, overpotentials, and electronic density of states can be analyzed. The oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) are fundamental processes in energy conversion technologies, such as fuel cells and electrolyzers.[81–83] In one study, authors systematically investigated the catalytic performance of platinum (Pt)-doped dual transition metal (DTM) Janus-MXenes, focusing on their potential as single-atom catalysts (SACs).[84] To explore the physical and chemical properties that influence catalytic overpotential, they employed first-principles calculations alongside advanced ML models. Initially, they assessed the stability of Janus-MXenes through cohesive energy calculations, phonon dispersion analyses, and *ab initio* molecular dynamics simulations. These evaluations confirmed the structural integrity and stability of the synthesized materials, laying the groundwork for further investigations. Following stability assessments, they delved into the electronic properties of Pt-doped Janus-MXenes. The results revealed promising candidates with ultralow overpotentials. The remarkable catalytic performance of these materials can be attributed to the effective tuning of the electronic properties of SACs through the DTM approach. Importantly, the ML models played a crucial role in elucidating the significance of various descriptors impacting overpotential. By analyzing these relationships, the underlying origins of the catalytic activity of the SACs examined could be uncovered.[84]

2.3.5. MXenes and neuromorphic systems. Neuromorphic computing, by emulating the brain's efficiency and cognitive capabilities, hold the potential to transform computing and enable innovative AI applications across various sectors, from autonomous systems to personalized healthcare. However, substantial engineering hurdles, particularly in software development, need resolution before neuromorphic computing can fully unleash its potential and compete with existing AI systems.[85] In robotics, these systems enable autonomous machines to navigate complex environments with precision and adaptability. In healthcare, neuromorphic systems aid in analyzing vast amounts of medical data to assist in diagnostics and treatment planning. Moreover, in cybersecurity, these systems enhance threat detection and response mechanisms by swiftly identifying patterns in large datasets.[86]

Advantages:

• Energy efficiency: neuromorphic systems can achieve high performance while consuming significantly less power compared to traditional digital systems.

• Scalability: the parallel architecture of neuromorphic systems allows for easy scaling to handle larger problems and datasets.

• Fault tolerance: neuromorphic systems can maintain functionality even in the presence of faulty components, similar to the resilience of biological neural networks.

Challenges:

• Complexity: designing and implementing neuromorphic systems requires expertise in various fields, including neuroscience, materials science, and computer engineering.

• Training and learning: developing effective training algorithms for neuromorphic systems is an active area of research, as traditional ML techniques may not directly apply to Spiking Neural Networks (SNNs).

• Hardware limitations: current neuromorphic hardware still has limitations in terms of scalability, programmability, and integration with other systems.

Key features of neuromorphic computing include:

• Massively parallel processing: neuromorphic systems employ numerous simple processing elements that work in parallel, akin to neurons in the brain, thus enhancing the efficiency of handling complex tasks.[85] The architecture of neuromorphic systems is designed to replicate the intricate network of neurons in the human brain. By leveraging this bio-inspired

design, these systems can process information in a highly efficient manner, enhancing their performance across various applications. The parallelism inherent in neuromorphic architecture allows for the simultaneous execution of multiple tasks, leading to faster computation and improved decision-making capabilities.

• Event-driven computation: computation in neuromorphic systems is triggered by events or spikes, mirroring the brain's communication method among neurons, leading to energy-efficient and real-time processing.[85]

• Adaptive learning: neuromorphic nisms by swiftly identifying patterns insystems know how to dynamically adapt and learn from their environment, enhancing performance and handling novel situations without explicit programming.[85]

• Low power consumption: through event-driven processing and low-precision analog computation, neuromorphic systems consume notably less power than traditional computers, making them suitable for edge AI and Internet of Things (IoT) applications.[85]

MXenes offer exciting possibilities for unique electronic devices, comprising innovative battery designs, energy storage solutions, and supercapacitors, with MXene serving as a versatile electrode material. The distinctive surface properties and 2D structure of MXenes open doors to a range of applications in cutting-edge electronic devices.[49,87–89] Memristors, artificial synapses based on diverse 2D materials, play a pivotal role in neuromorphic and data storage technologies. MXene, a notable 2D material, shows promise for memristor applications in view of its exceptional conductivity, rapid charge response, high stacking density, and strong hydrophilicity. Recent studies have highlighted the utilization of MXenes and their composites in creating artificial synapses with advantageous features like high power efficiency and scalability.[90] In one study, Sokolov and colleagues[91] investigated the outstanding insulating properties of partially oxidized MXene ($Ti_3C_2T_x$) sheets, highlighting their potential use in memory storage and electronic synapse functions. The device demonstrated intriguing resistive switching behaviors influenced by Ag^+ migration dynamics. Remarkably, the Ag^+ cation migration patterns resembled Ca^{2+} ion movements in biological synapses, allowing faithful replication of essential synaptic functions like Ag^+ intrusion/extrusion, paired-pulse facilitation (PPF), post-tetanic potentiation (PTP), short-term potentiation (STP), and the shift from STP to long-term potentiation (LTP). The advancement of such devices presented optimistic possibilities for incorporation into the next era of hardware-based AI systems, indicating MXenes' potential to transform electronic technologies and advance AI applications.[91]

The integration of optoelectronic capabilities into artificial neurons presents significant advantages, such as customizable device characteristics, varied functions, and enhanced computing efficiency for AI systems.[92] Though, existing studies predominantly focus on electric-driven mono-mode artificial neurons, but they lack an easy and effective method to merge electrical and optical signals seamlessly.[92] A multifunctional optoelectronic hybrid-integrated neuron leveraging Ag nanoparticles-decorated MXene was introduced.[92] This design targeted achieving optoelectronic spatiotemporal information fusion with a low operating voltage of 0.93 V and a high on/off ratio of 10^3, surpassing the capabilities of most artificial neurons. The creation of an integrated visual perception system involved combining artificial synapses, artificial optoelectronic neurons, and a robotic hand to mimic human conditional responses. By merging optical sensory signals with electrical training signals, the system displayed significantly reduced response times. Additionally, utilizing the spatiotemporal information integration ability, a multi-task pattern recognition activity was conducted within a spiking neural network incorporating artificial synapses and neurons. This system effectively recognized digit patterns and rotation angles simultaneously. As a result, this study demonstrated outstanding performance in sensory tasks and pattern recognition, establishing a groundwork for potential applications in neuromorphic circuitry.[92]

The synergy between Optical Neural Networks (ONNs) and MXenes heralds a new era in advanced computing. ONNs offer unparalleled advantages such as inherent parallelism and minimal energy consumption, aligning perfectly with the remarkable attributes of MXenes which with their exceptional conductivity and tunable optical properties, serve as ideal candidates for enhancing the performance of ONNs.[93] Nonetheless, a significant challenge hindering the adoption of ONNs is the absence of optical nonlinearity. This research focused on developing optical nonlinear activators for ONNs by blending $Ti_3C_2T_x$ MXene with microfibers, subsequently validating their operational principles.[93] Activation functions derived from experimental data were applied to simulate tasks such as multi-classification and super-resolution reconstruction, demonstrating performance levels comparable to traditional activation functions used in conventional computers. To assess the efficacy of the nonlinear activator, four essential criteria were introduced and verified: recovery time, deviation from linearity, proximity to an identity mapping activation function, and configurational re-configurability. Theoretically, the proposed nonlinear activator exhibited computing speeds potentially 100 times faster than standard electronic computers, serving as a promising nonlinear activation component for ONNs.[93] This advancement aims to facilitate the seamless integration of ONNs with AI systems.

3. Challenges

While MXenes have shown tremendous potential, further advancements and research are needed to unlock their full capabilities and overcome certain challenges. One area of focus is improving the scalability and production methods for MXenes. Currently, MXenes are primarily synthesized in the laboratory, and scaling up the production process to meet industrial demands remains an important hurdle. Another aspect being explored is the surface functionalization of MXenes. By modifying the surface chemistry, researchers aim to enhance the performance and tailor the properties of MXenes for specific applications. Functionalization techniques be able to improve stability, create selective adsorption sites, or

introduce additional functionalities, expanding the range of potential uses for MXenes. Additionally, efforts are being made to understand the fundamental properties and behavior of MXenes at the atomic and molecular levels. This knowledge is crucial for further optimizing MXene properties and engineering novel functionalities. Transforming scientific breakthroughs into tangible products requires the development of scalable manufacturing processes, quality control measures, and regulatory frameworks that ensure safety and sustainability.[94–99]

Before the advent of AI technologies, researchers primarily relied on conventional methods to explore MXenes and their properties.[100–103] These methods included:

• Trial and error approaches: researchers often used empirical techniques to synthesize MXenes, adjusting parameters such as temperature, time, and precursor concentrations without predictive models. This can lead to inefficient exploration of the material space.

• Experimental characterization: techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDX) have been commonly employed to analyze MXene samples post-synthesis. While effective, these methods can be time-consuming and labor-intensive.

• Limited data analysis: traditional data analysis methods often involved manual interpretation of experimental results. This process is not only prone to human error but also limits the ability to identify complex patterns within large datasets.

The limitations of conventional approaches in MXene research are multifaceted:

• Inefficiency: the trial-and-error nature of synthesis can lead to prolonged development cycles and wasted resources, as researchers may not effectively identify optimal conditions.

• Scalability issues: manual characterization methods are challenging to scale, especially when dealing with a vast array of MXene compositions, resulting in slower progress in material discovery.

• Limited predictive capability: traditional methods often lack the capacity to predict the properties of new or modified MXenes accurately, making it difficult to tailor materials for specific applications.

The integration of AI technology into MXene research offers several significant advantages:[26,67]

• Data-driven predictions: AI, particularly machine learning algorithms, can analyze extensive datasets to identify patterns and predict material behaviors. This enables researchers to make informed decisions about synthesis conditions with much higher accuracy.

• Efficiency and speed: AI can optimize synthesis parameters rapidly, reducing the time required for material discovery. For instance, using techniques like RF regression, researchers can predict optimal conditions efficiently, significantly shortening development timelines.

• Automation of analysis: AI tools can automate the analysis of spectroscopic data, freeing researchers from manual interpretation. This not only speeds up the characterization process but also enhances accuracy by minimizing human error.

• Enhanced material design: by utilizing AI, researchers can explore previously unconsidered combinations of terminal groups and structures, leading to the discovery of novel MXenes with tailored properties that may not have been identified through traditional methods.

Understanding the properties, synthesis, and applications of MXenes presents a myriad of challenges for AI technologies which stem from the complexity and variability inherent in MXenes, requiring sophisticated AI approaches to navigate effectively:

• Predicting novel properties: one of the primary contests is predicting novel properties of MXenes accurately. AI algorithms must contend with the vast array of structural variations and elemental compositions within MXenes to forecast their unique properties reliably. The non-linear relationships between different structural features and material properties further complicate this task, necessitating advanced ML models capable of capturing such intricate relationships.

• Optimizing synthesis routes: another significant question lies in optimizing synthesis routes for MXenes *via* the deployment of AI. The synthesis process of MXenes is intricate and involves various parameters that influence the material's final properties. AI algorithms need to decipher the complex interplay between synthesis conditions, precursor materials, and resulting MXene characteristics to streamline and enhance the synthesis process effectively.

• Enabling targeted applications: AI faces the dispute of enabling targeted applications of MXenes by correlating their properties with specific application requirements. Tailoring MXene properties to suit diverse applications, such as energy storage, catalysis, and sensing, demands a nuanced understanding of the material's behavior under different conditions. AI tools must decrypt the intricate relationships between MXene properties and application performance to facilitate the design of tailored materials for specific use cases.

4. Future perspectives

The integration of AI in the synthesis and application of MXenes has the potential to accelerate materials discovery, optimize processes, improve performance, and enable the development of MXene-based materials with tailored properties for a wide range of applications:

• Predictive modeling: AI is capable of being utilized to build predictive models that know how to forecast important MXene properties based on composition, structure, and processing parameters. These models be able to guide researchers in selecting the most promising MXene candidates for specific applications, reducing the need for extensive experimental testing.

• Materials design: AI algorithms know how to be deployed to propose new compositions, structures, or functionalization of MXenes that exhibit desired properties. By using generative models and optimization algorithms, researchers be able to explore the vast space of MXene possibilities and identify novel materials with optimized characteristics.

• Data-driven materials discovery: AI can analyze large databases of experimental and computational data to uncover hidden patterns, correlations, and trends related to MXene synthesis and properties. This data-driven approach is able to offer valuable insights and guide researchers toward new synthesis strategies and applications of MXenes.

• Process optimization: AI algorithms are capable of optimizing MXene synthesis processes by analyzing data from multiple experimental runs, identifying key process parameters, and suggesting optimal conditions. This can lead to improved yields, reproducibility, and efficiency in MXene production.

• Fault detection and quality control: AI is deployable to monitor and analyze various quality control parameters during MXene synthesis, enabling the real-time detection of process deviations or defects thus ensuring the consistency and high quality of MXene materials.

5. Conclusion

In this review, we examine the integration of AI in the study of MXenes and their composites, focusing on their synthesis, properties, and applications in energy storage, sensors and detectors, actuators, catalysis, and neuromorphic systems. We highlight recent advancements in AI methodologies that enable the prediction and optimization of MXene properties, addressing the complexities of their research. The review discusses the challenges associated with identifying novel properties of MXenes and emphasizes the necessity for sophisticated AI models to elucidate the intricate relationships between their structural features and material behaviors. Additionally, we explore how AI-driven approaches can optimize synthesis routes, streamline processes, and enhance the efficiency of MXene production.

The remarkable attributes of MXenes—such as electrical conductivity, thermal stability, and mechanical strength—make them highly desirable for applications ranging from energy storage and electronics to catalysis and biomedical fields. However, to fully harness the potential of MXenes, challenges related to scalability, surface functionalization, and fundamental understanding must be addressed. The integration of AI with MXenes presents numerous opportunities to enhance synthesis techniques, optimize processes, accelerate materials discovery, and develop MXene-based materials with improved properties for a wide range of applications. AI algorithms can predict and optimize the properties of MXenes based on their atomic structures, compositions, and processing conditions, encompassing electronic, optical, thermal, and mechanical properties tailored for specific applications. Moreover, AI is capable of facilitating the development of novel synthesis methodologies for MXenes by analyzing existing data and suggesting innovative approaches or modifications to traditional synthetic routes, thereby improving synthesis efficiency, scalability, and reproducibility. Importantly, AI excels in analyzing and interpreting complex characterization data for MXenes. By leveraging DL techniques, AI can extract meaningful insights from spectroscopic, microscopic, and diffraction data, leading to a deeper understanding of MXene structures and properties. Additionally, AI enables virtual screening and optimization of MXenes through computational modeling, allowing researchers to explore a vast array of MXene structures and compositions, which accelerates the discovery of materials with desired properties for specific applications. Finally, AI can synthesize and analyze extensive MXene-related literature, patents, and experimental data to create a comprehensive knowledge base, where AI algorithms recommend potential synthesis strategies, applications, and research directions, thus assisting researchers in making informed decisions.

Data availability

No data was used for the research described in the article.

Author contributions

A. K: writing – review & editing; E. N. Z: writing– review & editing; R. S. V: writing – review & editing; A. Z: supervision, writing – review & editing; S. I: supervision, conceptualization, writing – review & editing; P. M: supervision, writing – review & editing.

Conflicts of interest

Author(s) declare no conflict of interest.

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