

MXENE AND MXENE-BASED COMPOSITES FOR SENSING APPLICATIONS: A COMPREHENSIVE REVIEW OF PHYSICAL, PHYSICOCHEMICAL, AND PERFORMANCE ASPECTS

Abstract

The emergence of 2D materials, exemplified by graphene and MXenes, has revolutionized the landscape of materials science, offering a versatile platform for exploring novel structures and properties. MXenes, akin to graphene, have garnered substantial scientific and technological interest over the last decade due to their exceptional electron migration properties, high specific surface area, and remarkable thermal and chemical stability. This article delves into the expanding realm of MXenes as a promising foundation for advanced nano-biosensors capable of detecting harmful chemical and biochemical analytes. MXenes, characterized by their layered structure and metallic properties, have demonstrated outstanding potential in various applications, ranging from hydrogen production, catalysis, energy storage, and adsorption to sensor technology. This work particularly emphasizes the significance of MXene-based sensors in detecting biomolecules relevant to human health and environmental safety. Achieving early-stage detection is paramount for timely medical interventions, thereby enhancing the efficacy of treatments. Nano-biosensors designed using MXenes prioritize high selectivity and sensitivity, aligning with contemporary demands for ultra-sensitive detection platforms. The unique properties of MXenes, including high surface area and tunable surface functional groups, make them easily adaptable for specific biomolecule interactions, enabling tailored sensor design. Their semi-conducting metallic attributes, coupled with optimal bandgap characteristics, confer superior detection sensitivity compared to alternatives like graphene. Importantly, MXenes boast non-toxic elemental compositions, such as

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nitrogen, carbon, or titanium, ensuring their safety as biosensing platforms. Researchers are actively exploring innovative ways to combine MXenes with other nanostructured materials to create multifunctional biosensors, capitalizing on the distinctive biological and electrical traits of MXenes. This research article highlights the exciting prospects of MXene-based nano-biosensors, underscoring their potential impact in high-impact factor journals. The integration of MXenes into sensor technology holds promise for early disease detection, environmental monitoring, and a host of other applications that demand exceptional analytical performance and reliability. As MXene-based sensors continue to advance, they contribute significantly to the evolving landscape of materials science and biosensing technologies.

I. INTRODUCTION

1. Overview of MXenes and MXene-based Composites in Sensing Applications:

Graphene is a 2D material with a rich and diverse research landscape that has evolved over time. Following the advent of graphene and graphene-like materials, the exploration of novel structures and properties within the realm of materials science has garnered significant research interest. Over the last ten years, there has been a notable surge in scientific and technological attention towards MXene, a two-dimensional layered material that possesses a structure similar to that of graphene. In general, 2D materials are characterised by robust intracrystalline covalent bonding and feeble interlayer van der Waals forces. These materials demonstrate a comprehensive range of physical and chemical properties, including those of insulators, semiconductors, metals, and superconductors. The potential for exfoliation of MAX phases into 2D transition metal carbides or nitrides, commonly referred to as MXenes, has greatly expanded the scope of potential applications for MAX phases[1].

The MAX phases are a broad group of solid layered carbides or nitrides that possess a hexagonal lattice and the chemical formula $M_{n+1}AX_n$. Here, "M" denotes an early transition metal (Sc, Ti, Zr, Hf, V, Nb, Ta, Cr, or Mo), "A" represents an element from the main groups III-VI of the periodic table (Al, Ga, In, Tl, Si, Ge, Sn, Pb, P, As, Bi, S, or Te), "X" is either carbon or nitrogen, and n ranges from [2–5]. The MAX phase family has undergone recent expansion in terms of crystallinity. As per the available data, a total of 82 distinct crystalline MAX phases have been successfully synthesised through experimental procedures. In addition to the crystalline MAX phases, diverse alloys of MAX phases with varying compositions of transition metals and/or X elements have been synthesised. Theoretically, a multitude of crystalline or alloy structures for MAX phases have been predicted to exhibit thermodynamic stability.[6–10] All MAX phases exhibit metallic properties. The presence of partially filled d orbitals in transition metals near the Fermi level is responsible for the phenomena described in sections[11,12][13]

The electron migration properties of MXenes are exceptional, along with their high specific surface area and impressive thermal and chemical stabilities [14–17]. These characteristics make them highly appropriate for a range of applications in diverse fields, including hydrogen production, catalysis, energy storage, and adsorption [18–21]. Furthermore, MXenes have been found to possess exceptional sensitivity and selectivity as sensors [22–28]. The advancement of sensor technology with enhanced selectivity, sensitivity, and response/recovery is being pursued. The timely identification of early-stage detection has become a persistent and pressing objective.

2. Significance and Potential Impact of MXene-based Sensors in High-impact Factor Journals:

The research focus lies in designing and advancement of nano-biosensors that can detect chemical and biochemical analytes responsible for causing harm to both humans and the environment. The reliable detection of biomolecules, or analytes of interest, is of utmost importance in the development of nano-biosensors for the purpose of diagnosing the onset and progression of disease [29]. Consequently, the ability to intervene medically at an earlier stage, thereby facilitating prompt medical treatment, has the potential to improve the curative efficacy of the treatment. In the design of nano-bioelectrodes, it is crucial to prioritise high selectivity and sensitivity as the primary

analytical parameters, as noted by [30] and [31]. The increasing need for nanomaterials exhibiting exceptional analytical performance and superior characteristics has resulted in the development of novel nanomaterials that are well-suited for the creation of ultra-sensitive nano-biosensors. In the realm of materials science, 2D nanomaterials have garnered significant attention from researchers due to their potential as a biorecognition element in the creation of biosensors with exceptional sensitivity [32]. Materials that exhibit a crystalline structure with a limited number of atomic layers, typically ranging from 1-10 Å in thickness and submicron to few micrometres in lateral dimension, are classified as two-dimensional (2D) materials. The distinctiveness of 2D materials from their bulk counterparts arises from their substantial surface area and exceptional ultrathin layered structures, which exhibit intriguing electronic, electrical, optical, physical, and chemical properties [33]. 2D materials are classified into various categories such as superconducting, insulating, semiconducting, semi-metals or metals based on their chemical composition and structural characteristics.

Thin nanosheets of 2D layered MXenes have high surface areas and surface functional groups like -F, -OH, and -O, which make it simple to tailor them to biomolecules and change the conductivity, making them extremely versatile for detecting different biomolecules [34]. Additionally, due to their semi-conducting metallic characteristics with an adequate bandgap, MXenes display fewer current leakages in an off-state than graphene, leading to better detection sensitivity [35]. MXenes are safe to use as a biosensing platform because they are made of non-toxic elements like N, C, or Ti [36]. In addition, efforts are being made to combine MXenes with other nanostructured materials to create biosensors with a variety of functions that are motivated by the unique biological and electrical characteristics of MXenes.

II. SYNTHESIS AND FABRICATION TECHNIQUES

- 1. Synthesis Methods for MXene Materials:** In contrast to various other two-dimensional (2D) materials such as graphene, phosphorene, and MoS₂, MXenes exhibit distinct and enhanced properties pertaining to electrical conductivity, hydrophilicity, and redox activity. Although pure MXene [37] possesses remarkable electronic properties, there are several obstacles that hinder its practical use. These challenges include maintaining stability in colloidal suspensions, preventing stacking and aggregation, and addressing properties related to thermal, mechanical, and oxidative stabilities, as discussed in our previous review [37]. The synthesis method of MXenes is responsible for their inherent characteristics, which in turn give rise to distinct properties. Therefore, it is crucial to create structural features and defects during synthesis to achieve these unique properties. Functional groups have the potential to be incorporated into MXenes, thereby creating "anchor sites" that can offer advantages during the subsequent fabrication of hybrid materials involving MXenes.

Various etchants and their distinct combinations have been explored in addition to hydrofluoric acid (HF) [38]. These include HCl–LiF, HCl–NaF, NH₄HF₂, NaOH, and tetramethylammonium hydroxide. The process of fluorine-assisted etching involves the use of aqueous hydrofluoric acid (HF). The process of HF spontaneously dissociating results in the creation of an interlayer gap, accompanied by the formation of AlF₃ and H₂. Eventually, this leads to the departure of the MAX system [39]. During this particular

procedure, functionalized MXene materials are synthesized in the presence of hydrofluoric acid (HF) and water (H₂O). This results in the formation of MXene with surface terminations consisting of oxygen (O), hydroxyl (OH), and fluorine (F). As a consequence, these surface terminations impart distinctive and customized structural and electronic properties to the MXene material [40]. Since that time, hydrofluoric acid (HF) has been employed in numerous MAX phases to selectively remove A layers in widely studied 211, 312, and 413 MAX configurations, including Ti₂AlC, Ti₃AlCN, and Ta₄AlC₃, as reported in literature [41]. In the case of more intricate MAX-like structures, such as Hf-Al-C, Y-Al-C, and Zr-Al-C systems, it has been observed that the Al-C layer is eliminated instead of the conventional Al layer [42–44].

Therefore, the synthesis process that involves the use of HF necessitates a prolonged etching duration and the implementation of highly corrosive etching conditions, thereby demanding meticulous protective measures [45,46]. The utilization of fluoride-salt etchants and cation intercalation techniques. In a manner akin to the impact of hydrofluoric acid (HF), solutions containing fluoride salts have the ability to generate an in-situ HF solution that is capable of etching the A layer. Additionally, these solutions can employ cations to intercalate and weaken the bonds between sheets. Various solutions have been documented to include cobalt fluoride/HCl [47], FeF₃/HCl [48], bifluorides (NaHF₂, KHF₂, NH₄HF₂ in water) [49], and LiF, NaF, KF or NH₄F in HCl. Nevertheless, a notable disparity in the impact of exfoliation has been observed in comparison to hydrofluoric acid (HF). This evaluation involved the utilization of HF, NH₄HF₂, and LiF/HCl solution. The study found that the application of HF and NH₄HF₂ yielded comparable outcomes, as both substances caused an increase in the exposure of edge sites within the grain boundaries of polycrystal MAX particles to the etchant. The primary distinction lies in the interlayer spacing of multilayer MXene, which is observed to be greater for NH₄HF₂ compared to HF. This discrepancy can be attributed to the intercalation of ammonia ions in NH₄HF₂. In general, NH₄HF₂ is employed as a substitute for HF in order to mitigate potential hazards. This resulted in the successful exposure and propagation of the exfoliation of A layers, surpassing the performance of LiF/HCl in terms of both yield and rate. Nevertheless, the multi-layer MXene was acquired and remained in an uneliminated state as a result of the lack of intercalating agents.

The phenomenon of intercalation is contingent upon the structural characteristics of the cation, which enables its insertion into the vacant interlayer spaces within MXene sheets. However, following treatment with hydrofluoric acid (HF), the d-spacing expanded to 19.4 Å. The d-spacing was increased to 30.3 Å through the application of TBAOH (tetrabutylammonium hydroxide), leading to further delamination. In contrast, the LiF + HCl reaction exhibited a prominent peak corresponding to its MAX phase, while the presence of intercalated MXene was observed to a lesser extent. The impact of fluoride salts in a hydrochloric acid (HCl) mixed solution was assessed by Wang et al. [50] through the utilization of a hydrothermal-assisted technique. As an example, the compound MXene, produced through the synthesis of LiF and NH₄F, exhibits the ability to adsorb methane at elevated pressures and retain it under standard atmospheric conditions. This characteristic holds potential advantages in the capture of methane and other potentially harmful gaseous molecules. In the context of natural gas storage, it is noteworthy that MXene, which is produced through the synthesis of NaF and KF, exhibits the ability to absorb methane at elevated pressures and desorb methane at reduced

pressures. The utilization of intercalation techniques has demonstrated promising diffusion kinetics when applied to MXene/graphene heterostructures. In their study, Demiroglu et al. [51] examined the reduction of energy barriers within a heterostructure through the introduction of Na and K ions. They observed that the intercalation of these ions resulted in improved charge and discharge rates, making them advantageous for battery applications.

- 2. Synthesis without the use of Fluorine:** The utilization of hydrofluoric acid (HF) has been widely recognized as a prevalent method for the synthesis of MXene materials. Nevertheless, in addition to the negative impact on health that has been linked to the utilization of HF [52], it has been observed that MXene terminated with HF also has implications for both the theoretical and experimental determination of lithium storage capacity [53,54]. Understanding the distinction between materials can provide valuable insights in determining the preferred removal of one material over another. The removal of the A layer has consistently been the focal point for MXene. For example, it has been observed that M-A bonds exhibit lower strength compared to M-X bonds [55]. As a result, the utilization of HF has proven effective in the elimination of the A layer. The determination of the suitable voltage range for the electrochemical etching process of aluminum from titanium aluminum carbide (Ti_2AlC) in an aqueous electrolyte has been documented in previous studies [56,57]. This section will discuss HF-free techniques for the synthesis of MXenes, with a particular focus on their applicability to few-layer MXenes and their incorporation into hybrid materials. The process of alkali treatment. In order to gain a deeper understanding of the characteristics of an A layer, aluminum, which is an amphoteric element, is frequently utilized as an A phase due to its reactivity in both acidic and basic environments [58]. Several studies have employed alkali etchants, including potassium hydroxide (KOH) [59] and sodium hydroxide (NaOH).
- 3. Fabrication Techniques for MXene-based Composites:** Recently, researchers have been synthesizing new composite materials by combining MXenes with different carbon materials. The synthesis of MXene and its composites typically involves two steps. First, MXene materials are obtained by selectively removing atomic layers from MXene precursors like MAX phases. Then, MXene and carbon materials are combined using various methods such as ball milling, spray drying, electrospinning, and others. Previous reviews have focused on generalizing composites of MXenes with different elemental materials, but this review aims to systematically summarize the synthesis methods and applications of MXene and its composites for better understanding.

The review discusses different strategies for synthesizing MXene and its composites. Various strategies, including ball milling, self-assembly, spray drying, vacuum-assisted filtration, in-situ growth, and electrospinning, have been used to combine MXenes and carbon materials and create novel 3D structures. Ball milling relies on the impact of grinding bodies to pulverize and mix the components, while self-assembly allows for the spontaneous formation of ordered structures driven by electrostatic interactions. Spray drying quickly removes solvents to obtain powder and allows for control of particle size distribution. Vacuum-assisted filtration utilizes pressure differences to tightly combine MXenes and carbon materials into flexible structures. In-situ growth involves the growth of carbon materials on MXene-based materials, often using chemical vapor deposition. Electrospinning uses electrostatic atomization to

transform polymer solutions containing nanocomposites into fibers with tunable properties.

The review provides specific examples of each synthesis method. For example, in the ball milling method, MXenes' oxygen atoms interact with carbon atoms from carbon materials during the process, providing binding forces between carbon and MXenes. Self-assembly exploits the electrostatic attraction between MXene nanosheets and carbon nanotubes to prevent restacking and create a porous structure. Spray drying quickly removes solvents to obtain hierarchical composite microspheres with dispersed carbon nanotubes and magnetic nanospheres. Vacuum-assisted filtration combines MXenes and carbon materials tightly to create flexible substrates for batteries and supercapacitors. In-situ growth allows for uniform growth of carbon materials on MXene flake interlayers, suppressing flake stacking and improving composite stability. Electrospinning utilizes electrostatic atomization to create fibers containing MXene flakes and carbon nanofibers, enhancing electrochemical performance.

In summary, the review highlights different synthesis methods for MXene/carbon composites, discussing their advantages and specific examples. The diverse strategies offer options for tailoring composite structures and properties, enabling various applications in energy storage and other fields.

One-step in-situ growth methods refer to a process where the formation of MXene and metal oxide layers occurs simultaneously within a single reaction step. Within this methodology, there exist two prevalent approaches. The initial technique under consideration is in-situ oxidation growth. The deposition of metal oxides onto the MXene surface occurs via a redox reaction. The formation of MXene-metal oxide composites can be achieved in both liquid and gas phases. The deposition of various metal oxide compounds, such as Cu_2O , MoO_3 , Co_3O_4 , NiCo_2O_4 , and TiO_2 , onto MXene surfaces has been observed in previous studies [60–63]. Additionally, the process of in-situ hydrolysis growth involves the deliberate hydrolysis of metal ions, resulting in the creation of metal hydroxides. These metal hydroxides are then converted into metal oxides. Metal ions can be immobilised on the surface of MXene by manipulating the pH value, leading to the formation of metal hydroxide nanoparticles through hydrolysis [64].

- 4. In-Situ Conversion through Multiple Steps:** The process of multistep in-situ conversion entails a consecutive series of steps aimed at achieving the desired composite structure. The process commences with pre-generation, wherein precursor materials are synthesised on the surface of MXene. This is then followed by chemical transfer and subsequent thermal treatment or other chemical reactions, ultimately resulting in the formation of the desired composite [63,65–67]. This particular strategy facilitates meticulous manipulation of the composite's composition and structure. Through the utilisation of these synthesis strategies, it is possible to customise MXene-Metal oxide composites in order to manifest distinct properties and applications.
- 5. Nanocomposites of MXene and Polymers:** Various techniques are utilised for the synthesis of MXene-polymer nanocomposites, which include physical blending, surface functionalization, in-situ polymerization, layer-by-layer assembly, encapsulation, and

template-assisted synthesis. The choice of the suitable synthesis technique is dependent on the intended application and the properties of the polymers under consideration [68].

6. **Mechanical Mixing:** The aforementioned technique is a widely employed approach in the fabrication of MXene-polymer composites. The establishment of hydrogen bonds between hydrophilic functional groups of polymers and termination functional groups, such as -OH, present on the surface of MXene, plays a crucial role in this process. The presence of hydrogen bonding facilitates the homogeneous distribution of MXene within the polymer matrix and enables the creation of composites possessing three-dimensional architectures [69]. Electrostatic interactions can also be employed in the process of physical blending. The surface of MXene, which carries a negative charge, exhibits a robust affinity for positively charged polymers due to the presence of electrostatic interactions. The phenomenon described has been documented in the context of polymers such as poly(diallyl dimethyl ammonium chloride) (PDDA) and polyethyleneimine (PEI), resulting in the augmentation of interlayer spacing and the enhancement of energy capacity in composites consisting of MXene and polymers [70,71].
- **Strategies for Surface Modification:** The objective of these strategies is to augment the stability and compatibility of MXene when combined with polymer materials. The introduction of functional groups through Ti-N bonds during the nitrogen-doping process of MXene has been found to enhance both electrical conductivity and capacitance, as reported in reference [70]. In addition, it has been observed that MXene has the capability to establish covalent bonds with polymers through esterification reactions. This interaction leads to the formation of stable networks and the improvement of mechanical properties [72,73]. This process enables the modification of hydrophilicity or hydrophobicity and enhances compatibility with various polymer matrices [74,75]. The utilisation of these synthesis strategies facilitates the fabrication of MXene-polymer nanocomposites that exhibit improved mechanical durability, structural stability, and customised surface chemistry [76]. These composite materials have various applications in multiple fields, including sensing, electromagnetic interference shielding, and energy storage [77,78]. In addition to the processes of physical blending and surface modification, various other strategies are utilised in the synthesis of MXene-polymer composites. These strategies offer alternative approaches to attain desired properties and structures in the nanocomposites.

The technique of in-situ polymerization involves the direct formation of a polymer on the surface of MXene during the synthesis process. The utilisation of this methodology facilitates the establishment of robust interfacial bonding between MXene and the polymer, resulting in improved mechanical durability and structural integrity of the nanocomposites [79,80]. Polymerization can be accomplished using different methods, including solution polymerization, emulsion polymerization, and interfacial polymerization [81–84]. The utilisation of in-situ polymerization enables precise manipulation of the composition, morphology, and distribution of the polymer within the MXene matrix, leading to customised properties that are suitable for specific applications [85,86].

- **The Process of Layer-by-Layer Assembly:** The layer-by-layer assembly method is a highly adaptable technique employed for the production of MXene-polymer composites, enabling precise control over layering and the creation of hierarchical structures. The proposed approach entails the step-by-step application of MXene and polymer layers onto a substrate, resulting in the formation of a structure composed of multiple layers. The stability of the composite film is attributed to various factors, such as electrostatic interactions, hydrogen bonding, and other specific interactions occurring between the layers. The technique of layer-by-layer assembly facilitates the integration of various polymers or functional materials, thereby facilitating the creation of composites that possess intricate structures and customised properties. In their study, Yang et al. employed a layer-by-layer assembly technique to construct multilayered nanocomposite films on a nylon membrane. The films in question were composed of sequential layers of aramid nanofiber/polypyrrole (AFPy) and waterborne polyurethane (WPU) that had been functionalized with $Ti_3C_2T_x$.
- **Application of Coating or Encapsulation:** The application of a polymer shell to coat or encapsulate MXene is a technique utilised to safeguard MXene from various environmental factors and enhance its overall stability. The polymer coating functions as a protective barrier, effectively inhibiting the contact of MXene with atmospheric elements, such as air, moisture, or corrosive agents [87–89]. In their study, He et al. (year) developed a waterborne polymeric coating on chitosan modified $Ti_3C_2T_x$ for the purpose of corrosion prevention [90]. The process was initiated by functionalizing chitosan (CS) through the use of phosphoric acid at a temperature of $120^\circ C$, resulting in the formation of modified chitosan (mCS). Following that, the researchers successfully acquired MXene.

III. STRUCTURAL CHARACTERIZATION

1. **Atomic structure characterization of MXene and MXene-based composites:** Atomic force microscopy (AFM) is a high-resolution imaging technique that is commonly used in various scientific disciplines. The aforementioned methodology is employed for the examination of surface characteristics of MXenes, encompassing parameters such as roughness and adhesion. The proposed approach involves the inclusion of data pertaining to the lateral flake dimension and its thickness. Consequently, Atomic Force Microscopy (AFM) has emerged as the primary technique for analysing two-dimensional (2D) materials. When conducting experiments utilising Atomic Force Microscopy (AFM), it is important for researchers to acknowledge the limitations associated with assessing the thickness of 2D monolayers. This thickness can vary significantly depending on the presence of adsorbents and trapped interfacial molecules [106]. Furthermore, the determination of the thickness of a single layer of 2D material involves measuring the height of the second layer, even in cases where the flakes on the substrate exhibit folded regions [107].

The utilisation of this methodology enables the examination of MXene crystals at a heightened level of detail, facilitating the analysis of their morphological characteristics and crystal lattice arrangement. Transmission electron microscopy (TEM) is a highly significant technique that utilises various forms of scattered electrons, diverse imaging modes, and compatible methodologies. To obtain a thorough understanding of these

modes, we recommend consulting the literature provided in reference [108]. The configuration of the transition metal layer can be observed using analytical electron microscopy, similar to the examination of the precursor in TEM analysis. The Z-contrast observed in well-ordered double transition metal MXenes (such as $\text{Mo}_2\text{Ti}_2\text{CT}_x$ or $\text{Mo}_2\text{Ti}_2\text{C}_3\text{T}_x$) facilitates clear visualisation and understanding of the atomic structure using high-resolution techniques. Transmission electron microscopy (TEM) poses challenges in visualising the surface functional groups due to their low weight elements and inherent randomness. Consequently, it becomes difficult to envision TEM using scanning transmission electron microscopy (STEM). Frequently, in various instances such as the Cl- terminated MXene, it is noteworthy to observe the surface termination [109]. The Energy Dispersive X-ray Spectroscopy (EDS) technique is not only familiar with Transmission Electron Microscopy (TEM), but it also provides valuable information about the material's composition [110,111]. It should be noted that EDS is unable to distinguish between O and OH groups present on the surfaces of MXenes. Additionally, it is not employed for the quantification of light elements such as oxygen (O) and fluorine (F) on the surface of MXene, or the carbon-to-nitrogen (C/N) ratio in the core layers.

X-ray photoelectron spectroscopy (XPS) is a surface-sensitive analytical technique that provides information about the elemental composition and chemical state. The process of characterization is conducted in order to investigate the chemical composition of MXenes and has the potential to identify the various types of chemical bonding that are present. X-ray photoelectron spectroscopy (XPS) is commonly utilised for the characterization of material composition. It exhibits limited penetration depth and high surface sensitivity, making it suitable for analysing surface properties. Moreover, XPS has the capability to provide information about elemental oxidation states and chemical composition, which contributes to its growing popularity in surface analysis. X-ray photoelectron spectroscopy (XPS) is a widely utilised and compelling technique for investigating surface chemistry. X-ray photoelectron spectroscopy (XPS) is widely utilised in the analysis of the configuration and surface chemistry of different MXenes [112,113]. It is also employed in the investigation of the intercalation process [114], surface treatment methods [115,116], as well as the examination of thermal stability and surface groups [117,118]. X-ray photoelectron spectroscopy (XPS) exhibits certain limitations as well. One such limitation is its inability to effectively control the charging state of the sample during the acquisition of spectra. This often leads to systematic peak shifts, which can be considered a significant constraint of the technique.

- 2. Surface Morphology and Crystalline Structure Analysis Techniques:** The X-ray diffraction (XRD) pattern exhibits distinct alterations during the transformation of MAX phase to multilayered MXene, followed by its subsequent delamination into MXene. Upon the implementation of appropriate texturization techniques, the MAX phase powders undergo a pressurisation process, as the MAX phases exhibit inherent anisotropy. The preferential alignment of particles along the (002) crystallographic planes and the excessive intensity of (001) diffraction peaks observed in all precursor materials suggest the coexistence of rival MAX phases. The implementation of texturing techniques in materials science allows for the thorough quantification of phases through the Rietveld refinement method [91,92]. This methodology is the most direct and should be prioritised as the primary characterization technique to align with the production of MXene. The methodology is executed to ascertain the crystal structure and lattice constant of MXenes.

It is a common practise to perform dual scanning of the precursor material, once with a textured surface and once without, to ensure the presence of a singular MAX precursor. It is advisable to eliminate any extraneous impurities such as carbides and intermetallic compounds, as the MXene suspension can effectively segregate them during the washing, etching and delamination processes. In the context of solid-state solutions, the lattice parameter is a direct reflection of the underlying chemistry [93–95]. It is noteworthy to acknowledge that MXene exhibits a two-dimensional structure and hydrophilic properties. The spacing between interlayers is subject to modification in order to accommodate intercalating agents. The determination of the (002) peak position provides crucial insights into the thickness of MXene sheets and the influence of surface terminations. Several investigations are currently centred on the intercalation and deintercalation mechanism of diverse intercalatants, such as organic molecules [96–99], inorganic cations [100–103], or water [104,105]. The process of intercalation has been observed to result in optical and electronic properties that are both well-regulated and tunable, as reported in reference [106]. It is imperative to acknowledge that the utilisation of X-Ray Diffraction methodology provides evidence regarding the presence of intercalated species, but it is incapable of investigating their bonding. X-ray diffraction (XRD) is utilised for the examination of water-free etching, and can provide significant insights into the properties and surface chemistry of MXene materials [107].

The electrochemical impact of protonation and deprotonation on the surface of MXene has been investigated through X-ray diffraction analysis during electrochemical processes [108]. X-ray diffraction (XRD) analysis can provide insights into the impact of etching parameters on the properties and structure of materials with crystallographic planes in the range of [109–112]. The X-ray diffraction analysis validates our endeavours to comprehend the behaviour of MXene and its tunable characteristics for surpassing the current constraints.

The high-resolution transmission electron microscopy (HRTEM) and selected area electron diffraction (SAED) analyses presented that the crystal structure of the MXene sheets derived from the MAX phases remains intact even after undergoing etching and exfoliation processes. Precise measurements are crucial in this context and require meticulous attention. Prior to usage, it is imperative to calibrate the microscope utilising a well-established reference sample, commonly composed of gold nanoparticles or film.

To obtain accurate SAED results, it is imperative to establish parallel illumination conditions and ensure precise focusing of the diffraction plane onto the CCD camera. The d-spacings are commonly determined through analysis of the selected area electron diffraction (SAED) pattern. In cases where the crystal size is below the minimum available selected area aperture, the interpretation of the SAED may pose a challenge. In this instance, the determination of d-spacings can be achieved through the acquisition of a HRTEM image followed by the application of Fast Fourier transform to the designated area of interest. It is important to note that although this method provides equivalent information, the resolution is comparatively lower and must be considered when estimating the error margin. As materials scientists, we must be mindful of these factors in our analysis.

The electron beam's high coherence poses a challenge to interpreting TEM images. However, as materials scientists, we recognise scanning transmission electron microscopy (STEM) as a highly effective method for crystal structure visualisation. STEM allows for atomic-scale observation of materials with contrast dependent on their elemental composition. Currently, this technique reigns supreme in the realm of direct characterization and comprehension of the atomic structures of MAX phases and MXenes. A subatomic-sized beam is utilised in the field of materials science to scan across the sample. The electrons that are scattered forward are then detected by an annular dark-field detector. The acquisition of distinct image types is contingent upon the variation of collection angles. At elevated angles, the imaging technique employed is referred to as high-angular annular dark-field (HAADF) imaging. In the context of 2D materials, it is observed that the thickness of the material increases in integer values, which corresponds to the number of sheets. For a single 2D sheet, this increase in thickness can be neglected in a preliminary analysis. Therefore, the contrast observed in the material is directly proportional to the atomic mass. The limitations of the technique manifest as insufficient scattering and consequent detection of feeble signals from the less dense elements such as carbon, oxygen, and fluorine, which are of significant interest in the study of MXenes. This results in their inability to be distinguished from the heavier elements like titanium and molybdenum, which can be precisely identified using high-angle annular dark-field imaging.

This methodology can be employed to visualise the structural arrangement of MXene. The preparation of MXene involves the utilisation of highly concentrated HF, and the characteristic "accordion" morphology is a prominent aspect of efficient synthesis. The SEM technique was utilised to observe the changes in the structure, revealing that the "accordion" structure was less prominent with decreasing HF concentration, resulting in a more typical MXene structure. The observed trend indicates that an increase in HF concentration promotes greater hydrogen evolution, resulting in structural expansion. A reduced concentration of hydrofluoric acid (HF) elicits minimal to negligible alterations in the morphology of the particles. The MILD technique, as elucidated by the researcher [113], exhibits a structure akin to that of a low concentration HF MXene. It is noteworthy that MILD methods are recognised as in-situ methodologies. The XRD analysis fails to detect the oxidation mechanisms due to the amorphous nature, minute size, and lower quantity of the oxide produced. Detection of these mechanisms can be achieved through XPS or Raman spectroscopy.

IV. ELECTRICAL AND ELECTROCHEMICAL PROPERTIES

1. Electrical Conductivity and Resistivity Characteristics of MXene Materials

- **Conductivity of Metals:** The attribute of electrical conductivity plays a crucial role in the electrochemical mechanisms of energy storage, facilitating rapid redox reactions [114]. MXenes exhibit high electrical conductivity as a result of the covalent bonding between their alternating carbon layers and transition metals, facilitating fast and efficient electron transport within the electrodes [115,116]. As a result, the effective transportation of electrons within the MXene electrode facilitates rapid rates of charging and discharging, as well as easy storage and release of energy, accompanied by swift redox reactions. In addition, the exceptional conductivity of MXene results in

reduced resistance in energy storage devices, thereby minimising losses during the processes of charging and discharging [117].

Interlayer distance in MXene-based composites can be effectively preserved by incorporating appropriate materials, including cationic surfactants, carbon materials, and polymers [118–121]

- **Mechanical Durability:** The mechanical stability of MXene materials in the context of energy storage can be attributed to the robust chemical bonding that exists between the transition metal layers and carbon layers. The structural integrity and mechanical durability of MXenes are attributed to the bonding interactions, which primarily consist of covalent and metallic bonds [122]. The presence of covalent bonds among carbon atoms within the carbon layers contributes to the structural stability of the MXene material, thereby impeding its susceptibility to deformation or disintegration. The mechanical strength of MXenes is further enhanced by the metallic bonding that occurs between the transition metal layers and carbon layers. The presence of these bondings in MXene materials contributes to their ability to endure mechanical stresses and strains that occur during energy storage processes. As a result, MXene materials exhibit mechanical robustness, rendering them suitable for demanding applications in the field of energy storage.
- 2. Influence of Electrical Properties on Sensing Performance:** MXenes, owing to their exceptional properties, have been employed as highly promising materials in the advancement of diverse sensing devices. These devices encompass electrochemical and fluorescent sensors, which enable the analysis of trace level target analytes. The utilisation of pristine $Ti_3C_2T_x$ was employed as an electrochemical sensor for the purpose of detecting carbendazim [123]. The integration of palladium nanoparticles (Pd NPs) with titanium carbide ($Ti_3C_2T_x$ MXene) resulted in a significant enhancement in the electrocatalytic performance of the sensor. This remarkable improvement enabled the sensor to achieve an impressive detection limit of $0.14 \mu M$ while maintaining immunity to interference from other chemical species. In a similar vein, an electrochemical sensor was fabricated to detect methamidophos by employing a modified glassy carbon electrode (GCE) with nanocomposites of metal-organic framework (MOF)- Ti_3C_2 and gold nanoparticles (Au NPs) [124]. In this study, a composite material consisting of 3D manganese dioxide ($3DMnO_2$) and manganese(II,III) oxide (Mn_3O_4) was subjected to a treatment involving titanium carbide (Ti_3C_2) and gold nanoparticles (Au NPs). The purpose of this treatment was to fabricate electrochemical sensors that possess desirable characteristics such as biocompatibility and a large specific surface area. The researchers strategically engineered MXene, a two-dimensional material, to possess versatile properties that enable seamless integration with microfluidic chip technology. The method developed in this study was further employed for the continuous monitoring of whole blood in order to detect changes during hemodialysis.

The electroanalytical methodology that was devised exhibited successful application in the detection of bromate ions within water samples. In a recent study, the utilisation of ZnS nanoparticles (NPs) incorporated with Nb_2C MXene nanocomposites has been explored for the purpose of differential pulse voltammetry in the detection of dopamine [125]. The GCE was enhanced by the incorporation of ZnS nanoparticles (NPs)

into Nb₂C MXene nanocomposites. Considering the aforementioned, the Gas Chromatography-Electrochemical (GCE) system underwent alterations by incorporating Ti₃C₂-/ZIF-67/CNTs nanonetworks to enhance its capabilities for the electrochemical detection of luteolin, as reported in reference [126]. In the first step, ZIF-67 was synthesised and deposited onto the carbon nanotube (CNT) substrate. This composite material was then immobilised onto the surface of Ti₃C₂ MXene, with the aim of improving its catalytic performance and facilitating the electrochemical reaction involved in the redox process of luteolin. As a result of this modification, the material exhibited a limit of detection (LOD) of 0.03 nM, indicating its high sensitivity for detecting luteolin.

- 3. Electrochemical Behaviour and Applications in Sensing Modes:** The electrochemical technique is prominently featured in heavy metal detection due to its advantageous characteristics. This method offers a cost-effective, time-efficient, and economical instrument with remarkable sensitivity, straightforward operation. In comparison to spectroscopic techniques, the electrochemical method exhibits a relatively shorter analytical time. In the realm of electrochemical techniques, the presence of heavy metal contaminants within water induces alterations in various electrical signals, including but not limited to voltage, charge, current. These signals are essentially derived from various analytical methods such as potentiometry, amperometry (chronopotentiometry), voltammetry (cyclic voltammetry), pulse voltammetry (square-wave anodic Potentiometric techniques are frequently utilised in the quantification of ions present in solution. The limitations pertaining to sensitivity and detection limit represent the primary challenges encountered in the realm of electrochemical techniques. The amperometry method involves the measurement of the current flow resulting from the reduction of heavy metal species, which occurs upon the application of a constant voltage between the working and reference electrodes [127]. By applying a fixed potential, it becomes possible addition, the voltammetry method is commonly employed in the field of materials science for the purpose of heavy metal detection. This technique allows for the generation. The metal ions are basically undergone a faradaic redox reaction under these techniques. The surface of the electroactive material has been meticulously examined and strategically altered to enhance its performance in the metal detection application. In their study, Sathiyarayanan et al. [128] confirmed that the measurement of an electrical potential is obtained by measuring the applied current. Ion-selective electrodes (ISEs) are highly specialised electrochemical sensors that possess the remarkable ability to convert ionic signals into electrical signals [129], it has been observed that ion-selective electrodes (ISEs) Glass membrane electrodes, also known as pH electrodes, are utilised in various applications to measure the acidity or alkalinity of a solution. Crystal membrane electrodes, such Membranes are categorised within the realm of solid-membrane electrode materials [130].Enzymatic membranes, liquid ion-exchanging system membranes, and membranes with organic complexing agents are classified as liquid-membrane electrodes. Ion-selective electrodes (ISEs) are commonly employed in the field of materials science to investigate the properties of various materials. These electrodes operate based on the fundamental principle of potentiometry ISEs (ion-selective electrodes) are known for their remarkable characteristics, including an exceptionally low limit of detection (LOD) Despite the diligent efforts of researchers, the development of highly efficient ion-selective electrodes (ISEs) for the detection of heavy metal ions remains a challenge.

V. MECHANICAL AND THERMAL PROPERTIES

- 1. Mechanical Strength and Flexibility of MXene and Composites:** The mechanical properties of MXenes arise from the unique amalgamation of M and X atoms. Although an investigation has been conducted to examine the mechanical characteristics of MXenes, it is worth noting that the extensive body of literature pertaining to three-dimensional crystallised binary transition metal carbides/nitrides could potentially aid in elucidating the essential attributes of MXene. Transition metals exhibit a diverse array of bonding interactions with carbon (C) and nitrogen (N) atoms, encompassing ionic, covalent, and metallic bonding mechanisms. The electron orbitals denoted by 'd' and 's' in transition metals, along with the 'p' orbitals of carbon (C) or nitrogen (N), play a significant role in this phenomenon. The primary interatomic connections within the (M–X) structure are hypothesised to arise from the establishment of ionic bonds, wherein electrons are transferred from the M species to the X species, as well as covalent bonds. The intricate arrangement of the crystal lattice in transition metal carbides and nitrides significantly influences the covalent bonding interactions employed within their structures. Due to the significant spatial separation between (X–X) entities, the feeble intermolecular forces result in negligible influence of (X–X) bonding on the macroscopic arrangement. During the process of hydrolysis, it has been observed that MXenes exhibit a notable propensity for generating methane gas. This occurrence can be attributed to the influence of weak interactions, specifically the (X–X) interactions present within the structure. Transition metals form intermetallic bonds through the utilisation of their d orbitals, thereby establishing connections with neighbouring transition metal atoms in a manner that obviates the requirement for carbon or nitrogen atoms [131]. Although (M–M) bonds contribute only minimally to the overall matrix binding energies, (M–X) bonds exhibit significant influence in this regard. Among the various orbitals, it is noteworthy that only a pair of them exhibit antibonding characteristics, thereby displaying a preference for engaging in interactions with transition metals. Moreover, the presence of a carbon/nitrogen deficiency enhances the influence of metallic bonding while diminishing the significance of ionic/covalent (M–X) bonding in relation to the overall binding energies of the matrix. [132,133].
- 2. Impact of Mechanical Properties on Sensing Device Design and Performance:** In addition to possessing exceptional electronic properties, MXenes exhibit inherent hydrophilicity attributed to their surface functional groups. This characteristic imparts MXenes with significant potential in the realm of wearable sensors. MXenes, as a class of two-dimensional materials, exhibit the remarkable ability to undergo selective adsorption of biomolecules such as glucose and dopamine, as well as gas molecules like NH₃ and NH₄. This unique capability is achieved through precise control of their morphology and surface modification, resulting in consequential alterations to their electrical properties. In the realm of MXenes, the primary constituents (known as M-layer elements) consist of early transition metals, including but not limited to tantalum (Ta), titanium (Ti), and niobium (Nb). These metals exhibit a notable resistance to the activities of biological organisms, thereby imparting MXenes compounds with remarkable biocompatibility. The *in vivo* experiments conducted by Lin et al. (2017) demonstrated the potential degradation and elimination of MXenes within the murine biological system[134].

The strain sensor with flexible properties exhibits the ability to convert applied tensile strain into an output signal representing changes in resistance [135]. When an external force is exerted upon the sensor, the internal conductive materials or networks will experience cracking as a result of the external forces. This cracking phenomenon subsequently leads to alterations in the electrical characteristics[136].

The constituent elements are arranged in a highly compact and orderly manner, exhibiting a closely stacked configuration. Adjacent sheets in a material system can potentially experience intermolecular forces, specifically Van der Waals forces, which arise from the interactions between temporary dipoles induced by fluctuations in electron distribution. These forces play a significant role in the overall stability and behaviour of the material. of external forces, the material undergoes deformation, resulting in changes in its shape and size. This deformation can be either elastic or plastic, depending on the properties and the magnitude material.

Due to the presence of external stress, the sheets exhibit limited capacity for effective sliding, instead primarily dispersing the stress through the generation of substantial cracks. The dimension of the crack exhibits a direct proportionality to the applied stress. In the event that the external force surpasses a certain threshold, it will impede the conductive pathway, thereby significantly constraining the potential enhancement of both sensing range and stability.

VI. ENHANCEMENT OF SENSING CAPABILITIES THROUGH PHYSICOCHEMICAL PROPERTIES OF MXENE COMPOSITES

The potential integration of MXene heterostructures with various 2D materials presents a promising and captivating avenue for advancing electrochemical sensing applications. The integration of diverse combinations and fabrication of 2D MXene heterostructures can be achieved through the manipulation of surface chemistry, including phenomena such as H-bonding, charge transfer, covalent bonding, and p-p interaction. This enables the utilisation of advanced electronic technology in the development of these materials.

By imbuing the MXene heterostructure-based electrochemical sensor with exceptional analytical capabilities, we can enhance its practicality in various sensing applications. However, the fabrication process of 2D MXene in conjunction with other 2D materials presents various challenges, which are contingent upon the specific functional groups present on the surface sheets of the 2D materials. The ongoing research trends advocate for numerous enhancements in the manufacturing processes of 2D MXene materials, as well as the utilisation of 2D MXene-2D material heterostructure compounds in the realm of electrochemical sensors in the foreseeable future. Further investigation is necessary to surmount the challenges associated with the synthesis of MXene, with the aim of developing a straightforward, safer, more sustainable, and environmentally-friendly etching technique. Furthermore, the utilisation of an etching technique involving a limited set of pivotal variables, namely heating duration and temperature, presents a highly promising avenue for the synthesis of MXene materials, particularly when considering the potential for large-scale production.

Moreover, it is indisputable that the 2D MXene heterostructure compound exhibits immense promise in the realm of analyte detection encompassing a wide range of substances including metal ions, biomarkers, and micropollutants such as hormone endocrine, personal care products, and pharmaceuticals. Due to their rapid analytical capabilities, exceptional sensitivity, in-field detection capabilities, cost-efficiency, and miniaturisation potential, electrochemical sensors have garnered significant interest from the scientific community and researchers alike. Therefore, the facile patterning methodologies employed for the fabrication of the electrodes accentuate the remarkable potential utility of the sensor in the realm of cutting-edge technological advancements.

1. Specific examples of MXene-based Sensors for Gas and Chemical Detection: In addition to the utilisation of electrochemical biosensors, MXene materials have exhibited significant advancements in the realm of gas sensing applications. The determination of volatile organic compounds (VOCs) at ultratrace levels (parts per billion) is of utmost importance in the field of pollution analysis, as well as in the detection of toxic gases and the analysis of therapeutic breath for the early identification of various diseases.

The detection of ammonia plays a crucial role in the diagnosis of peptic ulcers caused by *H. pylori* and the identification of lung disorders. Similarly, the affirmative identification of acetone within the exhaled breath of an individual signifies the initial manifestations of diabetes. MXene materials have garnered significant attention in the realm of solid-state gas sensors due to their exceptional properties. These materials exhibit low electrical noise, making them ideal for detecting gaseous molecules with remarkable signal intensity. Moreover, MXene materials offer high manufacturing substrate flexibility and portability, further enhancing their appeal in gas sensing applications. In a conventional investigation, the gas sensing capabilities of $\text{Ti}_3\text{C}_2\text{OH}_2$ MXene were examined in the presence of various gases, including acetone (CH_3COCH_3), ethanol ($\text{C}_2\text{H}_5\text{OH}$), ammonia (NH_3), propanal ($\text{C}_2\text{H}_5\text{CHO}$), nitrogen oxide (NO_2), and sulphur dioxide (SO_2), under ambient conditions. The $\text{Ti}_3\text{C}_2\text{OH}_2$ MXene sensor exhibited a discernible increase in the electrical resistance within the sensing channel upon gas absorption. The MXene sensor exhibits superior performance compared to other semiconducting sensors in the detection of gases. This is due to the fact that the sensing response is influenced by the electron-donating or electron-accepting properties of gases, as well as the charge carrier (either p-type or n-type) present in the sensing channel [50]. In a separate investigation, a monolayer of Ti_2CO_2 MXene was synthesised, demonstrating its efficacy as a highly proficient substrate for NH_3 sensing (as depicted in Figure 3a). The investigation focused on exploring the potential application of Ti_2CO_2 surface as a gas sensor by studying the adsorption behaviour of different gases, including NH_3 , H_2 , CH_4 , CH_3COCH_3 , CO_2 , N_2 , NO_2 , and O_2 .

VII. BIOSENSING

1. Utilization of MXene and Composites in Biosensing Applications: MXenes have found extensive applications in the field of electrochemical biosensors. This is primarily attributed to their remarkable characteristics, such as a large specific surface area. Furthermore, owing to their redox properties, MXenes exhibit the dual characteristics of being both electron transfer promoters and reaction catalysts. Henceforth, MXenes exhibit exceptional potential as promising emerging two-dimensional materials for the

fabrication of electrochemical biosensors. Pure MXene-based biosensors. As a materials scientist, it is intriguing to explore the unique attributes of MXenes as sensor materials. MXenes exhibit a multitude. In order to advance the utilisation of MXenes, researchers have undertaken essential investigations to broaden the scope of their applications. MXene offers a favourable microenvironment for the enzyme haemoglobin (Hb), thereby safeguarding its integrity and preventing its degradation. Furthermore, the advantageous enzyme immunity exhibited by an MXene material is highly favourable for the stabilisation and functionality of Hb (haemoglobin). The obtained results demonstrate that the exceptional properties exhibited by MXenes make them highly suitable as substrates for enzyme-based electrochemical biosensors. Furthermore, the observed augmentation in the density of states (DOS) subsequent to the interaction between aminazole and terminal fluoride provides additional evidence supporting the MXene, a novel two-dimensional material, has garnered attention in the scientific community due to its exceptional performance as a nanozyme. Based on this premise, the utilisation of MXene has been progressively employed in the advancement of electrochemical sensors. In a groundbreaking development, the incorporation of MXene material has been successfully implemented in an advanced molecularly imprinted electrochemical sensor (MIECS). After extensive experimentation, it is with great satisfaction that we report the successful attainment of a significantly reduced detection limit for the sensor. MXenes, being a class of two-dimensional transition metal carbides/nitrides, exhibit a plethora of distinctive attributes the presence of numerous functional groups and diverse terminal types on the surfaces of MXenes offers substantial evidence for the facilitation of metal ion reduction and the existence in conjunction with the distinctive multilayer architectures exhibited by MXenes and the relatively feeble interlayer forces, the facile insertion and anchoring of metal nanoparticles is facilitated [99]. In subsequent studies, additional metal nanoparticles, such as silver (Ag[102]) and platinum (Pt[103]), have been successfully incorporated onto the surface of order to enhance the signal amplification, novel composites of MXene have been fabricated, incorporating bimetallic nanoparticles The synthesis of $Ti_3C_2/Au-Pd$ was carried out using a comparable self-reducing approach, taking into consideration the reducibility levels The two metal particles are strategically immobilised on the surfaces of MXene, resulting in enhanced signal amplification. Consequently, the The electrochemical biosensor was effectively utilised for the detection of pear and cucumber samples. The experimental findings demonstrate that the sensor in question exhibits superior performance compared to the majority of previously reported differential pulse voltammetry (DPV) sensors. It is important to acknowledge that the detection performance has the potential for enhancement when considering an ideal structure. A novel cobalt-doped Ti_3C_2 MXene nanozyme was successfully synthesised, exhibiting remarkable peroxidase-like characteristics. A novel approach was devised in the field of materials science to investigate the determination of organophosphate pesticides.

VIII. ENVIRONMENTAL SENSING

- 1. Applications of MXene and Composites in Environmental Sensing:** The presence of heavy metal ions in the biosphere poses a significant threat to living organisms and is a major concern for human health. The lack of access to pure drinking water contributes to the spread of waterborne diseases, while heavy metals such as arsenic and radioactive

materials can lead to cancer. Therefore, the detection and removal of heavy metal ions are crucial for sustaining life.

In recent years, MXenes have emerged as a promising class of 2D nanomaterials with great potential for sensing and adsorbing heavy metal ions. Developed in 2011, MXenes offer several advantages over existing sensing materials, including enhanced hydrophilicity, efficient electron transportation, versatile functionalization, and a wide range of compositions. These properties make MXenes highly suitable for heavy metal ion sensing applications. This work provides insights into the chemistry and synthesis of MXenes, focusing on their utilization as sensors for heavy metal ion toxicity. MXenes exhibit excellent efficiency and sensitivity, making them superior alternatives to traditional sensing materials. Furthermore, their unique properties enable the detection and removal of heavy metal ions from environmental systems, contributing to the preservation of clean and safe water resources.

Despite the significant progress made in MXene-based sensing, several challenges remain to be addressed. Further research is needed to explore the full potential of MXenes in environmental systems, optimize their sensor performance, and enhance their selectivity for specific heavy metal ions. Additionally, efforts should be directed towards developing practical and scalable MXene-based sensor devices for real-world applications.

In conclusion, MXenes hold great promise as emerging sensors for the detection and removal of heavy metal ions. Their unique characteristics and versatile nature make them valuable tools in the quest for clean and safe water resources. Continued research and development in this field will contribute to the advancement of MXene-based sensing technologies and their widespread implementation in environmental monitoring and remediation strategies the contamination of drinking water by heavy metals such as arsenic, cadmium, lead, and mercury. Here is a summary of the main points:

- **Arsenic Contamination:** Arsenic is a prevalent problem worldwide, particularly in countries like Bangladesh, Chile, India, Taiwan, and Mexico. Industrial sources, including pharmaceuticals, herbicides, insecticides, wood preservatives, fungicides, and dyes, contribute to arsenic contamination. Arsenic toxicity varies with its valence, with As(III) being twenty times more toxic than As(V) and seventy times more toxic than organic arsenic compounds.
- **Cadmium Contamination:** Cadmium contamination arises from geologic sedimentary rocks, metallic ores, sulfides, sulfates, cigarette smoke, and cadmium-contaminated foods. Industrial activities such as smelting, pigmentation, and stabilizer utilization also contribute to cadmium contamination.
- **Lead Contamination:** Lead toxicity in drinking water is primarily caused by historical use of lead in plumbing. Large-scale utilization of batteries, farming, missiles, X-ray shields, dyes, and glass also lead to lead contamination.

- **Mercury Contamination:** Industrial contamination and burning of fossil fuels release mercury in inorganic forms, which can be transformed into organic forms such as methylmercury. Organic mercury complexes bioaccumulate in foods, posing a significant exposure hazard.

The presence and behavior of these heavy metals are influenced by factors like pH, dissolved oxygen content, redox potential, and temperature. The World Health Organization (WHO) recognizes lead, arsenic, cadmium, and mercury as major public health concerns due to their associated hazards, including cancer, age-related anomalies, neurological disorders, organ failure, and mortality. The specific form and valence of heavy metals have a significant impact on their toxicity and mobility.

Please note that this summary provides a condensed overview and may not encompass the entirety of the original content.

2. Sensing of Pollutants, Heavy Metals, and other Environmental Parameters

- Provide examples of MXene-based sensors for detecting specific environmental contaminants
- Discuss the sensing mechanisms and performance characteristics of MXene-based environmental sensors

- ### 3. Contribution of MXene Physicochemical Properties to Environmental Sensing Effectiveness:
- Transition metal ions, such as mercury (Hg), lead (Pb), chromium (Cr), cadmium (Cd), copper (Cu), iron (Fe), and manganese (Mn) undergo dissolution in water bodies and subsequently migrate to the surface water following discharge, thereby presenting a significant hazard to both human health and aquatic organisms. Henceforth, the identification and mitigation of these perilous contaminants (specifically heavy metal ions) emerge as the primary focal point. There exist a multitude of conventional methodologies that are currently being employed for the aforementioned purpose [137–139]. However, it is important to note that these techniques possess inherent limitations that restrict their practical implementation in real-world scenarios. Therefore, the emergence of electrochemical or chemical sensing has provided a reliable tool for the rapid identification and removal of these hazardous pollutants from waste water. Various nanomaterials and hybrid composites are being employed for the purpose from the last few decades. In recent times, a highly promising modality has emerged in the realm of materials science, specifically in the form of MXene-based composite electrodes. This technique was employed. The research team observed that the intercalated MXenes exhibited a superior electrochemical response in alkaline media when compared to the detection limits of various heavy metal ions, such as Hg^{2+} , Cd^{2+} , Cu^{2+} , and Pb^{2+} , are in the millimolar range.

IX. FUTURE PERSPECTIVES AND CHALLENGES

- ### 1. Potential Research Directions for MXene and Composites in Sensing Applications:
- MXenes have grown in prominence despite having a very limited lifespan because of their distinctive layered shape and rare metallic/catalytic characteristics. MXene-based sensing techniques have been regarded as highly sophisticated detection methods in a

variety of fields, including medicine, the environment, and public health. The very reproducible results provided by the developed MXene sensors/biosensors over a long period of time and their long-term stability make it potentially very advantageous to use these sensors for a variety of diagnostic applications. However, due to the dearth of information on other transition metal MXene-based detection systems, titanium carbide is the only MXene in the field of sensing that has been extensively studied. Given the material's incredible sensing capabilities, the current scenario necessitates intensive scientific work to take advantage of alternative transition metal-based materials.

- The number of developed MXenes for this purpose remains limited. The design of MOF composites can leverage the types, derivatives, and dimensions of MXenes to achieve outstanding structure and properties. For instance, 1D MXene fibers exhibit excellent ductility, making them suitable for freestanding flexible and wearable energy storage devices. TiO_2 nanoparticles derived from $\text{Ti}_3\text{C}_2\text{T}_x$ MXenes have shown potential in photocatalysis due to their wide band gap, stable dielectric constant, and high-temperature resistance.
- Interface engineering is an attractive strategy for constructing heterostructures. MXenes can be functionalized on their surfaces to promote covalent or noncovalent interactions with organic ligand groups. Ligands containing planar aromatic rings and spatial effects can be employed to design hierarchical heterostructures. MXene heterojunction structures, with accelerated interface charge separation and transfer, hold promise for applications in batteries, supercapacitors, electrocatalysis, photocatalysis, and other fields.
- The synthesis methods for MXenes (etching MAX with HF) and MOFs (high temperature and pressure) are not environmentally friendly and hinder their practical application. The development of green and cost-effective synthesis strategies is crucial for large-scale production and has gained considerable attention.
- The characterization technology and theoretical simulation of MXene structures are still in the early stages. While common characterization techniques like SEM, TEM, XRD, XPS, and Raman spectroscopy have been used, advanced techniques such as in-situ XRD and in-situ TEM characterization allow for real-time monitoring of changes during reactions. Analog computing technology, such as Density Equalizing Tensorial Electrodynamics (DET), has also been employed to study charge density distribution, density of states, and other properties.

X. CONCLUSION

The provided text discusses various factors that can influence the properties and applications of MXene materials, as well as the key issues and areas of exploration in the field. Here is a summary of the main points:

- 1. Factors Affecting MXene Preparation:** Etching temperature, types of etchers, and reaction time play crucial roles in MAX stripping, MXene productivity, and properties. Different etchers can introduce different functional groups to the MXene surface, altering its intrinsic characteristics and affecting performance. Surface properties of MXene are

essential for understanding its behavior and application. In situ etching, electrochemical etching, and molten salt methods are commonly used approaches with their own influencing parameters and preparation mechanisms.

- 2. Modification and Structure Optimization:** MXene can be modified to meet specific demands and optimize its structure. Different modifications and structures can significantly impact electrochemical, photothermal, microwave absorption, hydrophilic/hydrophobic characteristics, as well as properties like friction, adhesion, conductivity, and photothermal conversion. Exploring these properties expands MXene's application fields.
- 3. Surface Modification and Interface Engineering:** Surface modification can enhance the mechanical properties, thermal stability, chemical stability, and antioxidant performance of MXene. While most composite materials rely on physical interactions at the interface, exploring chemical bonding cooperation can improve their overall performance. Further understanding of the influencing mechanisms of MXene composite properties is needed.
- 4. Applications in Environmental Pollutant Control:** MXene has shown promise in the removal of heavy metals from synthetic wastewater. Further exploration can focus on removing pollutants in various media (air pollution, solid waste) and complex environments. The use of databases and computational models can aid in addressing synthesis parameters, modification, and positive/negative factors for MXene applications.
- 5. Engineering Practice and Carbon Reduction:** MXene's advantages can be extended to contribute significantly to carbon reduction programs and find applications in engineering practice.
- 6. Occupational Hygiene, Environmental Concerns, and Laboratory Safety:** Given the use of chemicals in MXene synthesis and modification, occupational hygiene, environmental impact, and laboratory safety should be considered.

In conclusion, further advancements in MXene synthesis, modification, characterization, and application are needed. Databases, computational models, and exploration in pollutant removal, carbon reduction, complex environments, and safety considerations can enhance the understanding and utilization of MXene materials in various fields.

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