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ENHANCING WATER PURIFICATION EFFICIENCY THROUGH MACHINE LEARNING-DRIVEN MXENE FUNCTIONALIZATION

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ABSTRACT

Water purification is critical for sustaining life and safeguarding public health, yet existing methods face challenges such as low efficacy and high costs. This research examines the potential of MXENE materials to address these issues due to their unique structure and properties. The study aims to enhance MXENE functionalization techniques to maximize their effectiveness in water filtration through the application of machine learning approaches. By investigating various functionalization methods and leveraging machine learning to optimize MXENE characteristics, the research seeks to advance water purification technology. The novelty of this research lies in its integration of machine learning-driven methods for MXENE functionalization in water purification. By exploring novel approaches to modify MXENE characteristics and improve water filtration efficiency, the study contributes to addressing global water purification challenges. The study begins with an in-depth overview of MXENE substances, their synthesis techniques, and their relevance to water purification. It then delves into different functionalization procedures, emphasizing the importance of tailoring MXENE characteristics for specific water treatment applications. Machine learning approaches are proposed to forecast and optimize MXENE properties for enhanced water purification efficacy. The research demonstrates the potential of machine learning-driven MXENE functionalization in improving water purification processes. By optimizing MXENE characteristics, the efficacy of water filtration is significantly enhanced, addressing current limitations in purification technologies. The study concludes by highlighting the significance of its findings in addressing global water purification challenges. By overcoming obstacles through innovative approaches and leveraging machine learning techniques, the research underscores the potential impact of MXENE-based water purification methods in ensuring universal access to clean water.

Keywords: *Machine Learning, MXENE, Functionalization, Water Purification, Adsorption, Surface Chemistry.*

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1. INTRODUCTION

Over the past 50 years, there has been a sharp rise in the amount of water consumed worldwide as a result of urbanization and industrialization. The primary causes of the rise in water pollution are human activities and poor handling of natural water resources. For instance, many recent research proved that synthetic contaminants that are becoming more urgent may be discovered globally in raw and finished drinking water as well as wastewater influents and effluents at extremely low levels. Water and wastewater treatment facilities have used a variety of conventional and cutting-edge treatment techniques, such as membranes, ultrasonication, ozonation, chlorination, coagulation/flocculation/sedimentation/filtration, and carbon/nanomaterial adsorption, to treat both established and emerging contaminants. Recent years have seen a large increase in the usage of membrane technologies for the purification of water and sewage [1]. In the last several decades, membrane separation has emerged as a viable technology among traditional liquid-separation techniques including evaporated water, distillation, crystallization, and filtering due to ecological and energy concerns. The chemicals in nature, medicine, and water sectors have made substantial use of membrane separation as well as purification because of their many advantages, which include low carbon emissions, high dependability, ease of use, and less secondary contamination. However, the compromise between membrane flux and selectivity usually prevents membrane separation processes from proceeding. Numerous research has looked at creating new membranes with different nanomaterials, including MXenes, carbon nanotubes, graphene oxides, and metal-organic frameworks, to address this problem. 72 MXenes, a new family of two-dimensional materials made of titanium carbide (Ti3C2Tx), were first created in 2011 by researchers at Drexel University [2]. Because of their outstanding durability, huge surface area, high electrical/thermal conductivity, superior oxidation resistance, and hydrophilicity, these nanomaterials have grown in popularity [3]. Much recent research has looked at the ecological uses of various MXenes in membranes and adsorption catalysis.

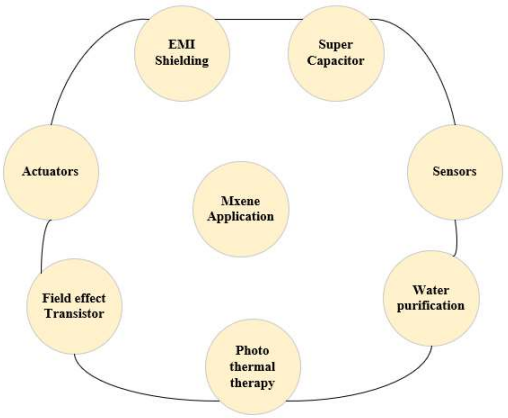

Figure 1: MXene Applications

MXene-based membranes should be able to separate materials effectively, operate safely over an extended period, and be manufactured using environmentally friendly methods. These factors are greatly impacted by the equilibrium, dispersion, and hydrophilic properties of MXenes. Fig 1 depicts the MXene applications. Due to its amazing features, two-dimensional (2D) materials gained considerable curiosity among scientists and scholars after the finding of graphene in 2004 [4]. MXenes have kept the curiosity of researchers and scientists since the day they were discovered because of their diverse range of intriguing mechanical, magnetic, electrical, and chemical characteristics. The MXene group consists of transition metals like C2-2,N-3,or MCN. These are two-dimensional nanolayers that have a planar size of a few millimetres and an outer layer of many atoms. Because of their many special qualities, MXene materials are appealing and fit for an extensive variety of uses. They have good mechanical, electrical, and physicochemical qualities, a substantial specific surface area, and outstanding biocompatibility, to name a few. Due to their distinct physicochemical properties, two-dimensional materials, like MXenes, received an abundance of interest. In this regard, MXenes are also highly intriguing due to their large interlayer spacing, great biocompatibility, atmospheric flexibility, and relative safety [5].

MXene nanomaterials can be expressed generally as M_(n+1) X_n T_x [6], where T stands for groups of terminal surfaces like (F) [7], (O) [8], (Cl) , and (OH) [9], and x is the number of surface functionalities. M is a newly formed metal (such as W,Mo,Cr,Ta,V,Nb,Hf,Zr,Ti,Y,or Sc) [10]. MXenes typically have a thickness of 1 nm, which varies according to the concentration of n in MXenes (M_(n+1)+X_n T_x). Typically, in the MAX phase, an octahedral M_(n+1)+X_n structure with a strong

MeX link and a comparatively weak bond encases the A layer. The initial Mxene was made of (Ti3C2) it was developed by using (HF) for etching the aluminium atoms specifically, over ambient temperatures in stacked hexagonal ternary carbide, or Ti3AlC2. Approximately thirty MXene compositions have been documented in the literature thus far, all of which were created from the progenitors of the MAX phase by adding more than one transition metal to the M layers. Ti3C2Tx [11] and Ti2CTx are two of the most often utilized titanium-based MXenes in environmental applications. Alternate MXenes compositions with nitride along with carbonitride were utilized as well in a variety of uses besides C2-2 [12]. MXenes' distinct layered structures and two-dimensional morphology make it simple to combine them alongside other materials to create a composite that improves both of their features. MXenes exhibit remarkable properties that render them a highly desirable option for a variety of purposes, such as nonetheless restricted to ecological rehabilitation, storing energy, gadgets, sensors, water separation, and catalytic processes. These attributes include high surface area, activated MOH, biocompatibility, quick functionalization, high metallic conductivity, and hydrophilicity. MXenes has also been researched as a potential new material for adsorption, membranes, and capacitive deionization processes used in water purification. The assessment of MXenes and MXene-based composite materials for the removal of different contaminants from water, including a focus on radionuclides, dyes, and heavy metals [13].

According to experimental data, the distribution of various functional groups on MXene surfaces varies depending on the etching process. Because of their varied chemistries, MXenes exhibit a wide variety of intriguing electrical, mechanical, magnetized, and electrochemical properties. MXenes in particular have high flexibility and can easily create composites using other substances because of their 2D shape and layered structures. This allows for the complementing integration of the exceptional capabilities of other materials [14]. Consequently, they now have MXenes as well as MXene-based compounds. garnered a lot of attention from researchers due to their promising nature. MXenes and MXene-based compounds are originally used in the storage of energy as powerful electrode materials for lithium-sulfur batteries and sodium-ion batteries because of their high permeability and strong electrochemical performance. That they have become even more well-known in environmental domains in recent times is remarkable. In particular, they can remove contaminants in water like ions of heavy metals, organic colors, saturated chemicals, and atomic waste; they have been used as efficient catalysts or co-catalysts for electro/photocatalytic extraction of water and photocatalytic carbon dioxide elimination. Their use has been utilized in biosensors and sensors for gases, exhibiting excellent performances.

MXenes exhibit a range of unique and beneficial properties, including tuneable Young's modulus, enhanced thermal and electric conductivities, and hydrophilicity. Their mechanical properties, characterized by strong M-N and M-C bonding, make them suitable for composite reinforcement materials despite lower elastic properties compared to graphene. MXenes also interact well with polymeric matrices, enhancing their utility in composites. The hydrophilic nature of MXenes, such as Ti3C2Tx, along with their bending characteristics, further distinguishes them. Electronically, MXenes can be tailored by altering functional groups and material balance, impacting their conductivity. Their electrical conductivities surpass those of graphene oxide and MoS_2 [15], and can vary significantly based on surface functionalities, defect concentration, and lateral dimensions. Surface variations through alkaline and thermal procedures can enhance electrical properties. Optically, MXenes exhibit notable light absorption in the UV-visible region, with transmittance affected by thickness and ion intercalation. They can absorb light energy effectively for applications like photothermal therapy [16]. Thermally and oxidatively, MXenes demonstrate stability challenges in the presence of water/oxygen, but stabilization techniques like carbon nano-plating and storage in oxygen-less environments improve their stability. MXenes can exhibit magnetic properties depending on surface functionalities and elemental compositions, although many are nonmagnetic due to strong covalent linkages. Their hydrogen storage capabilities, achieved through physisorption, chemisorption, and Kubas-type interactions, show promise for storing hydrogen under atmospheric conditions, with potential applications in hydrogen storage components. MXenes offer significant potential for various technological applications due to their versatile properties and tunability [17].

The combination of MXENE functionalization and machine learning approaches to streamline water purification procedures will be thoroughly examined in the suggested evaluation. It

will look at the predictive power of machine learning models for MXENE characteristics, evaluate experimental validation methods, and research the performance and stability of MXENEs in a range of water purification applications. This research will also point out important discrepancies between computational forecasts and actual results and suggest ways to close these differences to further MXENE usage in water purification. The need to accelerate the development and improvement of MXENE-primarily reliant materials for sustainable water purification is the driving force behind the use of gadgets mastering MXENE functionalization. Conventional MXENE functionalization experimental methods are often labour-intensive, aid-extensive, and constrained by the large parameter range related to optimizing MXENE characteristics for improved water purifying efficacy. By utilizing large datasets of MXENE characteristics and water purification metrics, machine mastering provides an information-driven approach to overcome such obstacles.

2. RESEARCH TECHNIQUES

The strategy employed to link articles to present research studies through the web community is covered in this section. This section covers the web community's approach to linking articles to current research findings. The research was built on the findings of the literature review. A few of the stated research questions are highlighted in the literature review, which makes it easier to find and evaluate the study material that is appropriate to the questions. The research is divided into many stages, one of which is obtaining materials for a systematic literature review (from sources like Springer, IEEE Xplore, Google Scholar, and Elsevier, among others). The requirements for inclusion and exclusion requirements have all been fulfilled in addition to the identification, screening, and eligibility stages of the review process. The processes included in a review procedure are shown in Figure 1. The stages involved in analysis are few. Listed below are a few of them:

- ❖ Resource selection
- ❖ Inclusion and exclusion criteria
- ❖ Review process

2.1 Resource Selection

Several journal information systems, such as Google Scholar, IEEE Xplore, Springer, Elsevier, and others, have been used in a web-based electronic search to look through online research databases. These internet databases were selected because they are considered the greatest sources of thorough information on the study issue and because they contain an extensive amount of information relating to ML research for MXENE.

2.2 Inclusion and Exclusion Criteria

This criterion makes it easier to select papers that are relevant to the current research endeavour. Only standard scientific publications that focus on water purification, MXene, and ML-based MXene are selected for this category; book series and review articles have been excluded. These papers are taken from the IEEE, Springer, and Elsevier collections. Furthermore, publications published between 2017 and 2022 were selected since they would provide a sufficient amount of time to complete the study's development.

Table 1: Inclusion and Exclusion

Criteria	Inclusion	Exclusion
Sort of publication	Research articles, conference papers, and review articles.	Preprints, Conference abstracts, News articles.
Language	Papers published in English.	Papers published in languages other than English.
Accessibility	Articles that can be accessed online	Inaccessible Publications
Timeline	Between 2017 to 2022	Articles classified as shaded papers (those published before 2017 or those lacking any bibliographic details like issues and volume numbers, publication dates, etc.)

The requirements for inclusion and exclusion are listed in Table 1. The proposed work's inclusion requirements include research publications, conference papers, and inventions that address MXENE materials, functionalization strategies, water purification approaches, and material science applications of machine learning. Pertinent studies must include empirical or theoretical data on the characteristics of MXENE, synthesis methods, surface chemistry adjustments, and performance measures for water purification.

Non-peer-reviewed publications, unrelated subjects, and research with insufficient practical or theoretical information regarding MXENE functionality for water filtration are among the exclusion criteria.

2.3 Review Process

The keywords employed in the study's search procedure are determined in the first step shown in Fig 1. Many terms that are comparable to and connected to the study topics have been employed for each online database, based on previous studies and thesaurus. In the beginning 350 articles including the records found via database searching and extra records discovered through other sources are taken for assessment.

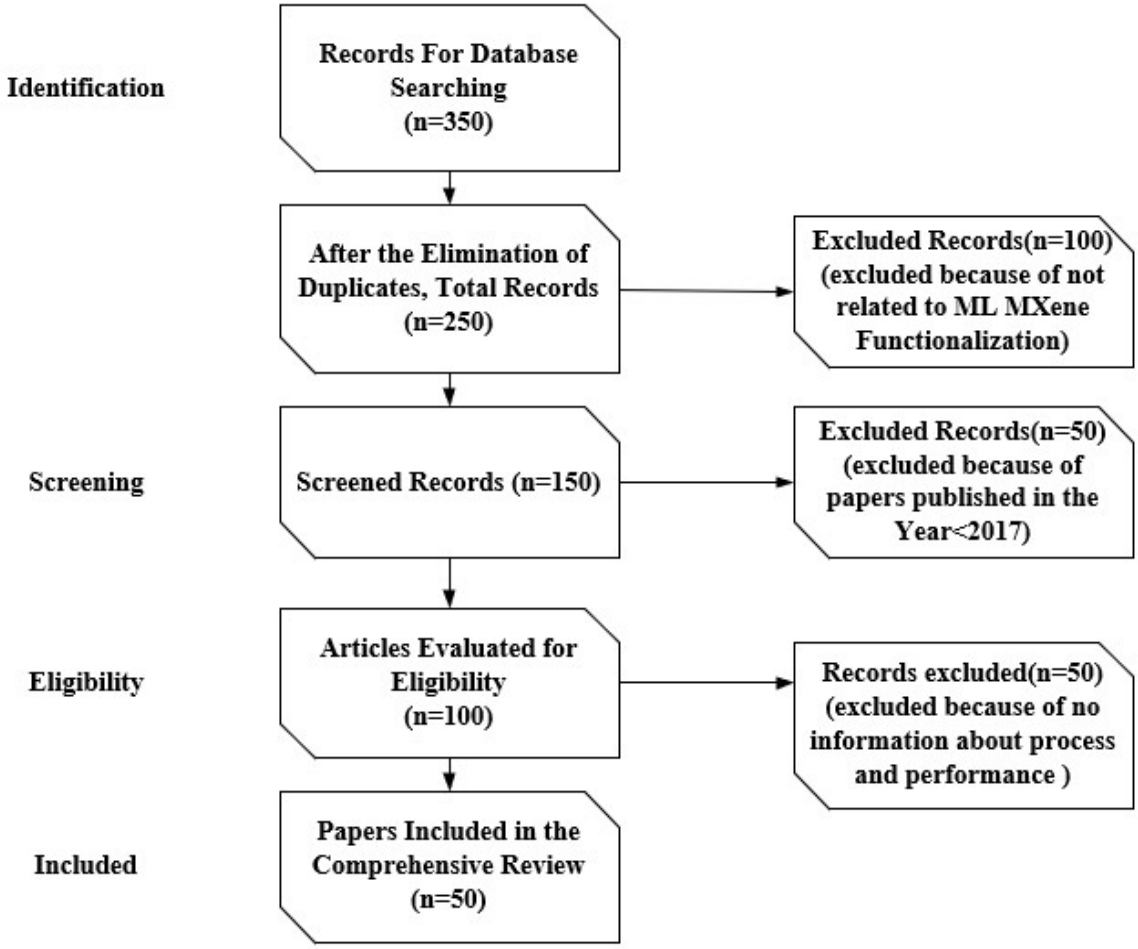

Figure 1: Review Process

3. LITERATURE REVIEW

Pogorielov et at., states that [18] Currently, a few atomic layers generated from nitride, carbide, and carbo-nitride pre-treatment agents have been selectively chemically etched to yield 20 or more MXenes. The etchants are primarily divided into two categories, including aqueous salts containing fluorine ions. In the early phases, MXenes are distinguished from MAX constituents by thoroughly immersing MAX systems in certain acids and breaking down M-A bonds. The two decisive criteria in such a technique are the length of the corrosion and full agitation. Top-down, as well as bottom-up mechanisms, are the two basic methods used in the creation of Two-dimensional mxenes [19]. The bottom-up synthesis manufacturing approach, which carefully constructs the structure, employs fewer inorganic or organic molecules/atoms than the top-down creation strategy, which frequently requires a large number of precursor materials. Using a crystal-growing process, the initial materials may be assembled into the precise 2D sequence that comprises the MXene structures. The advantages of the bottom-up technique allow for appropriate precise control over MXenes' form, dimensions, dispersion, and surface terminal functions. Three synthesis methods exist: top-down, top-up, and etching [20]. There are several methods for preparing MXenes. Different terminal functions can

be added to the M atom to finish the coordination of spheres and decrease their outermost Gibbs free energy [21], due to variations in their etching techniques. Therefore, their manufacture is greatly influenced by the MXenes' surface characteristics. The top-down approach has long been recognized, particularly in the creation and development of nanomaterials. These techniques frequently include splitting large, cumbersome precursor material into tiny, necessary quantum particles from 2D or 3D [22]. Using the top-down method, many bulk precursors, including graphite, carbon nanotubes, graphene, M_0 S_2 crystals, 〖WS〗_2 powder, black phosphorus, and g-C3N4, have been successfully converted into quantum dots. Among these are processes like Grinding balls, exposure to microwaves, water cleansing, chemical etching, electrochemical, intercalation, hydrothermal/solvothermal medication, and sound waves. Most top-down methods set up the catalysts' initial O2-containing functions on their surface, which makes it easier for defects to form in the catalysts. The bottom-up techniques use molecular materials as precursors as opposed to bulk material, which is used in top-down methods. MQDs might also be created from small precursors of inorganic and organic compounds using bottom-up techniques. The use of bottom-up techniques yields several benefits for QDs, including improved structures and characteristics due to quicker functionalization, more atomic utilization, and structural and morphological control. One-pot bottom-up approaches, on the other hand, will probably be used in the future to create MXene to meet the incremental application needs because of their comparatively easy working conditions when compared to top-down methods [23].

Chen, et al., [24] states that Harmful heavy metal ions (HMIs) like arsenic and chromate must be eliminated from drinking water to safeguard public health. Since heavy metal ions are extremely portable, biodegradable, and poisonous, they pose a serious threat to the world's water supplies. Even though a variety of adsorbents have been studied for the removal of HMI2,3, Since most adsorbents utilized for this function possess low capacities for adsorption, labour-intensive and intricate separation processes like spinning and dissolution are required. Additionally, adsorbent removal techniques are usually highly selective in identifying a specific HMI. Concerning the elimination of HMIs from water, coatings made from two-dimensional materials exhibit potential; nonetheless, they usually employ pressure-driven filtration. Utilizing Ti3C2Tx coatings to remove several both positively and negatively charged HMIs without force water is described in this work. Reduced graphene oxide was inserted between the layers of the Ti3C2Tx MXene-based material to optimize its microstructure. The film's surface underwent gradual hydroxylation to boost Ti3C2Tx accessibility, increase wettability, and promote HMI adsorption and reduction. Together, these actions increased the HMI removal effectiveness. The study offers a simple paradigm for exploiting two-dimensional materials-based films to control the crucial solid-liquid interactions for pressure-free water filtration. Additionally, it may provide a whole new world of adaptable, logically built Ti3C2Tx-based films for specific applications.

Sharma et al., [25] suggested a Nanocellulose-enabled membranes for water purification. When it comes to eliminating impurities from water, ranging from hydrated ions to micron-sized particles, membrane technology continues to be the most energy-efficient method. The poorest groups in the community, however, frequently cannot afford the relatively costly synthetic materials used in the present membrane technology. This paper presents viewpoints on the newly developing nanocellulose-enabled membrane technology, which is predicated on the extraction of nanoscale cellulose fibers from nearly any biomass. Many water purification systems have used the techniques of adsorption, absorption, flocculation, and coagulation because they are reasonably inexpensive and effective in eliminating pollutants like microorganisms and chemicals (metal ions, dyes, and organic compounds). It is well known that cellulose and its derivatives are a class of sustainable and useful materials that may be used for a variety of adsorption, absorption, flocculation, and coagulation processes. Given that nano cellulose membranes can eliminate a variety of pollutants in a single step through size exclusion and/or adsorption, their development from cheap, plentiful, and sustainable resources may reduce the membrane extraction expense. In addition to potentially solving the world's drinking water problems, the nanocellulose-enabled membrane method can offer a new, affordable platform for a variety of pressure-driven filtering methods, including reverse osmosis, microfiltration, ultrafiltration, and nanofiltration. A thorough discussion is held of a few pertinent factors that can regulate the filtering efficiency of membranes provided by nanocellulose.

Yehia et al., [26] recommended a Silica Nanoparticles for Water Purification. Global water supplies are becoming more and more contaminated, posing serious problems to public health since it is difficult to identify and treat a large range of pollutants quickly. In rural locations, where pipe infrastructure and organized water treatment systems are not always practical, this problem is especially urgent. Water storage, treatment, and quality monitoring may be accomplished economically and energy-efficiently using point-of-use (POU) water distribution networks. The POU systems that are now on the market, however, are not very effective in handling the growing range of pollutants, particularly those that are present in trace quantities. Furthermore, flexible POU systems that can identify and treat pollutants and provide clean water on demand are needed due to the fluctuation in pollutant species and quantities between sites. Because of their high level of activity and affinity toward chemical substrates, silica nanoparticles are one of the possible alternatives for creating quick and precise water purification procedures and sensors. Enzyme-nanomaterial composites, which increase the stability and activity of enzymes and increase their utility, have been created recently in large quantities. This advancement makes it easier to use silica nanoparticles in sophisticated POU systems. The use of silica nanoparticles in point-of-use water delivery systems for water monitoring and purification has demonstrated significant promise. These nanoparticles are perfect for eliminating impurities from water because of their special qualities, which include a large surface area, a significant adsorption capacity, and exceptional durability. Point-of-use water delivery systems can function more effectively and efficiently when silica nanoparticles are used in the water treatment process. This is especially true in rural locations where accessibility to clean water is scarce.

Rasool et al., [27] proposed a utilization of M_(n+1) X_n T_x for ecological cleanup and treatment of water. Because of their distinct characteristics and adjustable composition and structure, the diverse MXenes are considered to be among the most interesting 2D nanomaterials being explored for various implementation. MXenes, comprising water treatment/desalination membranes, adsorbents, catalytic substrates, and antibacterial agents, are being extensively investigated for use in ecological cleaning up and liquid /wastewater purification applications. To increase MXenes' efficacy in water purification applications, recent efforts have been focused on enhancing their durability, biological suitability, and recyclability in aquatic environments and atmospheric air conditions. By adjusting and managing the surface chemistry, which includes controlled oxidation and functionalization, MXene derivatives may be created. In a similar vein, several MXene-based composites using polymeric matrices were created to get around some of the drawbacks of pure MXenes, including aggregation and stability over time. More environmentally stable MXene structures need to be developed for situations where water interaction is unavoidable. More MXenes may arise and become accessible for purifying water and a variety of other environmental uses, since several of the more than thirty already known MXenes have also been theoretically anticipated. As of right now, Ti3C2Tx is the MXene family member that has been examined the most for environmental remediation and water purification applications. It is frequently employed as an adsorbent, for the photodegradation of pigments, and the reactive elimination of metal ions via water. Even still, compared to other 2D materials like graphene, it has received far less research. The non-toxic breakdown products produced by Ti2CTx and Ti3NC are identical to those of Ti3C2Tx and warrant special consideration.

Karahan et al., [28] suggested that with potential uses comparable to those of graphene's, a new class of multifunctional nanomaterials called MXenes is quickly taking shape [29]. The aim of this work is to give a current overview of the development and assessment of MXene-based membrane performance. The physicochemical properties and synthesis of MXenes are first described, with special attention to three important aspects of membrane fabrication: processability, dispersion stability, and exfoliation. Subsequently, several forms of MXene-based membranes found in the research are shown, including polymer-based nanocomposites and pure or intercalated nanolaminates. The main membrane processes that MXenes has so far investigated—gas division, sewage treatment, dehydration, and organic substance purification—are then assessed. Critical discussion is also given to the possible applications of MXenes in phase inversion, interfacial polymerization, and assembly of layers for the creation of nanocomposite membranes. Prospects include utilizing certain MXenes' high conductivity to electricity and catalytic activity for specialized uses that are difficult for other nanomaterials to fulfil. Additionally, the advantages of using modelling and simulation techniques to construct MXene-based membranes are demonstrated.

Overall, this analysis offers helpful guidance to the materials science as well as membrane sectors so they may better explore MXenes' potential for creating sophisticated separation membranes.

Table 2: Water Purification Techniques and Applications Using MXene Materials

References	Method	Advantages	Disadvantages	Inference
Chen, et al., [24]	MXene-based films	Pressure-free extraction of many HMIs	Potential challenges in scalability and large-scale production	MXene-based films offer a straightforward paradigm for pressure-free HMI elimination from water.
Sharma et al., [25]	Nanocellulose-enabled membranes	Sustainable and cost-effective membrane technology	Limited discussion on specific filtration performance parameters	Nanocellulose membranes offer an affordable basis for a range of pressure-driven filtering methods.
Yehia et al., [26]	Silica nanoparticles	Strong activity and selectivity toward chemical substrates	Potential environmental concerns related to nanoparticle usage	Silica nanoparticles show promise for water purification and monitoring in POU systems
Rasool et al., [27]	MXenes	Prospective applications in water treatment and environmental remediation	Limited studies on certain MXene derivatives and their stability in aqueous systems	MXenes hold potential for various water purification applications, but further research is needed.
Karahan et al., [28]	MXene-based membranes	Diverse formats and membrane processes explored	Challenges in exfoliation and dispersion stability of MXenes	MXene-based membranes show promise for advanced separation applications, with opportunities for niche uses.

The materials and techniques for treating water are given in the table 2. MXene-based films provide a straightforward method of filtering out dangerous substances from water, but scaling up might be a problem. Although particular performance criteria are not well addressed, the nanocellulose membranes offer an economical and sustainable filtration solution. Although silica nanoparticles have significant chemical activity, they are environmentally problematic. MXenes as well as MXene-based membranes have potential for treating water, but further study is required to determine how stable and dispersed they are.

Bjork et al., [30] proposed about the Functionalizing MXenes. Due to their chemical adaptability, two-dimensional metal carbides and nitrides, or MXenes, have garnered increasing attention in the last 10 years. This is because they hold great promise for applications in heterogeneous catalysis, energy storage, and superconductivity. Surface terminations, which typically consist of O,OH, and F, are a natural byproduct of the production of MXene. The surface terminations' chemical domain has been expanded to include more components, though, as a result of recent research, and this should be taken into account as a new factor influencing the characteristics of MXene. How different chemical species may function as terminations on distinct MXenes is not well understood. Specifically, little is known about the chemical conditions that are stable for various terminations. In this work, they give a comprehensive theoretical analysis of the surface terminations of MXenes in various atmospheres, taking into account twelve surface terminations (O,OH,N,NH,NH2,S,SH,H,F,Cl,Br,and I) and six experimentally produced MXenes (Ti2C,Nb2C,V2C,Mo2C,Ti3C2,and Nb4C3) [31]. They take into account MXenes that have been entirely terminated (single termination) as well as the effects of replacing individual terminations. With

forecast for methods for making single-termination MXenes and to determine which MXenes are durable in the surrounding settings, the work sheds light on which terminations are stable on which MXenes in various chemical surroundings. Furthermore, they suggest MXene production procedures that are still being used in trials. It is expected that the findings will offer design guidelines for customizing the surface expulsions of MXenes in addition to facilitating the creation of novel synthesis pathways.

Lei et al., [32] states that Two-dimensional nanomaterials, with their large surface areas and easy surface functionalization, have drawn more and more attention from researchers for a variety of uses, including energy storage, medicinal applications, environmental adsorption, and catalytic degradation. In this study, we exemplified the safer and easier extraction of the Al coating from Ti3AlC2 for the manufacture and ecological adsorption usage of 2D material MXenes. Through aromatic coupling-diazotization, sulfonic groups were added to the surface of Ti3C2. Additionally, an analysis and comparison of the Ti3C2 and functionalized Ti3C2 adsorption capacities and behaviors towards methylene blue were conducted. Numerous methods, including scanning electron microscopy, transmission electron microscopy, Fourier transform-infrared spectroscopy, X-ray diffraction, thermogravimetric analysis, and others, were used to successfully manufacture Ti3C2 and modified Ti3C2 [33]. Examined was the impact of several experiment parameters on how adsorption works towards MB, including the duration of contact, solution temperature, pH, and starting MB concentrations. The findings showed that Ti3C2—also known as Ti3C2–SO3H—that had been functionalized by sulfonic groups had better MB removal efficiency. Ti3C2-SO3H [34] has an optimal adsorption ability that's more than four times that of the initial components for MB. The outcomes of the isotherm and kinetics investigations showed that the Langmuir isotherm adsorption model and the pseudo-first-order model, respectively, provided a superior description of the experimental data. The formation of MB onto adsorbent surfaces was spontaneous and endothermic. The pH results of the experiments showed that an alkaline aqueous solution is optimal for dye adsorption. Those results demonstrate that Ti3C2-SO3H may be an excellent adsorbent for the removal of cationic dye molecules, which encourages the development of Ti3C2-SO3H for wastewater processing.

Mozafari et al., [35] states that because of their unique physicochemical characteristics and range of chemical compositions, MXenes, an innovative class of Ti3C2Tx and N3, are generating a lot of interest from researchers in a variety of fields, such as biomedicine, sensing, catalysis, energy preservation, and conversion, adsorption, and membrane-based separation. Many surface functionalization techniques, including single heteroatom doping and surface-initiated polymerization, have been deftly created in recent years to increase the potential of MXenes in many applications. This paper examines and contextualizes the latest developments in MXene surface functionality and the range of uses for the modified MXenes. It explains how surface functionalization affects the electrical, magnetically mechanical, visual, and hydrophilicity/hydrophobicity characteristics of MXene. MXenes have drawn a lot of interest over the last 10 years due to their desirable physicochemical, mechanical, magnetic, and electrical properties as well as their large surface area and abundance of surface terminations. Consequently, they have found use in several domains., including medical science, sensing, catalysis, energy conversion and storage, and membrane-based separation. The surface functionality of MXenes makes it possible to modify a number of their characteristics, expanding their range of applications and addressing some of their drawbacks, including limited flexibility, easy restacking, and unstable behaviour in a mixture of water as well as molecular oxygen. The most current developments in MXene surface treatment techniques, MXene-affected characteristics, and the useful uses of the resultant surface-modified MXenes were examined in this paper. Surface-modified MXenes have shown a lot of promise for a variety of applications.

Zhang et al., [36] states that several sectors such as energy storage, sensing, photothermal conversion, EMI shielding, nanogenerators, and MXene-polymer combinations are the most potential options. Polymers can be added to MXene to increase its conductivity, flexibility, and stability while reducing the restacking phenomena. They describe the methods used to prepare MXene-polymer composites in this review, which include physical mixing, in situ polymerization, surface modification [37]. When building MXene-polymer composites with desired shapes and qualities, these binding processes of MXene with polymer matrix might offer crucial assistance. Fascinatingly,

MXene's synergistic capabilities with polymers raise the bar for adaptability, resulting in better mechanical performance, increased electrical conductivity, and exceptional stability. As a result, they have potential uses in the domains of photothermal conversion, EMI shielding, nanogenerators, energy storage, and sensing. Nonetheless, the following associated difficulties still face MXene-based materials in real-world applications. First off, there are still issues with obtaining MXene-polymer compounds' long-term stability. During processing and storage, MXenes readily oxidize to metal oxides in the atmosphere. With the use of alkyl phosphonic acid ligands [38] and silane coupling agents, the surface-modification method enables MXene to be dissolved in nonpolar solvents such as chloroform and to show stable, long-term storage without oxidation. The utilization of MXene in multifunctional devices is hindered by the reduced electrochemical performance of the surface altered by binding substances made of silane. For practical purposes, therefore, alternate strategies to stop MXenes from oxidizing must be devised. Secondly, research on the underlying pathways is still lacking. A high-performing electrochemical device for energy storage may be built using the connection between each unique functional group on the MXene surfaces and its physiochemical characteristics. Regarding sensors along with EMI shielding gadgets, it is necessary to demonstrate the mass/charge movement characteristics amongst MXene and the various components in the structures that are intended.

Tong et al., [39] proposed a Surface engineering of MXenes for energy and environmental applications. MXenes are an innovative group of Ti3C2Tx, N3, and C3N4. Because of their unique electrical, electrochemical, optical, and chemical characteristics, they have drawn a lot of interest in energy and environmental applications. Two-dimensional materials have garnered a lot of attention because of their desirable characteristics. Numerous additional 2D materials, including TMDCs, multilayered double hydroxides, hexagonal boron nitride, transition metal oxides, nitrides, and MXenes, were discovered as a result of the identification of freestanding single-layer graphene. The intriguing electronic and structural properties of MXenes, which are transition metal carbides, nitrides, and carbonitrides, such as their large surface area, hydrophilic nature, high electrical conductivity, and easily adjustable structure, have drawn a lot of attention since their discovery in 2011 [40]. Applications for MXenes have been seen in the fields of biomedicine, rechargeable batteries, supercapacitors, electrochemical energy storage, photocatalysis, thermos catalysis, sensing as well as biosensing, and energy conversion and storage. Notably, MXenes' effectiveness in those applications is largely due to their adjustable surface chemistry. MXenes' physicochemical characteristics and functions are thought to be significantly influenced by their surface makeup. In this summary, they emphasize the application of various surface engineering techniques to MXenes, including surface functionalization, imperfections in the surface, surface doping, surface oxidation, and theoretical simulation of MXene surface engineering, in order to achieve an in-depth comprehension and the rational design of MXenes through surface engineering. Additionally, the connection between MXenes' physicochemical characteristics and surface engineering is explored. Ultimately, the present obstacles and prospects for the advancement of MXene surface technology are also suggested.

Table 3: Functionalization Methods and Strategies Applied to MXene Materials

References	Method	Advantages	Disadvantages	Inference
Bjork et al., [30]	Theoretical study	Gives information about stable terminations on various MXenes across a range of chemical settings.	Limited experimental validation of theoretical predictions.	Theoretical study offers valuable insights for designing MXenes with tailored surface terminations for diverse applications.
Lei et al., [32]	Surface modification	Enhanced adsorption capacity for methylene blue	Limited discussion on scalability and large-scale production.	Surface modification of Ti_3C_2 enhances its adsorption efficiency for wastewater treatment applications.

Mozafari et al., [35]	Surface functionalization	Expands potential applications of Mxenes.	Limited discussion on specific modification methods and their scalability.	Surface functionalization of MXenes enhances their versatility and enables various applications in different fields.
Zhang et al., [36]	Preparation strategies	Properties of synergistic amongst polymers and MXene for enhanced properties.	Challenges in establishing MXene-polymer composites' long-term reliability.	MXene-polymer composites show promise in various fields but face challenges in achieving long-term stability.
Tong et al., [39]	Surface engineering approaches	Extensive understanding and logical design of MXenes via surface engineering.	Limited experimental validation of surface engineering approaches.	Surface engineering approaches offer a pathway for tailoring MXene properties for specific applications.

This table 2 lists many ways to change MXenes along with the benefits and drawbacks of each approach. While theoretical research sheds light on MXene terminations, it is not supported by experimental data. Adsorption capacity is increased by surface modification; however, scalability is unknown. Applications for MXene are expanded by surface functionalization, although particular techniques require consideration. MXene-polymer composites are improved by preparation techniques, but stability over time is difficult to achieve. Although surface engineering methods provide customized MXene characteristics, they are not supported by experiments. With certain restrictions, these techniques work together to further MXene applications.

Roy et al.,[41] states that MXenes are M_(n+1) X_n T_x and N3 that resemble graphene and have variable compositions with rich surface chemistry. MXenes are used in electronics, energy storage, and catalysis due to their highly adjustable electrical, optical, and mechanical characteristics, which are the consequence of their compositional flexibility. An essential component that determines MXenes' viability for certain applications is its work function. To forecast the research's function of MXenes with generic compositions and surfaces terminated by bare metal atoms, O,OH, and F, they offer a set of machine learning models. This algorithm is trained using 275 points of information collected in the Computationally 2D Materials Database, using the fundamental chemical characteristics of the components that make up MXene as features. The neural network model estimates the experimental performance of MXenes with a mean absolute error of 0.12 eV on the training information and 0.25 eV on the testing data using 15 distinct MXene properties as inputs. The feature significance analysis shows that the work function is most substantially influenced by the electronegativity of atoms ending the MXene surface. Experimental observations on Ti3C2 also shed light on the adaptability of the work's component to the surface termination. To forecast the assigned operation, they offer reduced-order models with ten, eight, and five features. They show that these reduced-order models are transferable to new materials by projecting the function of work of MXenes with surface terminations that differ from those in the initial training set, such as Br,Cl,S,N, and NH. The ability to predict electrical characteristics, such as the work effectiveness, from the fundamental chemical characteristics of elements opens the door to the quick identification of customized MXenes with the precise range of attributes needed for a given application.

He et al., [42] states that nearly all material research should take into account the essential characteristics of material stability. In this work, they study material stabilities with an emphasis on the archetypal MXenes, utilizing machine-learning approaches and symbolic regression. The evaluation of MXene stabilities is conducted using a small dataset and machine learning techniques such as RF, KNN, Logistic regression, SVM, and GaussianNB. The results show that SVM achieves the greatest accuracy for classification purposes. More significantly, it is confirmed that symbolic regression is a workable technique for determining appropriate descriptors and creating new descriptors

that correlate with the material stability of MXene. This study shows that the symbolic regression and machine learning approaches are viable for classifying materials and characterizing their stability. The durability of the MXene materials is the study's output. The development of energy, the Gibbs free energy, the enthalpy, and other expressions may all be used to measure the long-term stability of the materials. Similarly, other derived parameters, such as thermal degradation, reduction in optical absorption efficiency drop, etc., may be retrieved from the trials to infer the stability. The stability value (output), which is used in line with the description in the OQMD databases and is thought to be more accurate, is described as the convex hull distance determined by the formation energy and the convex hull energy. The result value (stability) has to be labelled in order to categorize the materials as reliable or unreliable based on the replicated information. The SVM method provides the greatest accuracy for classifying materials based on stability when compared to the RF, KNN, LR, and Gaussian NB algorithms. Furthermore, it is shown that, in the absence of any earlier Designated chemical understanding by people, the symbolic regression technique can automatically discover the necessary descriptors to describe the material stability. It is confirmed that symbolic regression is a quick and effective way to handle material classification tasks and create new descriptors. It is anticipated that symbolic regression will be suitable for a range of materials classification problems in the future, such as deciding if a material is stable or not, if it is a superconductor, or if it is suitable for a particular application. This work confirms that the machine learning approach makes it easier to categorize and assess the stabilities of materials, and it proposes symbolic regression as a substitute for other ML based approaches for the descriptor design.

Priya et al., [43] proposed that a wealth of information may be found in published works that can be used to speed up the design and development of cutting-edge materials for a variety of crucial applications, such as the desalination of seawater. In this work, they create a machine learning model and train it using around 260 molecular dynamics computational outcomes to forecast the Quality of dewatering of 2D membranes found in published works. In addition to the pressure used, salt concentration, partial charges on the atoms, pore geometry, and membrane mechanical properties, 44 substance characteristics associated with the chemical reactions of the pores and the membranes are correlated with the desalination performance metrics of water flux and salt rejection rates. 3814 structurally optimized 2D materials were screened for maximal water flow and salt rejection rates through research using the ML model. They discovered some contenders that outperform the more well-known 2D materials, graphene, and MoS2, by a factor of three. Data from many 2D membrane MD simulations are used to validate this finding. Such established statistical models based on data from the literature may be highly helpful in directing functional materials research projects for a variety of uses. The functionalization of pores is a highly significant process that has been previously investigated. Partial charges on atoms generally are also shown to be important by the ML model characteristic significance list. A machine learning model has been created that links the computationally calculated salt rejection rates and water flux to 39 different features about the chemical, electrical, and structural characteristics of the membrane as well as its pore, as well as the utilized pressure, salt levels, pore region, membrane thickness, and pore radius. The factors that have the biggest impact on desalination performance are the membrane's maximal positive charge and pore atomic number. 3814 2D materials that are listed in public databases are screened using the model. It has been shown that non-metals such as halogens and chalcogens enhance the water flow, whereas transition metal near the pore improves salt rejection rates. It is anticipated that 2D transitional metal oxides as well as their combinations would work well for desalination. They present candidates that exhibit water fluxes three times higher than the innovative 2D membranes, a finding confirmed by molecular dynamics simulations. Increased average water density and more water-membrane interactions result from larger partial charges upon the membrane atoms, but lower average velocities.

Venturi et al., [44] recommended that the development of application-dependent design concepts for two-dimensional materials was made possible by machine learning. Two-dimensional materials are intriguing next-generation options for variety of applications due to their distinct mechanical and electrical characteristics. Finding high-performing 2D materials on a large scale requires computing descriptors using first-principles density functional theory, which is computationally intensive. In this study, they address this problem by training an ensemble of models to forecast thermodynamic, mechanical, and electrical characteristics by expanding and broadening crystal graph convolutional neural networks to phenomena

with planar periodicity. They examine around 45,000 structures for two distinct uses: photovoltaics and mechanical strength. They examine structural as well as compositional design concepts that influence the attributes of the buildings examined by gathering data from the screened candidates. This approach retrieves a few well-recognized design guidelines: Ti based MXenes often have high stiffness coefficients, and hybrid organic-inorganic perovskites containing lead and tin are likely to be excellent options for solar cell applications. It's interesting to note that more group 4 components also help to make MXenes stronger mechanically. They uncover some compositions of all-inorganic perovskites that have not been thoroughly examined in the area of photovoltaics, thereby providing avenues for further research. To encourage more advancements in this field, they have made the code base open-source. They have expanded the Crystal Graph Convolutional Neural Networks to include materials exhibiting planar symmetry in this study. Using this model, they searched through huge combinatorial produced datasets of perovskite and MXene materials to find materials that, based on the ensemble of trained Crystal Graph Convolutional Neural Networks models, had a high probability of possessing features of interest. They were able to identify the basic molecular design concepts for each application by using the screening procedure findings.

Zhu et al., [45] states that with the help of machine learning and graphene-like Ti2C Mxene /Au–Ag nano shuttles, a new bifunctional intelligent nano sensing platform for both electrochemical and surface-enhanced Raman scattering, intelligent analysis of ultra-trace carbendazim (CBZ) residues in tea and rice was successfully designed. Hydrofluoric acid was used to selectively etch the Al layers of Ti2AlC, and high-temperature calcination was used to create Ti2C MXene. Ti2C MXene/Au–Ag NSs revealed a broad and rough surface, improved conductivity, outstanding electrochemical responsiveness, noticeable raman enhancement, and an excellent level of steadiness. They were made by ultrasonically dispersing graphene-like Ti2C MXene into Au–Ag NSs [46] solution under dark circumstances. The compared and reviewed machine learning using several techniques, including relevance vector machines (RVM), artificial neural networks, and SVM, for the smart analysis of CBZ. With a low limit of detection of 0.002 μM for the electrochemical analysis of CBZ in a large linear range of 0.006 – 9.8 μM and a low limit of detection of 0.01 μM for the surface-enhanced Raman scattering detection of CBZ in a wide linear range of 0.033 – 10 μM, RVM demonstrated greater superiority. In addition to a new bifunctional nano sensing platform that utilizes the development of graphene-like nanohybrid for food and agro-product safety, this will deliver a new bifunctional intelligent sensing platform via various ML methods for improving the performance of the sensors via shared verification of more methods of detection. Based on graphene-like Ti2C MXene/Au–Ag nano shuttles, they successfully designed a new bifunctional intelligent nano sensing platform here, inspired by these considerations, via machine learning for both electrochemical and SERS intelligent analysis of ultra-trace carbendazim (CBZ) residues in tea and rice. The Ti2C MXene/Au–Ag NSs nanohybrid was created by ultrasonically dispersing Ti2C MXene, which was first produced by calcining titanium aluminium carbide (Ti2AlC) powder into Au–Ag NSs solution in the absence of light. They compared and explored the use of machine learning with several methods, including SVM, ANN, and RVM, for the smart evaluation of CBZ. Both electrochemical alongside Raman sensors have been used in enhancing the precision of the sensors through bilateral validation of two approaches of recognition, ML with RVM techniques has been employed for smart translation as well as information outputs for CBZ in actual samples.

Table 4: Application Of Machine Learning Techniques in MXENE Functionalization for Water Purification

References	Method	Advantages	Disadvantages	Inference
Roy et al.,[41]	ML models	Predicts the work function of MXenes with high accuracy	Limited experimental validation	ML models accurately forecast work function of MXenes, aiding in material design for specific applications.
He et al., [42]	ML and symbolic regression	Identifies descriptors for material stability	Limited dataset used for training	ML and symbolic regression offer viable techniques for classifying materials and describing material durability.
Priya et al., [43]	Machine learning model	Predicts desalination performance of 2D membranes	Reliance on computational simulations for validation	Machine learning model predicts desalination performance of 2D membranes, aiding in the discovery of high-performing materials.
Venturi et al., [44]	Crystal graph convolutional neural networks	Predicts thermodynamic, mechanical, and electronic properties of 2D materials	Computational intensity of first-principles density functional theory for data generation	Convolutional neural networks predict properties of 2D materials, enabling large-scale screening for various applications.
Zhu et al., [45]	Machine learning algorithms	Bifunctional nano sensing platform for electrochemical and Surface-Enhanced Raman Scattering analysis of ultra-trace CBZ residues in food products	Limited experimental validation	Machine learning algorithms enable intelligent analysis of CBZ residues in food products using a bifunctional nano sensing platform.

Several uses of machine learning algorithms for materials science are shown in this table 4. Although it depends on little experimental confirmation, machine learning forecasts MXene characteristics and membrane performance correctly. Using a tiny dataset, symbolic regression finds material stability descriptors. Convolutional neural networks with crystal graphs forecast 2D material qualities, assisting in material screening. Although there is minimal experimental confirmation, machine learning techniques allow for smart analysis of residual chemicals in food items. With certain limitations on validation, these techniques show the possibilities of machine learning within materials research.

Table 5: MXene-based Adsorbents for Contaminant Removal

MXene	Functionalization	Contaminant	Loading ($C0\ MXene$) mg	PH	Temperature	Time(h)	Maximum Uptake in mg/g	Refer ence
$Ti_3C_2T_x$	Regular	Ba	0.01-0.55	3-9	25	2	9.3	[47]
Ti_2CT_x	Alk-Ti_2C	Cd	0.06-2.2	2-9	20	1-1.15	326	[48]
$HTNs$	K-HTNs	Eu	0.1-1.5	2-10	25	4	203	[49]
MTC	Regular	Re (VII)	0.25	1-10	20	6	42.2	[50]
TCNs	Regular	Re (VII)	0.25	1-10	20	6	363	[51]

The table 5 presents a comprehensive overview of various MXene-based adsorbents used for contaminant removal, detailing their characteristics and performance under different conditions [52]. Each row corresponds to a specific MXene material, denoting its functionalization, the contaminant targeted, the initial loading of MXene, pH range, temperature, contact time, and the maximum uptake capacity for the respective contaminant. For instance, Ti3C2Tx and Ti2CTX

are two different types of MXene, each exhibiting distinct functionalizations such as 'Regular' and 'Alk-Ti2C.' The contaminants studied range from heavy metals like Ba and Cd to elements like Eu and Re (VII). The table also provides insights into the experimental conditions such as pH levels, temperature, and contact time, all of which influence the adsorption process. The maximum uptake capacity, expressed in mg/g, signifies the efficiency of each MXene material in removing the specified contaminant. This comprehensive presentation facilitates a comparative analysis of MXene-based adsorbents, aiding researchers in understanding their suitability and effectiveness for diverse environmental remediation applications

Table 6: Carbon-based Adsorbent Media

Adsorbent	Contaminant	Kinetic model (best fit)	Isotherm model (best fit)	Interactions	Uptake Capacity (mg/g)
MXenes	Ba	Pseudo Second Order	Freundlich	Electrostatic	12
Alk-Ti3C2Tx					46.5
Alk-MXene	Pb				140
Ti2CTx	Th				213
MXene	Methylene Blue			Hydrogen bonding	86.8
MXene-COOH					71
MXene-COOH			Langmuir		82
Graphene Oxide (GO) Magnetic cyclodextrin/GO				Ion exchange	84.32
Magnetic chitosan/GO					95.16
Carbon nanotubes	Hg			Electrostatic	127.6
MnO2 coated CNTs		Intrapartic le diffusion			58.82
Functionalized sulfur-CNTs		PSO			151.51
Fe3O4-CNTs					238.78
Adsorbent	**Contaminant**	**Kinetic model (best fit)**	**Isotherm model (best fit)**	**Interactions**	**Uptake Capacity (mg/g)**
MXenes	Ba				12
Alk-Ti_3C_2Tx					46.5
Alk-MXene	Pb			Electrostatic	140
Ti2CTx	Th				213
MXene				Hydrogen bonding	86.8
MXene-COOH			Freundlich		71
MXene-COOH					82
Graphene Oxide (GO) Magnetic cyclodextrin/GO					84.32
Magnetic chitosan/GO	Methylene Blue	Pseudo Second Order		Ion exchange	95.16
Carbon nanotubes					127.6
MnO2 coated CNTs		Intrapartic le diffusion			58.82
Functionalized sulfur-CNTs		PSO	Langmuir		151.51
Fe3O4-CNTs	Hg			Electrostatic	238.78

Adsorbent	Contaminant	Kinetic model (best fit)	Isotherm model (best fit)	Interactions	Uptake Capacity (mg/g)
MXenes	Ba				12
Alk-Ti_3C_2Tx					46.5
Alk-MXene	Pb			Electrostatic	140
Ti2CTx	Th				213
MXene				Hydrogen bonding	86.8
MXene-COOH			Freundlich		71
MXene-COOH					82
Graphene Oxide (GO) Magnetic cyclodextrin/GO					84.32
Magnetic chitosan/GO	Methylene Blue	Pseudo Second Order		Ion exchange	95.16
Carbon nanotubes					127.6
MnO2 coated CNTs		Intraparticle diffusion			58.82
Functionalized sulfur-CNTs		PSO	Langmuir		151.51
Fe3O4-CNTs	Hg			Electrostatic	238.78

Manuscripts must be in English (all figures and text) and prepared on Letter size paper (8.5 X 11 inches) in two column-format with 1.3 margins from top and .6 from bottom, and 1.25cm from left and right, leaving a gutter width of 0.2 between columns.

Centered at top of the first page should be the complete title of the manuscript, followed by name(s) of author(s), affiliation(s), mailing and email address(es). This is followed by the abstracts under the heading **ABSTRACT**, keywords under the heading **Keywords** and followed by the text. The text should be typed in single space, using a font similar to the one used in this text **(Times, 10 points)**. Paragraphs should be separated by single spacing. Each manuscript should **exceed 08 pages** including illustrations and tables.

2.1 Sections and Subsections

Sections and subsections should be numbered and titled as 1.0, 2.0, etc. and 1.1, 1.2, 2.1, 2.2, 2.2.1, etc. Capital letters should be used for the section titles. For subsections, the first letter of each word should be in capital letter and followed by small letters. One line space should be given above the sub section while no space should be given below the heading and text

2.2.2 Identification of sub subsections

Subsub section has to be in sentense case with no spacing above or blow the srat of it.

3. TABLES AND FIGURES

Figures should be labeled with "Figure" and tables with "Table" and should be numbered sequentially, for example, Figure 1, Figure 2 and so on (refer to table 1 and figure 1). The figure numbers and titles should be placed below the figures, and the table numbers and titles should be placed on top of the tables. The title should be placed in the middle of the page between the left and right margins. Tables, illustrations and the corresponding text should be placed on the same page as far as possible if too large they can be placed in singly column format after text. Otherwise they may be placed on the immediate following page. If its size should be smaller than the type area they can be placed after references in singly column format and referenced in text

Table 1: Center Table Captions Above The Tables.

Relevancy (%)	Score (%)
88.5	87.3
82.6	85.4
83.1	82.6

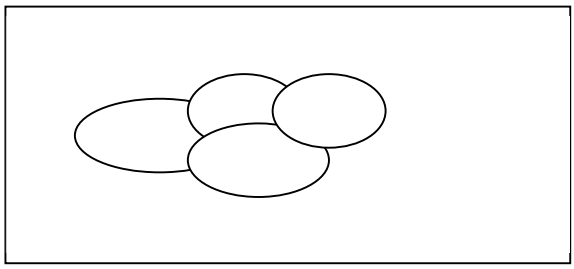

Figure 1: Description Is Placed Right Below The Figure

4. EQUATIONS

When numbering equations, enclose numbers in parentheses and place flush with right-hand margin of the column. Equations must be typed, not inserted.
(If nonstandard fonts are used its better to put equations as images instead of text)
Example:

$$Net_j = w_0 + \sum_{i=1}^{n} x_i w_{ij} \qquad (1)$$

REFERENCES:
[Author Name(s), Paper Title, Conference/Journal Title (Vol/Issue), Date, Page Numbers] Should be arranged/numbered in chronological order as they appear indexed [1],[2] in paper text.
Examples are as follows

[1] Author No.1, Author No 2 Onward, "Paper Title Here", *Proceedings of xxx Conference or Journal (ABCD)*, Institution name (Country), February 21-23, year, pp. 626-632.
[2] B.N. Singh, Bhim Singh, Ambrish Chandra, and Kamal Al-Haddad, "Digital Implementation of an Advanced Static VAR Compensator for Voltage Profile Improvement, Power Factor Correction and Balancing of Unbalanced Reactive Loads", *Electric Power Energy Research*, Vol. 54, No. 2, 2000, pp. 101-111.
[3] URL Date Stamp Time Stamp GMT and dd/mm/yyyy

Large Figures/Tables Or Any Other Annexures Can Be Placed At The End Of The Paper And Indexed In Paper Text Accordingly

Figure titles should be below figures
Figure x : Figure Title (Times New Roman 9pt Capitalize Each Word Italic)

Table x: Table Title(Times New Roman 9pt Capitalize Each Word Italic)
Table titles should be above tables

- ✓ Should effectively introduce the area and subareas under investigation.
- ✓ Critique available literature on the topic.
- ✓ Present a clear research problem derived from literature
- ✓ Present a valid detailed solution to the identified problem.
- ✓ Develop / Adopt/ Adapt a clear validation method/criteria.
- ✓ Follow a proper detailed method for validation and should present concrete and decisive evidence in from of research results. Discusses and evaluates the results in comparison to literature
- ✓ Provide difference from prior work
- ✓ Provide clear limitation and assumptions to achieve the solution or results presented.
- ✓ Provide clear conclusion and deduction based on work carried out and data presented.
- ✓ Provide clear Future Research Directions

REVIEW & SELECTION CRITERIA
Kindly visit the journal home page www.jatit.org to have a good look at what reviewers have in mind when conducting double blind review.

PAPER LENGTH
Number of pages is never a criteria to judge a paper but the content and its effective presentation matters. Following is just a guide for presentation of enough content to qualify as a good presentation

MINIMUM LENGTH
Minimum length to present sufficient content is 10 pages in journal format. Under 08 pages of text will

not qualify for an external review and shall be rejected in editorial screening

MAXIMUM LENGTH

Maxim allowed length is 45 pages in journal format. Can be relaxed to 50 pages in special cases

Adsorbent	Contaminant	Kinetic model (best fit)	Isotherm model (best fit)	Interactions	Uptake Capacity (mg/g)
MXenes	Ba				12
Alk-Ti3C2Tx					46.5
Alk-MXene	Pb			Electrostatic	140
Ti2CTx	Th				213
MXene				Hydrogen bonding	86.8
MXene-COOH			Freundlich		71
MXene-COOH					82
Graphene Oxide (GO) Magnetic cyclodextrin/GO					84.32
Magnetic chitosan/GO	Methylene Blue	Pseudo Second Order		Ion exchange	95.16
Carbon nanotubes					127.6
MnO2 coated CNTs		Intraparticle diffusion			58.82
Functionalized sulfur-CNTs		PSO	Langmuir		151.51
Fe3O4-CNTs	Hg			Electrostatic	238.78

The table 6 [52] provides a comprehensive summary of various adsorbents and their efficiency in removing different contaminants from solutions. Each row in the table represents a specific adsorbent, detailing the contaminant targeted, the best-fitted kinetic and isotherm models describing its adsorption behavior, predominant interaction mechanisms, and the uptake capacity expressed in milligrams per gram (mg/g). For instance, MXenes, graphene oxide (GO), and carbon nanotubes (CNTs) are among the adsorbents listed, targeting contaminants like Ba, Pb, Th, Methylene Blue, and Hg (mercury). The choice of kinetic and isotherm models such as PSO, Freundlich, and Langmuir offers insights into the adsorption mechanisms and equilibrium behavior of contaminants on these materials. The interactions between adsorbents and contaminants vary, including electrostatic interactions, hydrogen bonding, and ion exchange. The reported uptake capacities provide quantitative measures of the adsorbents' effectiveness in contaminant removal. This compilation of data serves as a valuable resource for researchers, environmental engineers, and policymakers involved in developing and optimizing adsorption-based technologies for water treatment and environmental remediation.

4. RESEARCH GAP IDENTIFICATION

Despite advancements in machine learning models for predicting properties and behaviours of MXenes, there remains a gap in experimental validation and scalability. The reliance on theoretical predictions and small datasets limits the robustness and applicability of these models [53]. Additionally, there is a need for further exploration into the stability and performance of 2D materials in real-world applications, such as desalination and sensing, to bridge the gap between computational predictions and experimental outcomes [54]. The proposed work aims to address these research gaps by conducting comprehensive experimental validations of machine learning models for predicting properties of MXenes. Additionally, the study will focus on expanding the dataset used for training these models to improve their accuracy and applicability. Furthermore, the research will investigate the stability and performance of 2D materials, particularly MXenes, in practical applications such as desalination and sensing, providing valuable insights for material design and development.

5. RESEARCH GAP

1. How precisely can machine learning algorithms anticipate the properties and behaviours of MXenes, and what are the key factors influencing their predictive performance?
2. What are the experimental validation techniques required to assess the reliability and scalability of machine learning models in anticipating the properties of MXenes?
3. How do the stability and performance of 2D materials, specifically MXenes, vary across different practical applications such as desalination and sensing, and what are the underlying factors influencing these variations?
4. What are the critical gaps between computational predictions and experimental outcomes in the study of MXenes, and how can these gaps be effectively addressed to advance the understanding and application of MXenes in various fields?

5.1 Research Question Results

1. How precisely can machine learning algorithms anticipate the properties and behaviours of MXenes, and what are the key factors influencing their predictive performance?

Machine learning models show promising potential in predicting the properties and behaviours of MXenes, but their accuracy is influenced by several key factors. Firstly, the quality and quantity of the training dataset significantly impact the predictive performance. A diverse and comprehensive dataset covering various MXene compositions, structures, and properties is crucial for training robust models. Additionally, the inclusion of experimental data for validation and refinement of the models enhances their accuracy and reliability. Another important factor is the choice of features or descriptors used as input for the machine learning models. These features capture the relevant chemical and structural characteristics of MXenes that correlate with their properties. Selecting appropriate features that adequately represent the complex nature of MXenes is essential for achieving accurate predictions. Moreover, the complexity of MXene structures and the diverse range of properties they exhibit pose challenges for machine learning models. MXenes can have different surface terminations, functional groups, and structural defects, all of which contribute to their properties.

Capturing these intricacies in the models requires careful consideration and feature engineering to ensure accurate predictions. Furthermore, the selection of machine learning algorithms plays a critical role in determining predictive performance. Different algorithms have varying capabilities in handling nonlinear relationships, high-dimensional data, and noise in the dataset. Choosing suitable algorithms and optimizing their parameters can improve the accuracy of the models. Additionally, the interpretation of machine learning models and the identification of relevant features affecting the properties of MXenes are crucial for gaining insights into the underlying mechanisms. Interpretability techniques such as feature importance analysis and model explainability methods aid in understanding the relationships between input features and output predictions, thereby improving model performance.

2. What are the experimental validation techniques required to assess the reliability and scalability of machine learning models in predicting the properties of MXenes?

Experimental validation techniques play a crucial role in assessing the reliability and scalability of machine learning models for predicting the properties of MXenes. One key validation approach involves comparing the predictions of machine learning models with experimental data obtained from various characterization techniques such as X-ray diffraction, scanning electron microscopy, transmission electron microscopy, and spectroscopic methods like X-ray photoelectron spectroscopy and Fourier-transform infrared spectroscopy. These experimental techniques provide valuable insights into the structural, morphological, and chemical properties of MXenes, allowing for direct comparison with the predicted properties from machine learning models. Additionally, validation studies can involve measuring specific properties of MXenes predicted by the models, such as electrical conductivity, mechanical strength, or catalytic activity, through experimental tests or simulations. Furthermore, cross-validation techniques, where the model is trained and validated on different subsets of the dataset, help assess the robustness and generalizability of the machine learning models. Longitudinal studies tracking the performance of the models over time and with additional experimental data contribute to evaluating their scalability and adaptability to new datasets. Overall, a combination of experimental validation techniques involving characterization methods, property measurements, cross-validation, and longitudinal studies is essential for comprehensively assessing the reliability and

scalability of machine learning models in anticipating the properties of MXenes.

3. How do the stability and performance of 2D materials, specifically MXenes, vary across different practical applications such as desalination and sensing, and what are the underlying factors influencing these variations?

The stability and performance of 2D materials, particularly MXenes, exhibit variations across different practical applications such as desalination and sensing due to several underlying factors. In desalination applications, the stability and performance of MXenes are influenced by their interactions with salt ions, water molecules, and applied pressure, which affect factors like water flux and salt rejection rates. The surface chemistry, porosity, and structural defects of MXenes play significant roles in determining their performance in desalination processes. On the other hand, in sensing applications, the stability and performance of MXenes are influenced by their interactions with target analytes, which determine factors like sensitivity, selectivity, and response time. Surface functionalization and modification of MXenes with specific functional groups can enhance their performance in sensing applications by facilitating target molecule adsorption and electron transfer processes. Additionally, factors such as environmental conditions, operational parameters, and device configurations also contribute to the variations in MXene performance across different practical applications.

4. What are the critical gaps between computational predictions and experimental outcomes in the study of MXenes, and how can these gaps be effectively addressed to advance the understanding and application of MXenes in various fields?

There are critical gaps between computational predictions and experimental outcomes in the study of MXenes, posing challenges in advancing their understanding and application in various fields. Computational predictions often rely on theoretical models and simulations to predict MXene properties and behaviours, which may not fully capture the complex interactions and dynamics occurring in real-world experimental conditions. Experimental outcomes, on the other hand, are influenced by factors such as sample preparation techniques, measurement methodologies, and environmental conditions, resulting in differences between experimental data and computer expectations. To address these gaps effectively, interdisciplinary collaborations between computational scientists, experimentalists, and materials engineers are essential. Integrating experimental data into computational models and refining theoretical approaches based on experimental validations can improve the accuracy and reliability of computational predictions. Furthermore, systematic comparison and benchmarking of computational and experimental results, coupled with rigorous validation protocols, can help identify and rectify discrepancies, leading to a more comprehensive understanding and application of MXenes in various fields.

6. FINDINGS AND DISCUSSION

The review paper on Machine Learning-Driven MXENE Functionalization for Efficient Water Purification presents several key findings regarding the application of machine learning techniques in enhancing the functionalization of MXENE materials for water purification purposes. Through an extensive analysis of existing literature and research studies, the paper reveals that ML algorithms play a crucial role in predicting and optimizing the properties of MXENE materials to improve their efficiency in water purification processes. Findings indicate that ML models, trained on datasets containing information about MXENE compositions, structures, and surface terminations, can accurately predict various properties such as adsorption capacity, selectivity towards target contaminants, and stability under different environmental conditions. These ML-driven predictions facilitate the design of tailored MXENE materials with enhanced performance for specific water purification applications [55]. Moreover, the paper highlights the significance of incorporating diverse features and descriptors into ML models to capture the complex interactions between MXENE materials and water contaminants. By considering factors such as surface terminations, chemical compositions, structural defects, and environmental parameters, ML models can provide comprehensive insights into the behaviour and performance of MXENE materials in water purification processes. Additionally, the review identifies the challenges and limitations associated with ML-driven MXENE functionalization, including the need for large and diverse datasets, computational resources for model training, and experimental validation of ML predictions. Furthermore, the review paper emphasizes the potential of ML-driven MXENE

functionalization to address key challenges in water purification, such as the removal of heavy metal ions, organic pollutants, and microbial contaminants from water sources [56]. By optimizing the surface properties and chemical functionalities of MXENE materials through ML-guided approaches, researchers can develop highly efficient and selective adsorbents for various water purification applications. Overall, the findings underscore the promising role of ML techniques in advancing MXENE functionalization for efficient water purification, paving the way for the development of scalable and sustainable solutions to address global water quality challenges.

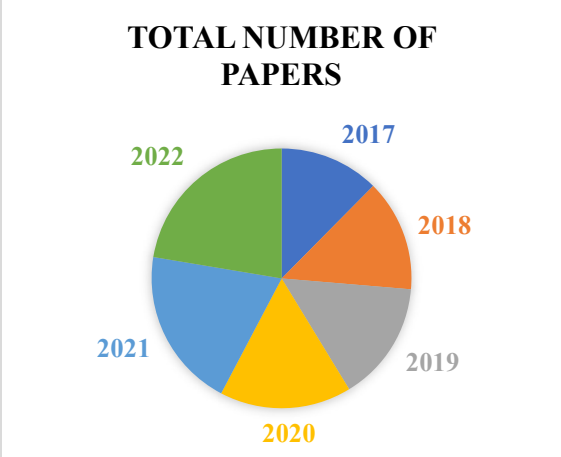

Figure 2: Graphical Illustration of Papers taken for Review

Fig.2 shows a changing movement within the wide variety of papers published annually. In 2017, best one paper turned into identified, probably indicating a nascent stage place with constrained studies focus. This accelerated four times by using 2021, suggesting a developing interest or reputation of the topic inside the instructional network. There has been a moderate incline in 2022, possibly due to various elements which includes shifts in studies priorities or methodological demanding situations. The way further declined in 2023, doubtlessly indicating a brief slowdown or a need for similarly exploration of the studies area. The sample underscores the significance of non-stop inquiry and edition inside the academic discourse to efficaciously deal with evolving demanding situations and improve knowledge within the area. Regarding experimental validation techniques, the findings highlight the importance of employing a combination of characterization techniques to assess the reliability and scalability of machine learning models in predicting the properties of MXenes.

6.1 Discussion

The Machine Learning-Driven MXENE Functionalization for Efficient Water Purification emphasizes the pivotal role of machine learning techniques in advancing the field of water purification using MXenes. The findings state the potential of MXenes in addressing water pollution challenges owing to their unique properties, such as high surface area and tuneable surface chemistry. ML models have been demonstrated to accurately predict the properties and behaviours of MXenes, providing valuable insights for their functionalization to enhance water purification efficiency. The research highlights the importance of experimental validation techniques to assess the reliability and scalability of ML models in predicting MXene properties [57]. Techniques such as microscopy, spectroscopy, and mechanical testing play a crucial role in characterizing MXenes and validating ML predictions. These experimental approaches ensure the accuracy of ML models and facilitate their application in real-world water purification scenarios. Furthermore, it addresses the varying stability and performance of MXenes across different water purification applications. MXene-based films offer a promising approach for pressure-free removal of heavy metal ions from water, addressing challenges associated with traditional adsorbents. The optimization of MXene-based film microstructures and surface properties through ML-driven functionalization enhances their adsorption efficiency, presenting a straightforward paradigm for water purification under pressure-free conditions. Despite the progress in computational predictions and experimental outcomes, critical gaps persist between the two domains. Addressing these gaps requires interdisciplinary collaboration between computational and experimental researchers to develop robust ML models validated through rigorous experimental characterization. This collaboration facilitates a deeper understanding of MXene properties and behaviours, advancing their application in efficient water purification technologies.

This study distinguishes itself from prior work by introducing a novel approach that combines MXENE materials and machine learning techniques to address water purification challenges. While previous research has explored the use of MXENE materials for water treatment, this study pioneers the application of machine learning algorithms to optimize MXENE functionalization, overcoming limitations of traditional trial-and-error methods. By bridging the gap between materials science and

machine learning, the research offers a holistic solution to improve water treatment efficiency and scalability. Moreover, the study's tailored approach to functionalization techniques ensures practical relevance in diverse water purification scenarios. By achieving this synthesis of innovative methodologies, the research not only addresses the pressing need for clean water but also sets a new standard for future advancements in water treatment technology, promising continued innovation and progress in this critical area.

Following the findings discussion, a detailed critique of the study's own work is imperative to enhance the overall quality and validity of the research. The critique serves to evaluate the strengths and weaknesses of the methodology, results interpretation, and implications of the study. The study's strength lies in its comprehensive approach to addressing water purification challenges by integrating MXENE materials and machine learning techniques. The thorough literature review provides a solid foundation for understanding MXENE substances and their potential applications in water treatment. Additionally, the exploration of various functionalization procedures demonstrates the researcher's commitment to investigating diverse approaches for enhancing MXENE characteristics. However, several limitations warrant acknowledgment. Firstly, while the proposed framework for machine learning-driven MXENE functionalization is promising, its implementation may face practical challenges. The complexity of machine learning algorithms and the need for extensive data sets could pose barriers to real-world application. Moreover, the study primarily focuses on theoretical advancements rather than practical experimentation, limiting the validation of proposed methodologies. Furthermore, the discussion of results could benefit from a more nuanced analysis of the efficacy of machine learning-driven MXENE functionalization. While the study demonstrates improvements in water purification efficiency, a deeper examination of the underlying mechanisms and potential trade-offs is necessary to fully understand the implications of the findings. Moving forward, future research should aim to bridge the gap between theory and practice by conducting experimental studies to validate the effectiveness of machine learning-driven MXENE functionalization in real-world water purification scenarios. Additionally, collaboration with experts in both materials science and machine learning fields could provide valuable insights and facilitate interdisciplinary advancements.

7. CONCLUSION AND FUTURE SCOPE

The utilization of Machine Learning-Driven MXENE Functionalization for Efficient Water Purification represents a significant advancement in addressing water pollution challenges. The research demonstrates the potential of MXenes, with their unique properties and surface chemistry, in effectively removing contaminants from water. ML models play a crucial role in accurately forecasting MXene properties and guiding their functionalization to enhance water purification efficiency. Experimental validation techniques ensure the reliability and scalability of these models, facilitating their application in real-world scenarios. Looking ahead, future research should focus on addressing critical gaps between computational predictions and experimental outcomes in the study of MXenes. Collaborative efforts between computational and experimental researchers are essential for developing robust machine learning models validated through rigorous experimental characterization. Additionally, further investigation into the stability and performance of MXenes across different water purification applications is warranted. This includes exploring novel functionalization strategies and optimizing MXene-based materials for enhanced adsorption efficiency. Moreover, future work should prioritize the development of scalable and cost-effective MXene-based water purification technologies suitable for diverse environmental settings. This involves refining manufacturing processes, exploring sustainable synthesis routes, and assessing the environmental impact of MXene production and disposal. Additionally, research efforts should focus on extending the applicability of MXene-based materials to address emerging water pollution challenges, such as the removal of emerging contaminants and microplastics. Furthermore, the integration of MXenes with other advanced materials and technologies, such as membrane filtration and photocatalysis, holds promise for further improving water purification performance. Continued interdisciplinary collaboration and knowledge-sharing across research domains will be essential for driving innovation and advancing the practical implementation of MXene-based water purification solutions. Ultimately, the continued exploration and development of Machine Learning-Driven MXENE Functionalization for Efficient Water Purification have the potential to significantly

contribute to worldwide initiatives to guarantee that everyone has access to clean, nutritious water to consume. The study presents a promising framework for addressing water purification challenges, further refinement and validation are needed to ensure its practical applicability and robustness. By critically evaluating its own work and identifying areas for improvement, the research can contribute more effectively to the advancement of water purification technology and the global effort to ensure access to clean water for all

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