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Strategic Insights for Bulk Production of MXene: A Review

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Abstract. The remarkable versatility of MXene materials has propelled them into the forefront of advanced material science, with applications spanning energy storage, catalysis, water treatment, and electronics. Bulk production of MXene materials is essential to meet the demands of applications, enhance commercial viability, support research efforts, integrate MXene into industries, and drive technological advancements. It is a key step in realizing the full potential of MXene materials and ensuring their widespread use in diverse fields. However, the problem is that MXene synthesis methods, especially those developed at the laboratory scale, face challenges when transitioning to large-scale production. Maintaining the quality, consistency, and yield of MXene materials on a large scale can be complex. The paper provides a comprehensive overview of current synthesis methods, critical parameters that influence bulk production, precursor materials and post-synthesis characterizations, and innovations in scaling up MXene production. The necessary environmental and safety measures were also reviewed. This comprehensive review work is critical for developing the area of MXene bulk manufacturing and has major implications for the larger community. By thoroughly addressing problems, investigating crucial factors, and emphasising breakthroughs in large-scale synthesis, the study serves as a road map for researchers, industry experts, and maybe policymakers.

1 Introduction

MXene materials are two-dimensional transition metal carbides, nitrides, and carbonitrides—have revolutionised modern materials research. Born from the MAX phases family, MXenes were discovered in 2011 [1]. and have since captivated academics, researchers, engineers,

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and industries with their unique features. MXenes' unique mix of metallic conductivity, hydrophilicity, and mechanical flexibility makes them versatile candidates for many applications [2]. These materials are ideal for energy storage applications like batteries and supercapacitors due to their excellent electrochemical performance [3]. MXenes are promising for water filtration [4], sensing, and catalysis due to their catalytic characteristics [5].

Bulk manufacturing is crucial to integrating MXene materials into numerous industries and technological advances. MXenes' unusual electrical, mechanical, and chemical characteristics make them promising for energy storage, catalysis, and electronics [6]. They must go from laboratory-scale synthesis to large-scale, commercially feasible manufacturing to reach their full potential. Bulk production meets rising MXene demand and allows cost-effective and scalable manufacture [7]. This scalability is pivotal for meeting the requirements of industries such as electronics, energy, and environmental remediation, where MXenes can play a transformative role [8].

This work provides an in-depth overview and analysis of current MXene synthesis techniques, including mechanical exfoliation, chemical etching, electrochemical delamination, and other emerging methods systematically. These are to identify and address the challenges that hinder the bulk production of MXene materials, such as scalability issues, cost considerations, environmental and safety concerns, material inconsistencies, and impurities. Critical parameters related to bulk production, encompassing raw material selection, process parameters, precursor materials, and post-synthesis treatments are discussed. Economic consideration is concerned to result in cost-effective strategies to be implemented. The quality control and standardization in MXene bulk production is explained. Safety measures, and regulatory compliance to ensure environmentally sustainable and safe MXene production are included as well. The review is ended by providing future perspectives and insights about the impact contributed by the bulk production of MXene with the advance of emerging technologies and collaborations between academia and industry. The review paper aims to contribute to the advancement of MXene research and guide researchers, industry professionals, and policymakers in catalyzing the development of strategies for precision and efficient large-scale production of MXene materials by addressing and tackling possible challenges.

2 Challenges in MXene Bulk Production

The technique of MXene bulk manufacturing must be carefully chosen since it has a considerable influence on total production efficiency, quality, and costs. Diverse techniques, including chemical etching and exfoliation, produce MXene with distinct characteristics, such as surface area, morphology, and layer thickness [2]. The selected technique has an impact on the material's electrochemical, mechanical, and thermal characteristics, directly impacting its performance in applications like energy storage and catalysis. Furthermore, the scalability, environmental effect, and economic feasibility of the preferred manufacturing technique are critical in determining the overall success and broad acceptance of MXene-based technology. Thus, technique selection is essential for obtaining the required material properties and optimising production procedures. **Fig. 1** depicts various problems in the bulk synthesis of MXene.It is critical to select an appropriate reactor for the large-scale production of MXene due to its significant impact on the material's quality, scalability, and economic feasibility. Reactor selection influences factors such as temperature, pressure, and mixing, which affect the structural and chemical characteristics of MXene [9]. The reactor design also influences yield, production rate, and energy consumption. To ensure that MXene manufacturing can be scaled up for large-scale applications, selecting an appropriate reactor is essential for obtaining consistent and repeatable results. Furthermore, factors like reactor materials and safety designs have a big impact on the overall performance and economic viability of MXene bulk production.

Selecting appropriate precursors for MXene bulk production is essential as it significantly impacts both cost and quality [10]. Precursors determine the composition and properties of the final MXene material. Choosing cost-effective and readily available precursors can reduce production expenses. Moreover, precise precursor selection influences the purity and uniformity of the MXene product, affecting its performance in applications like energy storage and catalysis. Inconsistent or impure precursors may lead to variations in material properties, impacting product quality and reliability [11]. Thus, careful consideration of precursor choice is integral to achieving a balance between cost efficiency and high-quality MXene production for optimal performance and market competitiveness.

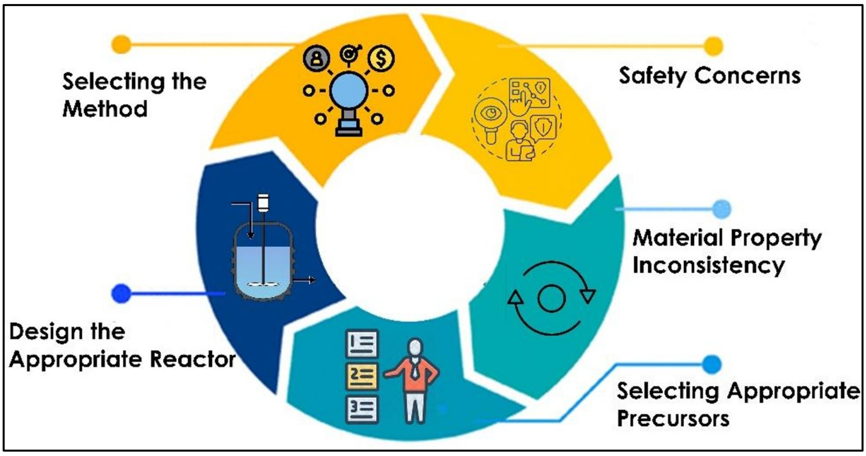

Fig. 1. The challenges in MXene bulk production.

In the bulk production of MXene, material property inconsistency is of the utmost importance, as it has a direct effect on both cost and quality [12]. Inconsistent material qualities can cause differences in product performance, making it difficult to fulfil specific application needs. This discrepancy may necessitate extra testing and quality control methods, boosting production costs. Furthermore, it might jeopardise the dependability and effectiveness of MXene-based goods, lowering market adoption. Uniform material qualities guarantee constant product performance, decreasing the need for significant quality control and waste reduction. As a result, correcting material property inconsistencies is critical for lowering production costs and providing high-quality, dependable MXene materials for a wide range of applications.

Safety considerations in MXene bulk production are critical since they affect both cost and quality [13]. Safety procedures minimise accidents, protect workers, and reduce environmental dangers, avoiding liability. Safety requirements may increase production costs due to protective equipment, training, and facility adjustments. They must be justified and balanced with the production costs. However, failure to prioritise safety can result in accidents, production delays, and significant legal ramifications. A safe manufacturing environment fosters uniform and regulated procedures, improving MXene quality. Safety is essential for production efficiency, risk reduction, and industrial reputation.

3 MXene Synthesis Methods

Hydrofluoric acid (HF) is the principal etchant in the widely used and well-established etching process, which is used to synthesise MXene [14]. This process breaks the metallic bond between titanium and aluminium, which leads to the erosion of aluminium layers. To address the concerns related to the high toxicity of HF, new methods have been developed to decrease its use in the process. In fact, the process of etching with HF has both benefits and cons. The main benefit is that it efficiently produces MXene by selectively eliminating aluminium layers from MAX phase precursors [15]. Strict safety standards and environmental safeguards are required because of the major safety issues posed by HF's high toxicity [16]. Particular precautions must also be used while dealing with and disposing of HF. Environmental and safety considerations make HF-based bulk production unlikely; hence, novel approaches are needed to address these issues and pave the way for industrial-scale MXene synthesis that is scalable, sustainable, and cost-effective [17]. One possible option for mass production is shown in **Fig. 2**, which shows several synthesis processes.

An adaptable method for synthesising MXene, fluoride salt etching, makes use of chemicals such as lithium fluoride (LiF), sodium fluoride (NaF), or ammonium bifluoride (NH_4HF_2) [18]. Using a carefully regulated reaction with fluoride salts, this technique selectively removes aluminium layers from MAX phase precursors. There are benefits and drawbacks to the modified acid etching method, which uses lithium fluoride (LiF) and hydrochloric acid (HCl), in the production of MXene. When compared to HF etching, the accurate removal of aluminium layers from MAX phase precursors is ensured by its controlled and customised method. A precise equilibrium between the amounts of LiF and HCl is required for this procedure [19]. Among the benefits is the possibility of less hazardous handling and disposal, which helps alleviate worries about HF's toxicity. The enhanced safety profile of modified acid etching makes it an attractive option for large-scale manufacturing [20]. However, there are still obstacles to overcome when it comes to maximizing efficiency, standardisation of processes, and scalability in large-scale MXene synthesis when employing the modified acid etching method.

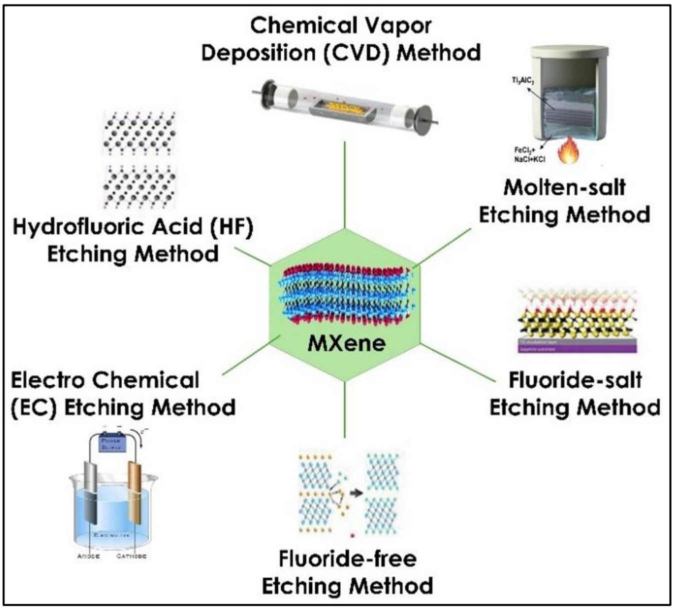

Fig. 2. Different synthesis methods of MXene.

By avoiding the use of potentially harmful fluoride chemicals, fluoride-free etching in MXene production offers a safer alternative. This strategy prioritises safety precautions and addresses environmental problems related to fluoride-based etching methods [21]. It typically employs concentrated hydrochloric acid (HCl) or nitric acid (HNO3). By doing away with the use of potentially harmful fluoride compounds, fluoride-free etching in MXene production improves safety, among other benefits. This technique avoids the potential toxicity of fluoride-based etching by using other etchants such as strong hydrochloric acid (HCl) or nitric acid (HNO3). The lack of fluorides, on the other hand, might lead to less controlled etching, which could affect the process's selectivity and repeatability [22]. To ensure consistent and controlled synthesis, address challenges in scalability, cost-effectiveness, and standardisation for large-scale MXene production while maintaining the safety benefits associated with fluoride-free alternatives, and refine the method, fluoride-free etching could be able to be used in bulk production [23].

A novel approach to MXene production, molten salt etching selectively removes aluminium layers from MAX phase precursors using high-temperature molten salts like lithium chloride (LiCl) or potassium chloride (KCl). By using high temperatures, this method may dissolve aluminium under regulated conditions without damaging the MXene structure [24]. By employing high-temperature molten salts such as lithium chloride (LiCl) or potassium chloride (KCl) to selectively remove aluminium layers, molten salt etching in MXene synthesis offers benefits like improved safety and less environmental impact compared to conventional acid-based methods [25]. However, optimising temperature conditions and guaranteeing scalability for large-scale production are problems. The energy consumption might be affected by the high temperature requirements, and the effects on the characteristics of MXene should be carefully considered. The environmentally benign profile of molten salt etching is promising, but the approach needs further work before it can be considered viable for large-scale production; problems need to be addressed, and conditions optimised for industrial-scale synthesis [26].

Chemical vapour deposition (CVD) is a method used in MXene synthesis to create films by carefully depositing precursor gases onto a substrate. Precursors, including organic ligands and metal chlorides, are commonly utilised [27]. With CVD, one may fine-tune the MXene characteristics to suit certain uses by controlling the film's thickness, composition, and structure. Among the many benefits of CVD for MXene production is the ability to precisely regulate the film thickness and composition, resulting in material qualities that may be tuned to specific needs [28]. Yet, there are obstacles, such as the need for regulated gas conditions and high temperatures, that restrict scalability and may affect the structure and characteristics of MXene. Substrate dependency, which might limit applications' adaptability, can also result from the deposition process [29]. Successfully navigating these obstacles, fine-tuning process parameters, and creating efficient, large-scale deposition techniques are crucial for the prospect of CVD bulk production. Striking a balance between the benefits and drawbacks of CVD for MXene synthesis to achieve practical, scalable applications is the goal of ongoing research.

4 Critical Considerations for Bulk Production

4.1 Reactor Design

Mass production of MXene requires a very tedious synthesis process, and one major part is the designation as well as the arrangement of an effective reactor reaction chamber. This reactor is a crucial factor in determining whether the synthesis process succeeds or fails because it determines not only how much money has to be spent but also what its quality will be. The decision on which reactor to use is also dependent upon the chosen synthesis route for the long-scale MXene production. It was stated that in the previous discussion, an appropriate selection of the etching method is a key factor, under its influence subsequent redesigning. Some important points of reactor design require consideration, such as the surface area; stirring process; heating and cooling systems, and pressure overflow [30]. **Fig. 3** presents the synthesis reactor consisting of all aspects required for MXene preparation in a scale-up approach.

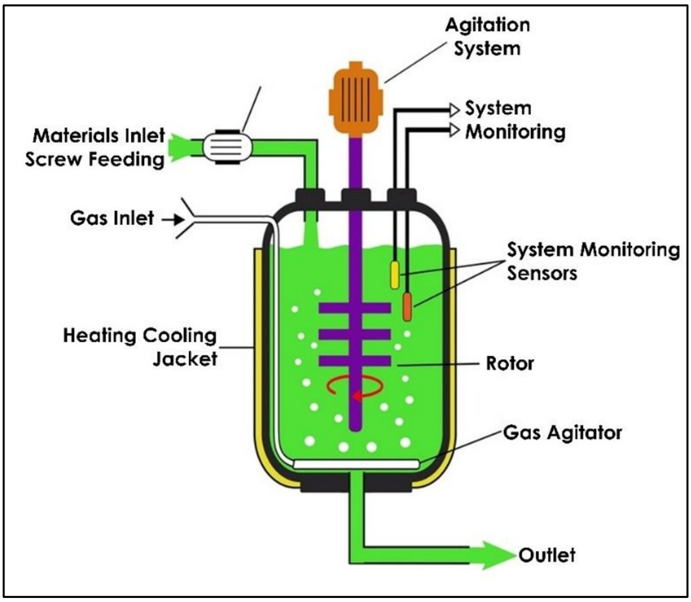

Fig. 3. A proposed reactor setup for the synthesis of MXene in bulk.

Initially, the area of the reaction chamber is a very important parameter. When constructing the reactor, it is recommended to have a large chamber instead of having one that is too tall. This design option increases the surface area of the liquid, which leads to a much better interaction between the reactants. More efficient etching is achieved due to the larger surface area, leading to a higher yield and better quality of MXene production. Secondly, mixing is a very crucial process. Adequate mixing facilitates the complete elimination of the aluminum (Al) layer from the MAX phase during the etching process. They include several stirring methods including the mechanical or magnetic type. The right stirring method needs to be chosen, as the incomplete disposal of the “Al” layer might impair the quality of the MXene product. Poor mixture can also lead to an increased reaction time, thereby increasing the production duration and thus the cost. The third major concern is the establishment of a heating and cooling system for the reactor. The synthesis of MXene is an exothermic process, producing a lot of heat during the reaction. Temperature adjustment is very critical to keep the process within the limits. With the introduction of MAX phase material into the etching solution, there is a fast temperature rise. Managing this requires an effective cooling system to capture the heat that is produced during this stage of the reaction. Moreover, controlled heating is very necessary to increase the etching process. Thus, the heat transfer behaviors of the reactor should be adequate to provide efficient temperature control. It is very critical to choose the materials for the reactor that can resist highly corrosive acidic environments and still provide a high efficiency of heat transfer. For instance, the use of alloys which include nickel-molybdenum can provide good acid resistance and heat transfer characteristics.

For the reaction chamber, PTFE is widely used in lab-scale production because of its acid-resistant properties. Nevertheless, PTFE is not an ideal material for the efficient transfer of heat. To overcome this weakness, particularly in mass-based production environments, alloys such as nickel–molybdenum become vital. These alloys are very essential for the resistance to acidic environments and proper heat conductivity, helping ensure the great success of MXene synthesis in a practical situation. The other aspect is the inward environment of the reactor. In the scale, a loosely sealed container is usually needed as the reaction could be exothermic and this can lead to gaseous productions such as carbon monoxide (CO) and carbon dioxide (CO_2). Running the reactor in a fume hood is proposed as a lab-scale synthesis. But in mass production, this may not be very convenient. In such instances, an exhaust system having a non-return valve that is controlled by the pressure sensor should be integrated. This delivery enables the controlled gas release, thus ensuring safety and productivity in the manufacturing process.

In conclusion, the choice and configuration of the reactor required for MXene bulk production is a very important stage that greatly defines both the price and final product quality. Factors like the surface area, vertexing process, and heating and cooling setups along with pressure controls enable to achievement of efficient yet controlled synthesis of MXene for different applications. To promote the scalability, reproducibility, and overall effectiveness of large-scale MXene production, investing in a robustly designed or manufactured reactor is very inevitably necessary.

4.2 Precursors Selection

Precursor selection in the bulk production of MXene is very crucial because it determines not only the cost but also the quality of this process. Precursors are also the raw materials in MXene synthesis, and their nature leads to different products concerning composition, purity, and properties. For example, $Ti_3C_2T_x$ MXene can be synthesized by using (e.g., Ti: Al, Ti: Graphite; Carbon black; TiC and the formation of different precursors that can produce MXene **Fig.4** Different precursors are sold with various prices, thus effectively affecting the product's price [31]. Precursor selection directly influences the cost of production. The choice of cost-effective and easily accessible raw materials makes it possible to reduce production costs [32]. Further, the accessible and stable prices of the selected precursors may affect whether MXene production on a larger scale is economically viable and sustainable. By choosing the readily available precursors, cost efficiency is achieved, and when the rate of production can be multiplied. Besides the financial factors, precursor choice is also an important factor in deciding on the quality of MXene products. The purity and homogeneity of the initial ingredients directly affect the business composition type, and properties synthesized by MXene. The final product may vary irreproducible due to the impurities or inconsistent quality in the precursor, which affects its performance for different applications.

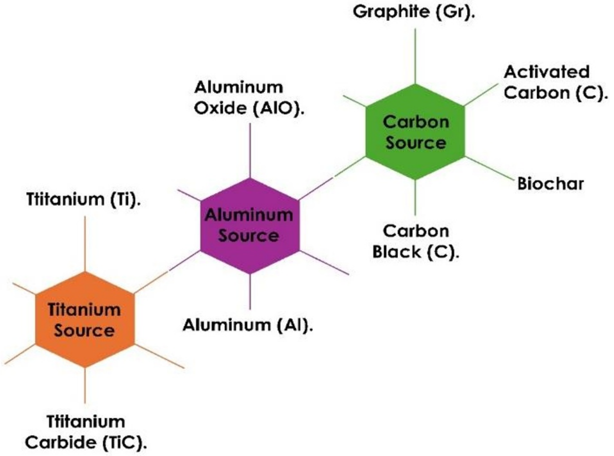

Fig. 4. Different precursors are needed for the synthesis of MXene.

In addition, the chemical properties of the precursors have an impact on the entire synthesis process. There may be some unique reaction conditions that affect the different precursors, such as the temperature and time applied in a particular case. The compatibility of the chosen precursors with the selected synthesis method plays a very important role in achieving a controlled and reproducible process that is vital for maintaining quality output on a large scale. Precursor selection goes far beyond the consideration of cost and quality to encompass the environmental impact during production. The use of eco-friendly and sustainable precursors helps to advance greener manufacturing while reflecting modern trends that promote green practices. To conclude, the precursor selection in MXene bulk production is a very important parameter that affects both the cost and quality of manufacturing significantly. The choice of cost-effective, quality, and environmentally friendly precursors is very critical for achieving an efficient production process while also ensuring the stability of final MXene products and supporting economic feasibility in the large commercial scale synthesis processes.

4.3 Operating Parameters

It is crucial to have optimal operating conditions for the synthesis of bulk production of MXene as it provides adequate control over the material properties, high-purity products, and improved scalability [33]. Parameter optimization, involving reaction temperature and time as well as the precursor ratios is a capability that allows the researchers and manufacturers to customize MXene for uses such as energy storage or sensing. Such an optimization leads not only to the materials with required features, such as specific surface area and shape but also ensures yield advancement and purity levels improvement accompanied by the quality of resource usage diminution [34]. The scalability and productivity created by the optimization allow for a transition from laboratory-based experiments to large-scale industrial production of MXene materials due to the increased demand. **Fig. 5** shows various critical parameters, which play an essential role in the synthesis of MXene and affect its quality. Additionally, the uniformity and repeatability achieved through precise parameter optimization can increase the credibility of MXene's performance between various batches for researchers as well as end-users [35]. In addition, the cost savings obtained by streamlining processes, such as reducing precursor material costs and using cheaper manufacturing techniques also lead to the economic feasibility of MXene production. Consequently, not only does optimization guarantee the quality and customized features of MXene but also it facilitates progress in technology, material science as well as eco-friendly manufacturing approaches.

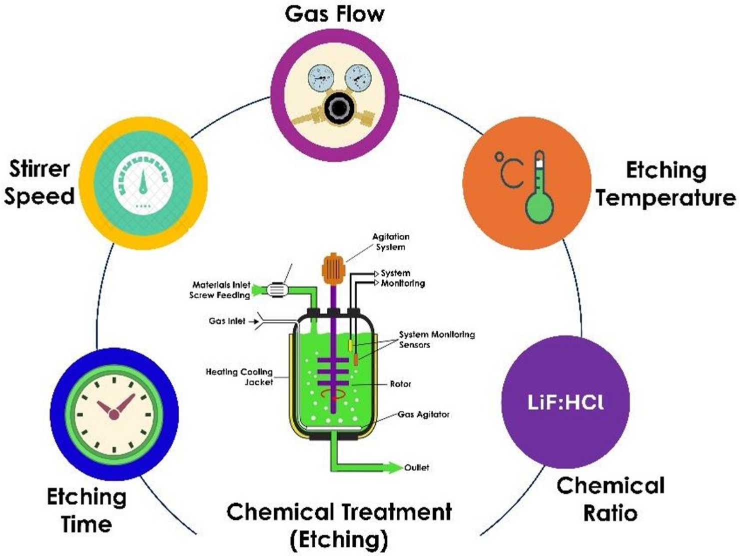

Fig. 5. Different critical operating parameters for the synthesis of MXene.

4.4 Economic Considerations and Cost-effective Strategies

The MXene cost analysis encompasses an examination of the different aspects that lead to the total costs incurred during fabrication. Some important factors affecting the production costs are precursor selection, reactor design, and materials; also, energy consumption; labor cost, and purification processes. Precursors selected play a very critical role in determining the overall material cost of manufacturing, which considers various aspects such as availability, price stability, and environmental effects. Reactor design and materials encompass both the initial capital expenditure and operating cost only to require thermal-insulating materials that can withstand reaction conditions alongside efficient heat transfer. Energy usage however plays a very key role in the operational costs especially when it comes to heating and cooling. Labor costs include the workers who are engaged in synthesis, quality control, and maintenance. Further, the purifying processes to get the required MXene quality might add some extra cost. To capitalize on the production efficiency, scalability, and competitiveness in the MXene market resource allocation decisions need to be made based on a detailed cost analysis that will determine process refinements.

Economies of scale are a very important factor in the MXene mass production, which determines the efficiency and cost-effectiveness as well as overall competitiveness. In any case, it should be noted that attaining economies of scale involves a lot of strategic investment planning and effective operation. Challenges can include specialist equipment, effective supply chain management, and consistency at increased production volumes. As the scale of production increases, balancing economies of scale against maintaining high-quality standards becomes a critical element for successful bulk manufacturing, especially in advanced materials such as MXene where precision and consistency should be emphasized.

Lowering the synthesis costs during the MXene manufacturing process requires a comprehensive approach. Cost-effectiveness and availability were important elements of the strategic precursor selection. Economies of scale are achieved through the increase in production volume, the distribution of fixed costs, and the application of equipment that can be scaled up. Improving parameters such as the temperature and reaction time using continuous process optimization leads to high efficiency and yield. Energy efficient technologies with their advanced reactor designs contribute to the minimizing of power consumption. Supply chain management is very efficient, there are many massive purchases, and waste minimization strategies all further help cost reductions. Automation and robotics help in reducing labor costs while also enhancing accuracy at the same time. Innovation and cost-effective solutions are often promoted through collaborative research, strategic outsourcing, as well as a culture of continual improvement. The life cycle assessment helps ensure a comprehensive view of the environmental effects that can determine decisions for sustainable and cost-effective MXene synthesis [36]. The alignment of these strategies is very essential to a production process that will be cost-effective and competitive. Some of the research works demonstrate that using recycled materials as a precursor material (for instance, Beverage cans, Biochar, and Activated Carbon) for synthesizing MXene leads to a reduction in cost being more than 10%. The last product cost is approximately 20.33$ [37].

4.5 Safety Concern

Safety issues that arise concerning MXene bulk production are also pivotal in defining the well-being of human personnel as well as the costs involved. The particularities of the MXene display its exothermic synthesis processes with a notable gas release emphasizing how very important it is to have adequate safety measures [13]. The introduction of comprehensive safety strategies involves a lot of initial expenses on the specialized equipment, training programs, and necessary facility alterations to eliminate the risks resulting from hazardous materials and reactions. Not emphasizing safety may result in a lot of accidents, production stoppages, and sometimes legal liability that can dramatically increase the overall cost of MXene manufacturing [38]. Moreover, safety considerations also go beyond the personnel to the environmental consequences because handling materials improperly or inadequate measures can lead to contamination or harmful effects. Although safety measures may appear to incur an initial cost, these investments are inevitable for the long-term production efficiency that reduces many risks and protects both the workers as well as environmental surroundings [39].

4.6 Quality Control and Standardization in MXene Bulk Production

Quality assessment of MXene encompasses a wide range of characterization techniques to analyze the structural and chemical properties, shown in **Fig. 6** below. XRD exposes crystallographic details and phase purity as well. SEM and TEM images elucidate the MXene morphology & and layer thickness. Raman spectroscopy and XPS investigate the MXene's chemical composition, confirming its presence of elements as well as possible impurities or defects [40]. The electrochemical characterization methods are used to assess the performance of MXene in energy storage. The optical and chemical characteristics of MXene are investigated by the UV-visible, as well as Fourier transform infrared (FTIR) spectroscopies [41]. The holistic approach promotes a complete quality assessment, determines the applicability of this material, and advances the MXene technologies.

Fig. 6. Different quality assessment instruments are required to characterize MXene.

Industrial standardization has a very key role in lowering the cost of MXene manufacturing at an industrial level, while simultaneously delivering superior quality products. Standards allow for the standardization of processes relating to optimizing synthesis, economies of scale in supply chains, and streamlining production. Even with the expense of such quality assurance measures, standards serve to significantly reduce the sub-standard materials produced and therefore reduce rework costs. Standardized procedures also streamline the training programs and allow personnel to operate the equipment more effectively, thus reducing labor costs. In addition, compliance with the industry standards reduces the potential risks concerning the safety of processes and outcomes, environmental impact as well as regulatory requirements. Market confidence and trust in the customer terms are supported when products coincide with the established standards of quality which allows for competitive prices. In general creation of industry standards helps in innovation and cooperation which results in increasing productivity at a lower cost but with high-quality products.

4.7 Future Perspectives and Research Directions

The advancement of MXene manufacturing on an industrial scale is dependent on new technology and breakthroughs. Continuous flow systems and automated platforms are examples of modern reactor designs that improve efficiency and cut down on labour expenses. Innovative energy-saving techniques, such as microwave-assisted synthesis, reduce power use [42]. Modern corrosion-resistant alloys and other state-of-the-art materials are used to build reactors, which increase their longevity and endurance. Consistently high-quality MXene output is guaranteed by process intensification techniques and advanced monitoring systems, which optimise synthesis parameters. Improved production efficiency, lower prices, and the capacity to scale are all results of these technical developments, which are essential for the broad industrial uses of MXene. Additionally, the advancement of industrial-scale MXene synthesis relies heavily on collaboration between academics and industry. Academic study yields ground-breaking understandings, novel approaches to synthesis, and fresh material findings. On the other side, industries provide insights into practical applications, specifications for scalability, and the means to execute projects on a grand scale. By working together, we can speed up the process of turning research results into practical applications in industry, which in turn improves production efficiency, cuts costs, and boosts quality. The sharing of information and resources between academia and industry fosters a collaborative ecosystem, resulting in advances in MXene manufacturing that are both academically sound and commercially feasible for a wide range of applications.

5 Conclusions

Ultimately, MXene materials have established themselves as trailblazers in the realm of innovative materials, discovering uses in a wide range of sectors, including electronics, water treatment, energy storage, and catalysis. Nevertheless, there are obstacles to preserving quality, consistency, and yield when moving from small-scale synthesis in the lab to large-scale manufacturing. This review carefully looks at these problems by looking at the latest ways to produce MXene, the precursor materials used for starting the production process, and new ways to make MXene production more efficient. Environmental and safety concerns are also highlighted in the article. This review provides essential insights into MXene, as its promise is dependent on its ability to be successfully produced on a large scale. The document supports scientific breakthroughs and ensures broad use of MXene materials by providing a roadmap for researchers, industry experts, and policymakers. It promotes the area of MXene bulk manufacturing and simplifies its integration into industries. Overall, this joint effort between academics and industries is necessary to fully utilise MXene materials in solving current issues and promoting innovation across numerous fields.

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