

Review Article

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A mini-review on MoS₂ membrane for water desalination: Recent development and challenges

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Abstract: This review provides comprehensive studies of molybdenum disulfide (MoS₂) for water desalination. The most recent molecular dynamics simulation and experimental work on the design, fabrication, ion rejection, and water flux of MoS₂ were summarized. Since MoS₂ has excellent properties such as physicochemical, mechanical, and biological properties compared to other 2D materials such as graphene-based nanomaterial, it is necessary to have a critical study on MoS₂-based membranes. Hence, a critical review of MoS₂-based membranes has been found essential for us to investigate and evaluate the findings in this field and objectively assess the current state-of-the-art in water desalination. The advantages of desalination technology and the primary approaches that have been used up until now are first outlined in this study, deeply emphasizing membrane technology. The primary mechanism of salt rejection in membrane technology is explained. Then, the types of MoS₂-based membranes for water desalination are reviewed based on the different published works while critically reviewing the performance of each type of MoS₂-based membranes.

Keywords: water desalination, MoS₂ membranes, water flux, ion rejection, nanosheets

1 Introduction

Water scarcity has been a significant issue worldwide. As the population grows, agricultural activities rise, and industrialization continues, the gap between supply and demand widens, and natural water supplies deteriorate; this has become one of the most significant challenges [1]. By 2025, it is estimated that almost 70% of the world's population will confront water scarcity, considering that roughly 50% of the world's population reside within 200 km of the shore [2]. As a result, the technology for obtaining clean water at the lowest possible energy cost becomes increasingly crucial. Aside from the tiny amount of fresh water available, the oceans and seas contain nearly all of the world's water (up to 97% of the total amount) [3].

Water desalination is the most promising method for creating an unending water supply [4]. It offers an enticing prospective solution to the age-old issue of plentiful seawater's practical inaccessibility for potable use. It involves removing salts and other dissolved contaminants from various sources, including brackish surface and groundwater and industrial and municipal wastewater, among others. Since freshwater sources are limited, the world has turned to seawater and water recovery from marginal sources such as brackish groundwater and seawater [5–7].

The desalination process or technology can be categorized into membrane technology and thermal technology [8], as shown in Figure 1. Membrane-based desalination uses a membrane (molybdenum disulfide [MoS₂], graphene *etc.*) to filter the water, enabling it to flow through while keeping salt and other minerals, *e.g.*, nanofiltration (NF), reverse osmosis (RO), and electrodialysis [9–13].

Membranes have numerous advantages, including low energy consumption, continuous separation, mild process conditions, simplicity of scaling-up, the absence of additives, and the flexibility to combine with other separation methods. Fouling tendency, limited membrane lifetime, low flux selectivity, and more or less linear scaling-up factor are the most typical restrictions, regardless of membrane type [7,12,14–16].

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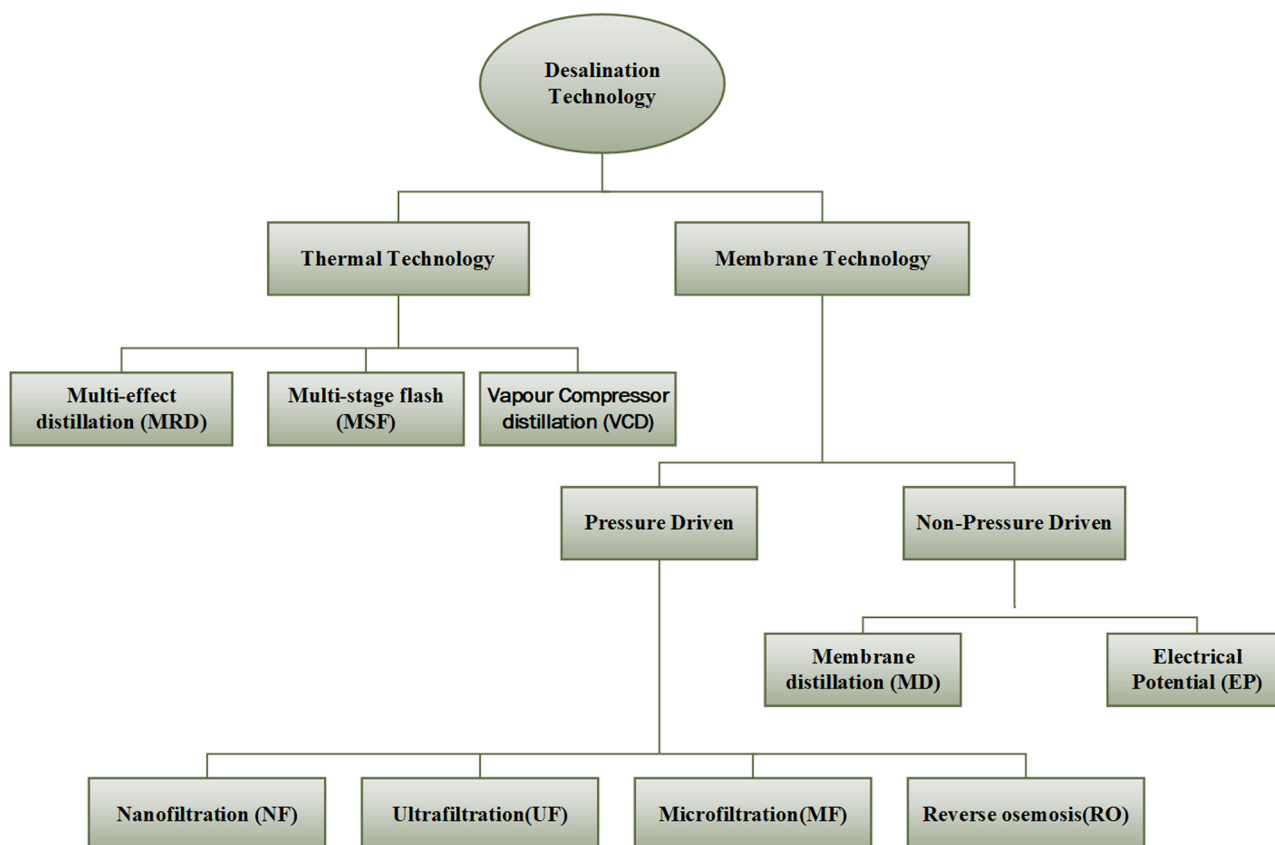


Figure 1: Desalination technology categories.

The most commonly used desalination technique in membrane technology is RO [17,18]. The mechanisms of salt rejection in membrane technology [19–21] are explained, which are as follows:

- Dehydration impacts (steric exclusion of the hydration shell) [22]
- Size exclusion (bare ion) [20,23]
- Subtler effects, such as those seen in biological channels, involve particular interactions with the pore
- Charge repulsion [24,25]
- Interactions between solutes and the chemical structures of the pore and
- Differences in entropy

2D materials have been adopted for water desalination, treatment, and purification due to their outstanding properties such as hydrophobicity, easily controlled thickness and shape, charge density, high bandgap, and water transfer channel, which offer excellent permeability, selectivity, flux, and antifouling [19–22]. In the current literature, those 2D materials with higher permeability-incorporated nanomaterials are called ultra-permeable membranes [26], as shown in Table 1.

One of the most well-investigated 2D materials is graphene and their derivatives, such as graphene oxide (GO) and reduced graphene oxide (rGO) [23,24]. Graphene is a single-atom-thick membrane (0.34 nm) that has been shown to have higher flux rates than conventional membranes. Chemical functionalization of a graphene nanopore (*e.g.*, adding hydroxyl groups) has been demonstrated to improve permeability but lower desalination efficiency [25,27,28].

However, other 2D materials such as MoS₂, MXene, boron nitride [29], metal–organic frameworks [30], and covalent organic framework [31,32] are fast-emerging synthetic water nanochannels for desalination application [33,34]

Hence, both MoS₂ and graphene have excellent performance for water desalination, and several literature studies have shown that MoS₂ is better than graphene and its derivatives. For example, Song *et al.* [35] compared the performance of porous graphene and MoS₂ nanosheet *via* molecular dynamics (MD), and their simulation results show that MoS₂ performs better than graphene in terms of water permeability. Table 1 shows the comparison of different properties of MoS₂ and graphene and its derivatives in terms of their advantages and disadvantages in water desalination.

Table 1: Comparison of different properties of 2D material membranes and their advantages and disadvantages in water desalination

2D material membrane	Interlayer spacing/pore size (nm)	Surface area (m ² /g)	Zeta potential (mV)	Advantages	Disadvantages
GO	0.85	–24 to –46	90	• Atomic thickness • Easy to synthesize • Functional group	• Membrane swelling • Unstable in an aqueous environment
rGO	0.7–1.2 nm	–24	130	• Lower swelling • More swelling • Narrower nanochannels	• Membrane swelling • Low permeability
MoS ₂	0.65 nm	–45	165	• Medium permeability • Long-term stability • Rigid nanosheet. • High water flux • Excellent salt rejection. • Long-term stability	• Requires functionalization • Hydration of the membrane is required at all times for efficient water transport

MoS₂ is an inorganic transition metal dichalcogenide (TMD) molecule containing one molybdenum atom and two sulfur atoms. Dichalcogenides are chemical compounds made up of transition metals such as molybdenum and chalcogen (a periodic table element in group 16) such as sulfur(s) [36]. MoS₂ nanosheets and MoS₂-based membrane have many advantages over other 2D materials, and MoS₂ has been widely involved in membrane design and application of water desalination and treatment. Some of the benefits of MoS₂ are as follows:

- A higher elastic modulus (200–300 GPa) facilitates water treatment.
- It can be obtained naturally from molybdenite mineral.
- It has better performance in many aspects such as catalysis and electrochemical properties.

According to Sun *et al.* [37], the MoS₂ membrane had an Evans blue rejection of 89% and a water flux of 245 Lmh/bar, indicating that the water flux was 3–5 times larger than GO membranes.

Researchers have been conducting extensive research on MoS₂-based membranes for the past few years. NF, RO, and forward osmosis are separation methods using MoS₂-based membranes. However, there are few review publications on MoS₂-based membranes for water desalination, purification, and treatment, to the best of our knowledge. For instance, the fully hydrated MoS₂ membranes displayed moderate-to-high water permeability and ionic rejection at 1.2 nm interlayer spacing [38]. In contrast, different reports on separating the layer of MoS₂ nanosheet frameworks without tunability lacked water–salt selectivity [39]. Therefore, it is necessary to summarize the key results of MoS₂ membranes, understand the present research status of the separation mechanism, and improve the membrane performance in water desalination.

In this review, we discussed the main MoS₂ nanopore preparation techniques related to the membrane fabrication. Then, the manufacture and design of MoS₂-based membranes are thoroughly outlined in terms of nanoporous membranes, MoS₂ composite membranes containing MoS₂-incorporated membranes, layer-stacked membranes, and MoS₂-based membrane surface modification. The overview is based on a thorough examination of the present state of 2D-based membrane development and the classification of classic membrane technologies. Then, emphasizing desalination, we critically analyzed current advancements in MoS₂-based membranes for water treatment and purification. Meanwhile, MoS₂-based membranes are compared to other kinds of 2D-based membranes for their new features and great performance (mainly GO-based membranes). Finally, we will discuss upcoming difficulties

and chances to fully realize the potential of MoS₂-based membranes in water treatment and purification.

2 Fundamental structure of MoS₂

MoS₂ is a TMD that belongs to a popular type of layered material in which metal layers are sandwiched between two layers of chalcogen atoms [40]. The structure of MoS₂ is made up of weakly linked layers of S–Mo–S, with an Mo atom layer sandwiched between two S atom layers, as in Figure 2. Weak van der Waals forces hold these interlayers together, but strong covalent forces have the individual atomic interlayers together [36,41,42]. It has a band gap of ~1.8 eV [43–45] that changes from an indirect gap to a direct one in monolayer structures, and the interlayer of spacings of the MoS₂ monolayer is 0.62 nm with a spacing of 0.3 nm [46–48]. A single-layer MoS₂ is formed with a thickness of almost 1.0 nm, and it is a mechanically robust material with applicable Young's modulus of 270 ± 100 GPa [49,50], which can be compared to steel. The possibility of crafting the pore edge with both Mo and S or using them individually allows the nanopore to be designed with the appropriate functionality. Protein channels and other nanoscale membranes have recently been revealed to have a nozzle-like structure that improves water permeability [49,51].

MoS₂ fish-bone structure allows for a nozzle-like sub-nanometer (sub-nm) pore for quick water permeation; while theoretical membrane efficiency studies are crucial in desalination technology, some other issues of membrane manufacturability must be addressed, such as precise pore creation, well-defined sealed membranes, and large area synthesis with defect-free. In MoS₂ membranes, adaptable nanopores with sizes varying from 1 to 10 nm were effectively sculpted using a highly concentrated electron beam and transmission electron microscope. Waduge *et al.* [49,52,53]

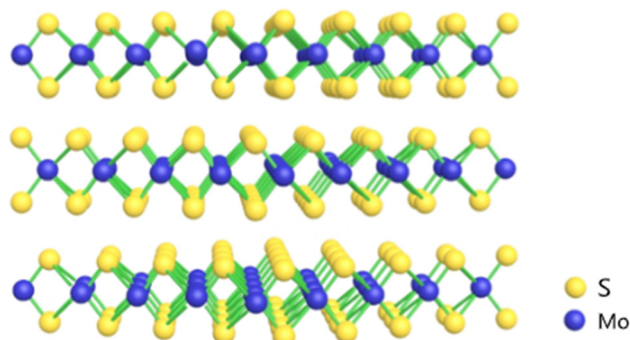


Figure 2: Laminar MoS₂ structure [54]. Yellow atoms represent S, and blue atoms represent Mo.

reported the fabrication of a large area, tightly sealed membrane with nanopores as small as 2.8 nm.

MoS₂ structure differs from 3D, 2D, 1D (three, two, one dimensional, respectively), or dot structures, which determine the characteristics and applications that change from one dimension to another. For example, 3D can be used as semiconducting, metallic, or superconducting [42]. Its bulk (3D) structure exists in tri-agonal (T), hexagonal (H), and rhombohedral (R), where 2H MoS₂ refers to the MoS₂ compound's two-layer hexagonal shape. There are three primary structures, which are 1T, 2H, and 3R, where 1T phase coordinates form an octahedral structure, and 2H and 3R in trigonal prismatic structure, as shown in Figure 3. 1T-MoS₂ has one S–Mo–S layer per unit cell, with octahedral coordination. It is a metallic MoS₂ with Pauli's paramagnetism and a negative temperature coefficient for electronic conductivity [36,55,56]. 2H-MoS₂ is composed of edge-sharing trigonal prisms with two layers per unit cell to form a hexagonal system's planar. 2H-MoS₂ electronic structure is semiconducting [55]. The layered structures of 3R-MoS₂ polytypes are regular due to the Mo atoms' six-fold trigonal prismatic cooperation with the S atoms. The prismatic S coordination of the common 2H phase and the high-pressure 3R phase is contrasted with the octahedral coordination in the 1T coordination [45]. Three layers of 3R-MoS₂ are layered and have rhombohedral symmetry; it is also semiconducting. MoS₂ nanosheets can produce the 2H or the 1T phase, depending on the exfoliation techniques. These two phases can be changed from one to the other by annealing (1T to 2H) or intralayer atomic sliding caused by Li intercalation (2H to 1H) [57].

2D is used mainly for membrane separation; we focus on the 2D MoS₂ structure for water purification for this review. MoS₂ exist in different 2D structures such as nanosheets and nanoribbons.

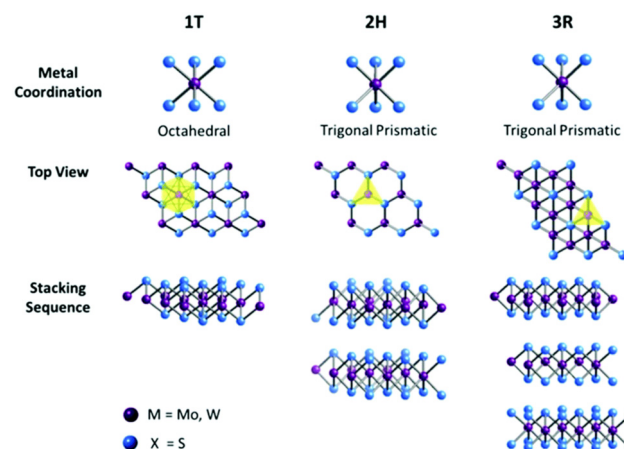


Figure 3: Different stacking and coordinating arrangements for the three MoS₂ structures [53].

3 Synthesis for MoS₂ and its composites

The critical synthesis techniques used to prepare MoS₂ and related composites are briefly discussed. There are different methods used to obtain the material layer. Each of them is different in terms of quantities, sizes, and shapes. The approaches used in synthesizing MoS₂ nanostructure are (1) the top-down approach and (2) the bottom-up approach [42,52], as shown in Figure 4.

3.1 Top-down method

The top-down technique is an exfoliation technique for obtaining MoS₂-layer materials, including mechanical, liquid, and sputtering. There were weak van der Waal forces between TMD layers, which allowed for various exfoliation synthesizing methods [58,59].

3.1.1 Mechanical exfoliation

Mechanical exfoliation is an approach used to prepare 2D nanosheets from the bulk-layered material by mechanical fragmentation [60]. It is also recognized as the scotch-tape method, which detaches or peels bulk crystal rubbing

against a solid surface, effectively overcoming van der Waal's force among the layers and residue and electronic-grade MoS₂ nanosheets for fundamental studies (*e.g.*, photoluminescence [PL] and field-effect transistor performance have unique characteristics) [43,61].

Mechanical exfoliation does not require specialized machinery, and it is the most straightforward and affordable method for producing the cleanest, most crystalline, and atomically thin nanosheets of stacked materials. It has the potential to achieve quality materials. Its limitation is that it cannot be used for high-quality, large-scale production of clean water from desalination due to the presence of defects. Miyake and Wang processed an MoS₂ with a radius of less than 50 nm at the nanoscale scale using an atomic force microscope [62], as shown in Figure 5.

3.1.2 Liquid exfoliation

There are two types of liquid exfoliation: sonication-assisted and shear force-assisted.

3.1.2.1 Sonication-assisted liquid exfoliation

It helps to exfoliate layered compounds in liquid solutions, which may help to intercalate the activation barrier [18,63]. Based on strong sonication power and components (ions, polymers, surfactants) that improve adhesion to the

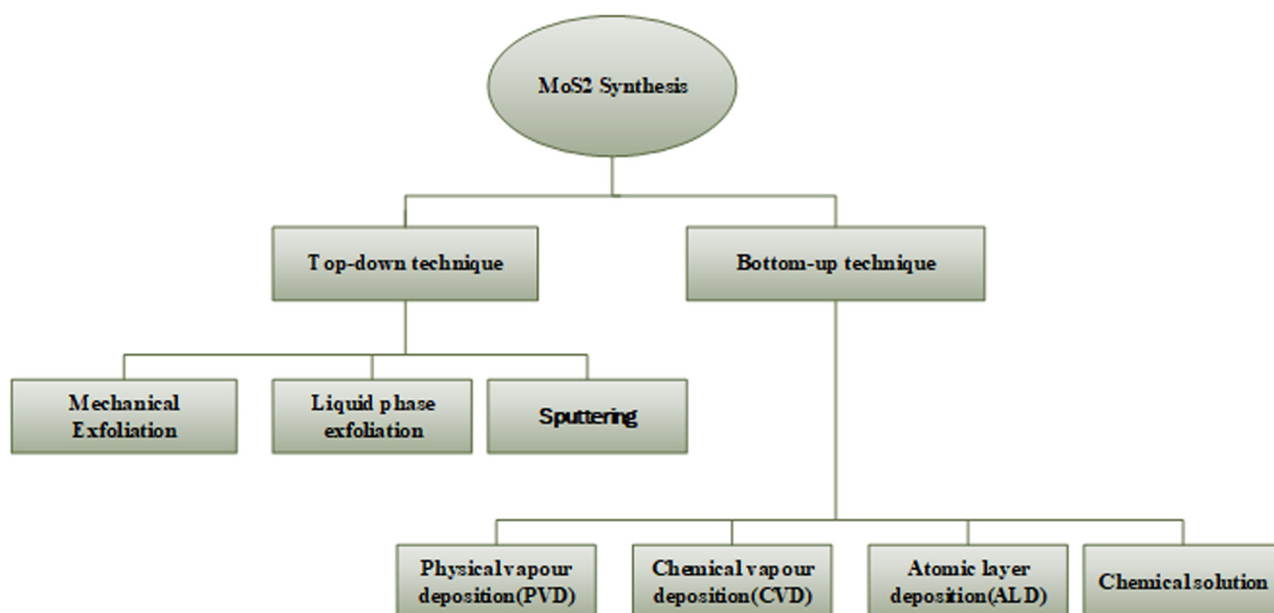


Figure 4: Different MoS₂ synthesis techniques.

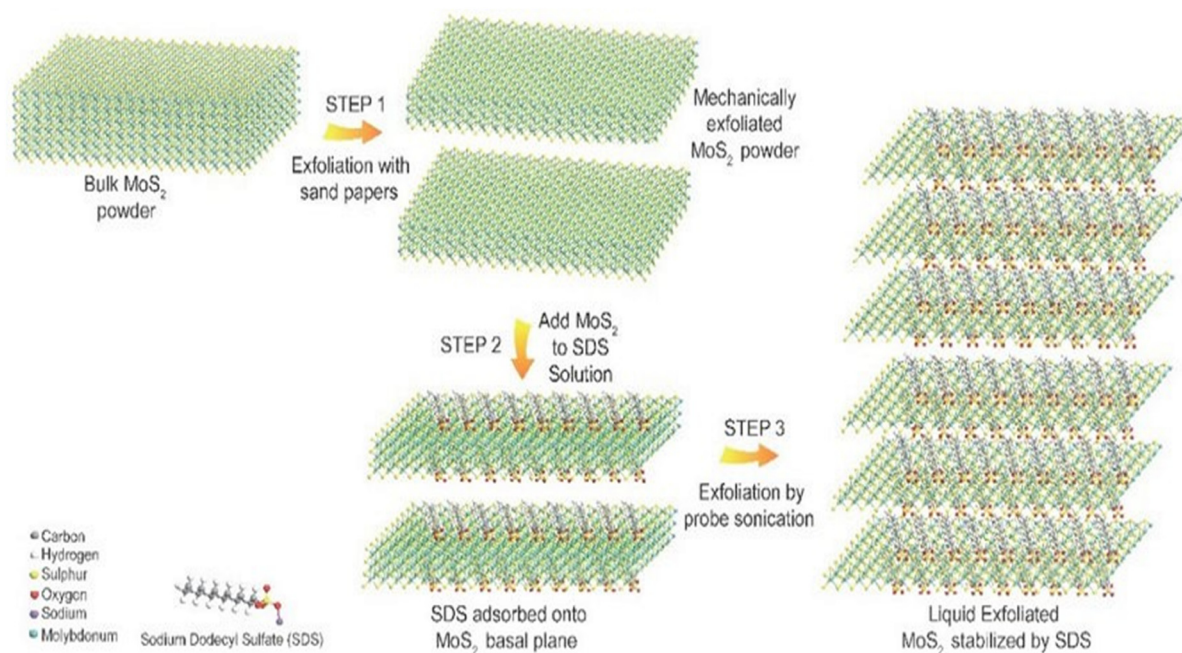


Figure 5: A top-down approach from mechanical exfoliation to liquid-exfoliated MoS₂ [41].

stratified MoS₂ surface and permit exfoliation, the process yields an exceptional amount of dispersion of few-layered MoS₂. TMD nanosheets tend to accumulate in the absence of a surfactant or a polymer because they remain hydrophobic even after being exfoliated in water, *i.e.*, following a lengthy sonication time [64].

Liu *et al.* [65] established a basic exfoliation procedure with salt in a liquid phase, and they were able to make

MoS₂ nanosheets, as shown in Figure 6. They exfoliated with isopropyl alcohol and salts such as sodium tartrate, potassium sodium tartrate, and potassium ferrocyanide as assistants. These salts have an impact on how MoS₂ in isopropyl alcohol exfoliates. With MoS₂ nanosheet dispersion concentrations of 0.240 mg/mL, it was discovered that the isopropyl alcohol–K₄Fe(CN)₆ method could increase the exfoliation efficiency by about 73 times. The resulting MoS₂ nanosheets

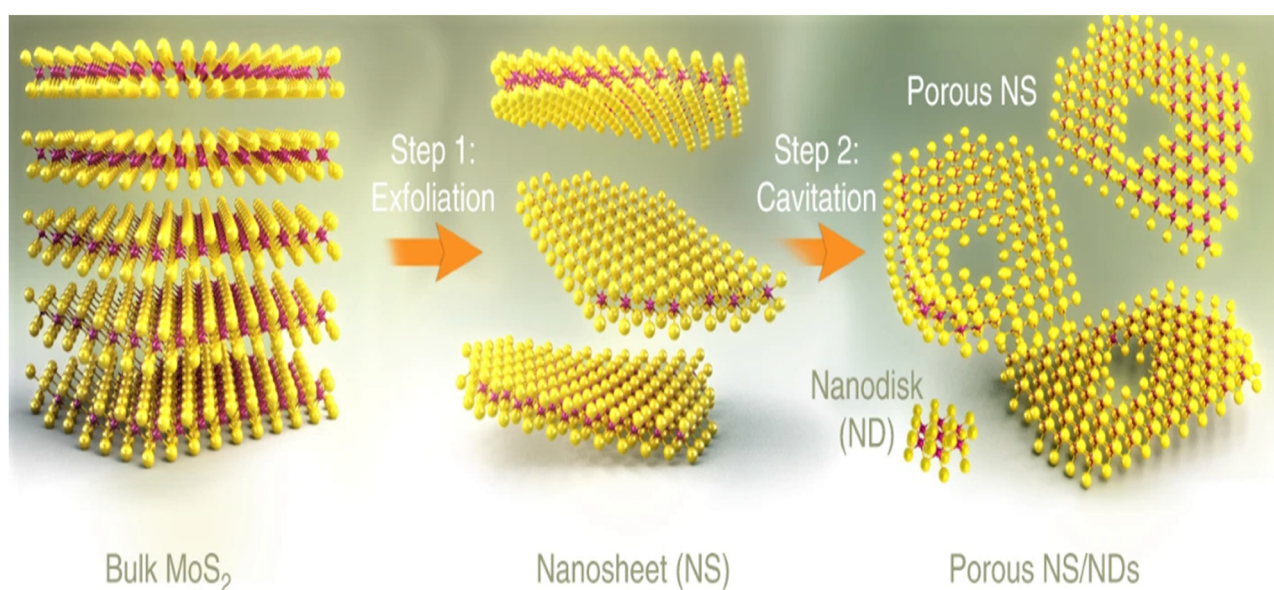


Figure 6: Schematic exfoliation process [67].

have a tiny dimension (relatively small area) due to their prolonged period of induced scission and the production of non-homogeneous MoS₂ layers, which is a drawback in sonication-assisted exfoliation. Recently, according to Kaushik *et al.* [66], combining bath and probe sonication produces faster exfoliation than sonication alone.

3.1.2.2 Shear force-assisted liquid exfoliation

It is a process of using high-speed mechanical mixers, such as shearing laboratory mixers, ball mills, and even domestic blenders, to produce bulk MoS₂ by exfoliating in suitable surfactant solutions or organic solvents to provide a local shear rate in a mixing vessel (usually with a 1 L or higher capacity). A simple, effective, and scalable approach for MoS₂ exfoliation was reported using a mixture of low-energy ball milling and sonication. Ball milling causes layered materials to exfoliate, forming two-dimensional nanosheets from the edge by applying compression and shear stresses. The MoS₂ suspension as-fabricated was 0.8 mg/mL, while nanosheets of MoS₂ with diameters ranging from 50 to 700 nm and thicknesses range were reported by Yao *et al.* [68].

Varrla *et al.* [69] successfully fabricated MoS₂ using exfoliation shear of MoS₂ nanosheets in a surfactant, which was shown on a wide scale using a kitchen blender. By optimizing mixing variables, they obtained 0.4 mg/mL concentrations and 1.3 mg/min production rates (time of mixing, rotor speed, MoS₂ concentration, and solution volume); by adjusting the surfactant content, the length and thickness of the film could be adjusted between 40 and 220 nm and 2–12 layers.

Apart from the elaborate ones, there are other methods in top-down techniques: sputtering, which is used to prepare layers of MoS₂ to be used as lubricants. The coating has a low coefficient of friction; however, under humidity, particularly for thin layers of MoS₂, these frictional qualities can vary.

3.2 Bottom-up techniques

Bottom-up techniques are used to obtain 2D nanosheets by direct growth using a precursor, and the most difficult technological challenge is ensuring the growth of 2D nanosheets in one direction while having a minor influence on the growth in the other two directions. However, the centimeter-scale MoS₂ and GO nanosheets have recently been successfully created *via* a bottom-up synthesis technique [46]. Bottom-up is an alternative approach that has the potential to produce less waste and is cost-effective. Bottom-up approach refers to the fabrication of material from the bottom-up: atom by atom, molecules by molecules, or cluster by cluster. Many of these techniques are

still in development or are only now being used commercially to produce nanopower [70]. Therefore, large-scale production is difficult but remains a cheaper technique compared to the top-down approach. Bottom-up approaches can be classified into physical vapor deposition (PVD), chemical vapor deposition (CVD), atomic-layer deposition (ALD), and chemical solution.

PVD is a bottom-up technique that incorporates ion embedding similar to molecular beam epitaxy. This technique can be applied only to a thin layer of MoS₂; the resultant grain has varying diameters at low temperatures and is environmentally friendly [71].

CVD is used to apply a thin and thick layer, where Mo is placed over a substrate, and sulfur vapor flows over it. It is proven to be the most efficient way to make a millimeter-scale homogeneous monolayer MoS₂ on a variety of substrates, including SiO₂ on Si (SiO₂/Si), mica, and strontium titanate [72]. Three methods can be used to create MoS₂ nanosheets using CVD: (i) direct sulfurization of Mo-based films (such as MoO₃ or Mo metal) [73,74], (ii) thermolysis of Mo and S atoms [75], and (iii) vaporization and disintegration of Mo and precursors followed by the production of MoS₂ layers on a growth substrate.

Choi *et al.* [76] used CVD to synthesize MoS₂ *via* a liquid organic precursor on an insulating substrate. This approach is more repeatable and can produce more significant portions of the MoS₂ layer than the methods involving molybdenum oxide and sulfur power. However, because traditional CVD growth techniques have a small surface area, mass development of monolayer or few layers of MoS₂ is unfeasible. Using a micro-sized cubic NaCl crystal power as a pattern, MoS₂ nanosheets were created. Zhu *et al.* [77] used NaCl as a substrate because it is cheap, scalable, and chemically stable, allowing it to produce highly crystalline MoS₂ power in batches. The average nanosheet thickness of MoS₂ rose from 1.93 to 2.62 nm when the temperature was raised from 500 to 650°C, and the optimum growth range was determined to be 550–650°C [60]. Its drawbacks include working at high temperatures in a vacuum and producing films of excellent quality with adjustable thickness, and different CVD procedures include sulfurizing films made of Mo, thermolysis precursors containing S and Mo, and vaporizing and decomposing precursors containing Mo and S atoms.

ALD is used to create thin and thick films [78]. It is efficient, and the layers contain fewer pollutants, making it suitable for various applications such as electronics, sensors, and water purification membranes. Chemical solutions can be used to make MoS₂ layers using hydrothermal and solvothermal reactions, in which both Mo and S react in an aqueous solution above the boiling point and a non-aqueous solution at high temperatures. This approach

allows us to manage the size and shape of the layers, resulting in power and thin sheets of MoS_2 . It is both affordable and scalable [79]. Kim *et al.* [80] used metalloporphyrin as a promoter layer in thermal and ALD experiments. The carrier density and conductivity of MoS_2 can be adjusted with this approach depending on the thickness of the metalloporphyrin used. On a large scale, it is used to make MoS_2 nanosheets (Figure 7) (Table 2).

4 Classification of MoS_2 -based membranes for water desalination

4.1 Nanocomposite MoS_2

Graphene, as is well identified, can be used as an ultrathin separation membrane by drilling nanoscale pores along the graphene planar [90]. As a result, similar concepts are being applied to investigate MoS_2 membranes. MoS_2 is a graphene-like nanomaterial that offers good structural strength, atomic thickness, chemical stability, and mechanical stability in a single sheet [53]. A nanoporous membrane for separating water and other components with efficiency and minimal energy consumption can be created by artificially producing nanopores in monolayer MoS_2 in the right size. The desalination process is the focus of the majority of studies on nanoporous MoS_2 membranes because the nanopore size is becoming near the diameter of the hydrated

ions. The first illustration of the possibilities for a thin layer of MoS_2 as water-related separation membranes was achieved using MD simulations. The effectiveness and consequences of using nanoporous MoS_2 membranes for water filtration were examined by Heiranian *et al.* [91] using MD simulations. They discovered that monolayer MoS_2 with pore areas varying from 20 to 60 $\text{\AA}^2$ could reject >88 % ions and had water flux that was 70 % better than nanoporous graphene under the ideal circumstances. In a separate investigation, Kou *et al.* [92] used all-atom MD simulations to confirm that nanoporous MoS_2 membranes exhibited higher desalination performance. Furthermore, they discovered that the ideal nanopore diameter was 0.74 nm and the nanoporous MoS_2 membranes had good water permeability and flawless salt rejection. Moreover, Wang and Mi [46] indicated that in order to produce the best water flux and salt rejection, the nanopore size should be kept in the range of 0.44–1.05 nm. The majority of current studies on nanoporous MoS_2 membranes focus on MD simulations, with very few experimental studies. Many experiments are being conducted to verify the outcomes of theoretical calculations and simulations. The possibility of making and controlling nanoporous on the monolayer MoS_2 has been demonstrated by using different approaches such as ion bombardment [93], electron beam [53,94], and defect engineering [95,96], even though the pores created at this point (a few nanometers) are still too large for the porous MoS_2 membrane to be classified as a desalination membrane. In particular, electrochemical processes offer a practical and scalable method for producing a large number of nanopores with essentially uniform diameters since they may sequentially remove individual atoms around flaws or single-atom vacancies [97].

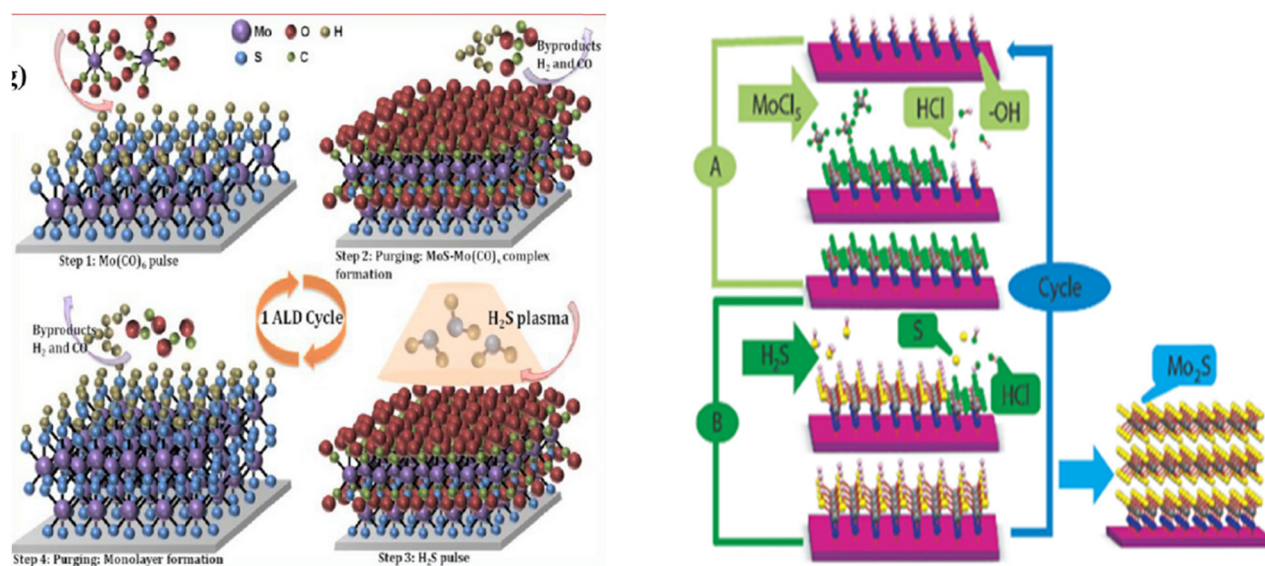


Figure 7: MoS_2 is grown using Mo(CO)_6 and H_2S plasma in a two-step ALD process [81,82].

Table 2: Summary of synthesis techniques

Technique	Characteristics of the MoS ₂ sheets obtained	Ref.
Liquid-assisted sonication	Studied PL and Raman analyses produced by the bath and probe sonication	[66]
Liquid exfoliation and ultrasonic cavitation	Studied and obtained less defective and high-concentration nanosheets in a short time (within 10 min)	[83]
Liquid-phase exfoliation	Studies show that grinding solvent was critical in sin flake dimensions and morphology	[84]
Liquid exfoliation and sonication	Motilities of about 10 cm ² /V, on/off ratio of 10 ⁶	[85]
PVD	Growth of MoS ₂ (1-x)Se _{2x} monolayer alloys with controlled morphology	[86]
PVD and magnetron sputtering	They deposited MoS ₂ films with thicknesses from 10 to 1,000 nm on SiO ₂ /Si and reticulated vitreous carbon substrate	
CVD and organic liquid precursor	This procedure enables complete MoS ₂ coating while using water to eliminate contaminants such as carbon and sulfur	[76]
CVD	Formation of MoS ₂ monolayer triangular flask using MoO ₃ and S power	[87]
CVD	MoS ₂ domains are highly dependent upon the spatial location on the silicon substrate, with variation from triangular to hexagonal geometries.	[88]
ALD	Obtained monolayer sample of grain sizes up to 420 nm, and a five-layer sample of grain sizes up to 400 nm	[89]

Liu *et al.* [98] successfully produced nanoporous MoS₂ membranes with 1–10 nm diameters using an intensely focused electron beam and transmission electron microscope; nevertheless, these membranes were designed for DNA translocation rather than water-related membranes. Thiruraman *et al.* [99] researched nanoporous MoS₂ membranes based on experimental results. They used Ga⁺ ion irradiation to induce sub-nm vacancies in the suspended monolayer MoS₂ [44]. Nanoporous MoS₂ membranes had 300–1,200 pores with average and maximum sizes of 0.5 and 1 nm, respectively. Figure 8 shows a more thorough description. Additionally, pores with dimensions smaller than 0.6 nm were found too small for ions to flow through, essentially identical to the simulation results.

The formation of single-chain hydrogen bonds, steric effects, and electrostatic repulsion between charged species and nanopores are the main separation mechanisms of this kind of membrane. According to separation mechanisms, the performance of a nanoporous MoS₂ membrane is primarily affected by pore characteristics (such as nanopore size and shape, pore density, and atom type at the pore edge), filtrated species (such as hydrated radius and valence state of ions), and external pressure.

Theoretical calculations and modelling studies have revealed that nanoporous MoS₂ membranes can achieve high salt rejection and quick water transport capabilities, which will most probably result in the breakthrough of the permeability–selectivity trade-off. Membrane performance is heavily influenced by pore properties, applying external pressure, and filtrated species. The production of large-scale, defect-free monolayered MoS₂ and the controlled development of uniform pores on the planar surface are two critical challenges in developing nanoporous MoS₂ membranes.

Creating a large-scale, defect-free monolayer MoS₂ is the first step toward nanoporous MoS₂ membrane applications. The CVD approach may aid in creating large-scale, defect-free monolayers [100].

Furthermore, it has been claimed that a modified CVD technique may achieve a more mechanically stable monolayer of MoS₂ with a high degree of crystallinity [101,102]. The large-scale production of nanoporous MoS₂ membranes differs from nanoporous graphene membranes in some ways [100]. Since graphene's Young's modulus is greater and monolayer MoS₂'s is less [103,104], MoS₂ monolayers are more likely to be malleable, allowing uniformly dispersed pores to form. Furthermore, the regulated production of pores in the monolayer MoS₂ remains a significant issue, as most current studies focus on MD simulations, with few experimental studies. Some methods for making nanopores in graphene, such as oxygen plasma etching [91,105], helium ion beam [106,107], and electron beam radiation [108,109], may serve as a guide for making pores in a single layer of MoS₂.

4.2 MoS₂ composite membranes

Polymeric membrane is still the best membrane-based separation method for treating and purifying water. The flux permeability, selectivity, and antifouling properties of MoS₂ composite membranes may be enhanced using the hydrophilic and negatively charged MoS₂ nanosheets [110,111]. These polymeric membranes are used mainly in designing and manufacturing MoS₂-incorporated and MoS₂-surface modification membranes. In other words, the intriguing properties of MoS₂ nanosheets or pre-functionalized MoS₂ nanosheets are used to

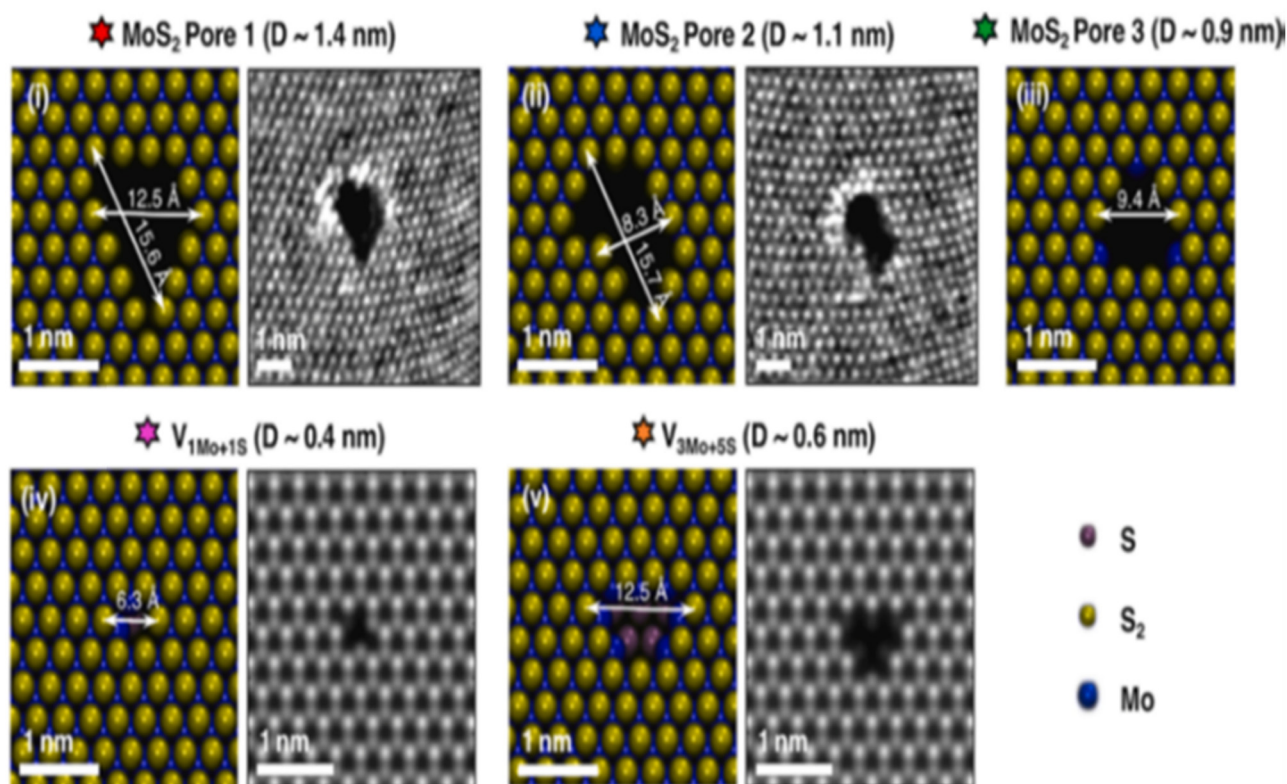


Figure 8: Schematic illustration of the sub-nm pathways of water through the porous MoS₂ membrane [99].

improve the membrane performance of porous and dense polymeric membranes by integrating MoS₂ into the organic phase as casting solutions and coating the surface of polymeric membranes with MoS₂ [111]. The mixture of MoS₂ nanosheets and polymer solutions should be homogenous during fabrication.

Furthermore, the layer-by-layer (LbL) assembly approach is frequently used to precisely control nanomaterial loading on the membrane surface modification. LbL assembly was used to create MoS₂ nanosheets as well. In a dopamine solution, poly(ethyleneimine) solution, MoS₂ dispersion, and finally, poly(acrylic acid) solution, Li *et al.* submerged the base polyethersulfone membrane [112]. The creation of a tri-layer FO membrane was the outcome of such LbL deposition. Figure 9 provides a schematic representation of the fabrication information. The MoS₂-coated-FO membrane demonstrated strong antifouling properties in addition to a high water flux of 27.15 L m⁻² h⁻¹ and a low salt reverse flux of 16.4 gMH.

Desalination and removing some impurities (such as microorganic pollutants, heavy metals, and oils) have received much attention thanks to the coupling of MoS₂ nanosheets and commercial NF/ultrafiltration (UF)/RO membranes.

4.3 Layer-stacked MoS₂ membranes

By stacking 2D nanosheets, researchers have created innovative water-related separation membranes with high performance thanks to the sheet-like structure and adjustable physicochemical features of 2D materials. The capillary width (also known as the free-layer spacing) between 2D nanosheets allows for efficient sieving of molecules and ions of various sizes.

Vacuum and pressure-assisted filtration has been the most popular approach for fabricating layer-stacked MoS₂ membranes. The layer-stacked MoS₂ membranes are simple to assemble, environmentally beneficial, and can be produced in large quantities [114]. The layer-stacked MoS₂ membranes without tunability showed good stability, high water flux, and rejection of big molecules, suggesting that they could be useful for molecular separations from aqueous solutions but not for desalination [115,116]. The tunability and control of interlayer spacing were carried out to accomplish high ion selectivity and permeability. Covalent bonds and electrostatic forces are primarily responsible for the observed regulation of interlayer spacing.

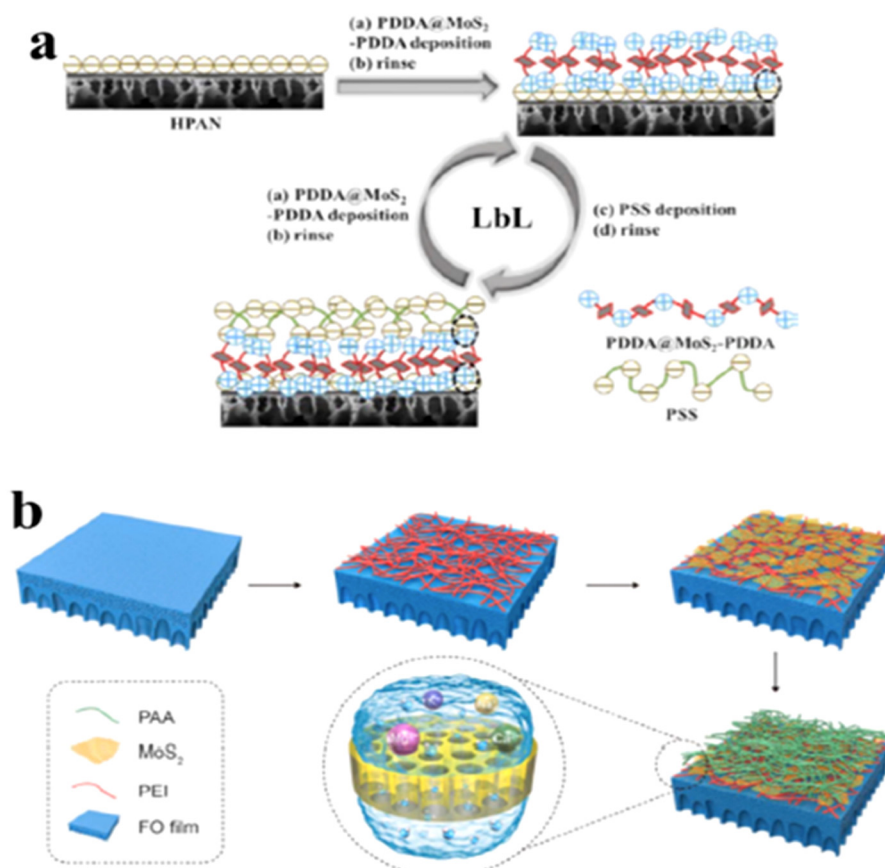


Figure 9: Surface modification by MoS₂ nanosheets: (a) MoS₂/polyelectrolyte hybrid NF membranes and (b) MoS₂-coated-FO membrane [113].

Layer-stacked MoS₂ membranes have demonstrated good stability in aqueous solutions since comparable van der Waals and hydration forces may preserve the inter-layer gap of layer-stacked MoS₂ membranes [38]. The outstanding water stability of layer-stacked MoS₂ membranes is one of its most remarkable features. Without any stabilizing treatment, a layer-stacked MoS₂ membrane was reported to demonstrate consistent water permeance and molecule rejection under testing for a week [37]. The exceptional integrity of plain MoS₂ membranes in water under varied pH levels has recently served as another recent example of the characteristic [114,117]. However, MoS₂ nanosheets are relatively rigid due to their three-atomic structure, which makes MoS₂ water channel less susceptible to mechanical compaction under high transmembrane pressure applied during membrane operation [34,118].

To control the membrane structure and properties, MoS₂ could be adjusted according to the physicochemical properties of the nanomaterial and membrane fabrication settings to adjust the spacing between the layers. To modify the distance between layers, materials with unique qualities, such as amphiphilic molecules and nanoparticles, can be

introduced to the membrane production process. Operational parameters such as filtration pressure and speed could all impact the spacing between MoS₂ nanosheets, the orientations of the nanosheets (parallel alignment or micro-domains), and membrane thickness. As a result, filtering factors in the fabrication process must be considered for interlayer spacing adjustment and optimization.

In recent years, studies on MD have been carried out to try to explain this phenomenon; these theoretical studies have shown that water molecules can create a planar multi-layered structure between two MoS₂ layers [119–121], increasing the interlayer distance of stacking layers. Additionally, these results showed that water intercalation did not affect how S-Mo atoms were arranged on the planar surface [121]. In order to maintain sufficient big free spacing for the water transport, it is suggested that the layer-stacked MoS₂ membrane either needs to be kept wet/hydrated or needs to be rewetted using solvents (such as isopropanol).

Layer-stacked membranes' structural features, such as their crystal phase, interlayer spacing, and vacancy defect, should be highlighted because they show great promise for integrating membrane technology with other water

treatment technologies such as advanced oxidation, photocatalytic, and adsorption technologies. Future investigations will speed the discovery of novel multifunctional MoS₂-based membranes due to the rising demand for effective and energy-efficient treatment processes in water treatment and purification.

5 Computation simulation

Researchers have used simulation to examine the membrane performance of nanoporous MoS₂ for the desalination of water. They have used MD to investigate the water permeability and flux through a membrane. In this section, we summarized recent previous work carried out on MD for this review.

In water desalination, MD simulation is used to develop a membrane and investigate its characteristics. Simulation gives us the behavior of the MoS₂ membrane, and it has been confirmed that water is transported faster in MoS₂ than other 2D materials such as graphene and CNT [100]. Heiranian *et al.* [91], carried out a study on single-layer MoS₂ nanoporous using MD simulation to analyze the possibility and prospect of nanoporous MoS₂ for water purification, as shown in Figure 10. They anticipated that monolayer MoS₂ with hole areas ranging from 20 to 60 Å² would be able to reject more than 80% of ions. However, water flux was 70% better than that of nanoporous graphene, proving that pores play a key role in the mode of water flux.

Another study by Cao *et al.* [122] compared the water permeability and ion rejection rates of various 2D materials such as MoS₂, graphene, phosphorene, and boron nitride. It

was discovered that the single-layer MoS₂ consistently outperforms graphene by 27% better, 38% phosphate, and 35% boron nitride in terms of water permeability while retaining more than 99% ion rejection under the same condition. They showed that MoS₂ could desalinate water more quickly than other 2D materials and ensure that the filtered water contains relatively very few undesirable ions.

The effect of multilayer MoS₂ membranes on water desalination was investigated by Oviroh *et al.* [123]. Their result revealed that the pore size increased from 3 to 6 Å, water permeability increased, but salt rejection decreased. Salt rejection increased from 85% in the monolayer MoS₂ membrane to about 98% in the trilayer MoS₂ membrane.

The relationship between permeability and membrane thickness was investigated by Abal *et al.* [124] using MD simulation. They anticipated that contrary to the expected hydrodynamic behavior, permeability did not rise with the inverse of membrane thickness (Table 3).

6 Summary of experimental studies of MoS₂ for desalination

Several experimental studies [38,46] have been performed on MoS₂ for water desalination, but when compared to graphene, it is minimal. In this section, we focus on previous work on experimental work, its fabrication, and the performance of MoS₂ membrane in the past 5 years. Water desalination relies heavily on membrane separation. The efficiency and performance of membranes for desalination are primarily affected by salt rejection and water flux. The interlayer spacing of the MoS₂ nanosheet plays an essential role in desalination applications [125]. However, it has been researched how to enhance desalination performance by combining commercial UF/NF/RO membranes with MoS₂ nanosheets, namely, MoS₂-coated membranes and MoS₂-surface-modification membranes.

In this regard, numerous initiatives and fabrication techniques have been used to manage the interlayers and enhance the functionality of MoS₂ membranes. Table 4 shows MoS₂-based membrane types, their performance, and the synthetic method. The basic desalination processes, which include nanoporous membrane, layer-stacked membrane, composite membrane including MoS₂, and membrane surface modification using MoS₂ nanosheet, mainly include size exclusion and electrostatic repulsion for the MoS₂ membrane.

As previously mentioned, the desalination performance of the nanoporous MoS₂ membrane can be significantly influenced by the size, type, and chemistry of the pores. A

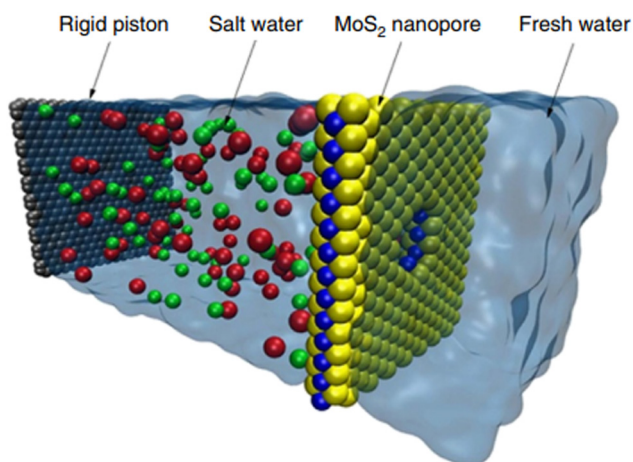


Figure 10: MD simulation of MoS₂ for water desalination [91].

Table 3: Previous work on simulation of MoS₂ for water desalination

Membrane	Membrane types	Ion rejection (%)	Water flux	Pressure (MPa)	Pore size (Å)	Ref. (Å)
Nanoporous MoS ₂	Monolayer	85	767.02 N/ns	5–50	3–6	[123]
	Bilayer	95	604.71 N/ns			
	Trilayer	98	580.70 N/ns			
Nanoporous	Single-layer MoS ₂	99	9.36 L/m ² /day/MPa	100	4–6	[122]
Nanoporous	Single-layer MoS ₂	88		<10	20–60	[91]
Nanocomposite MoS ₂	TiO ₂ /MoS ₂ bilayer	97	6 × 10 ⁻⁸ mmg/cm ² sbar	<250	6.4	[45]

critical pore size of 0.55–0.60 nm in interlayer space may be necessary for the passage of water molecules because the diameter of water molecules is 0.264 nm, which allows free movement through the pore [126]. The free spacing between MoS₂ layers significantly impacts the salt rejection in layer-stacked membranes. Layer-stacked MoS₂ membranes have a considerable separation distance because different ions can travel through them without being tuned. It is highlighted that the accurate design of interlayer spacing should be carried out to narrow the nanochannels. For example, Sapkota *et al.* [67] used the interlayer spacing of 0.6 nm to achieve 98% salt rejection, and Wang *et al.* [38] compared the interlayer spacing of 1.2 nm and 0.6 nm and they reported that 1.2 nm has higher salt rejection than 0.6 nm. However, the flux permeability and selectivity of composite membranes are enhanced by using the hydrophilic sites and negative charge of MoS₂ nanosheets in both MoS₂-incorporated membranes and membranes with the modified MoS₂ surfaces.

Various researchers have modified NF membranes to effectively reject self-utilizing NF membranes using MoS₂ nanosheets to increase their selectivity and permeability. The MoS₂-based membrane with a typical negatively charged NF membrane, according to Yang *et al.* [131], showed the highest rejection of Na₂SO₄ (94%) and the lowest rejection of NaCl (60%). According to this research team, adding oxidized MoS₂ nanosheets to the PA selective layer in the NF membrane improved the salt rejection even more [132]. When each salt was present in a solution containing 2,000 mg/L at 3.5 bar and 25°C, the rejection rates for Na₂SO₄, MgSO₄, MgCl₂, and NaCl were 97.9, 92.9, 86.3, and 65.1%, respectively.

However, MoS₂ nanosheets and polymers could also be added to positively charged NF membrane construction to increase the rejection of multivalent cations. For instance, the MoS₂/polyethyleneimine composite NF membrane had outstanding desalination performance when the transmembrane pressure was 6 bar, and the starting concentration of MgCl₂ was 0.01 M [133], *i.e.*, pure water permeance of 4.6 Lmh/bar and high MgCl₂ rejection of 95.5%.

Sapkota *et al.* [67] studied the high-permeability sub-nm sieve composite MoS₂ membrane, as shown in Figure

11; their results suggest that porous MoS₂ nanosheet–nanodisk laminate has both high and efficient ion rejection and small molecular pathways for water penetration through the sub-nm voids in the highly laminate structure.

The Donnan theory, which states that the charge was repelled by electrostatic repulsion and the counter ions were also retained to maintain electrical neutrality, played a significant role in both the negatively and positively MoS₂-based NF membranes during the desalination process [118]; the order of rejection rates for multivalent salts may be better understood in light of this.

The layer-stacked MoS₂ membranes with no tunability were not capable of effectively rejecting ions, while the nanoporous MoS₂ membranes were often developed for desalination procedures. It is interesting that a recent study created a novel, high-performance membrane by combining the distinct qualities of the two different types of membranes [67], *i.e.*, the composite layer-stacked MoS₂ membranes were made from one to two layer-thick porous nanosheets and nanodisk, as illustrated in Figure 10. Their experiment output showed 99% rejection of NaCl at an initial concentration of 0.5 M under optimal conditions. The multimodal porous network topology with adjustable surface charge, pore size, and interlayer was credited with superior membrane performance.

The fabrication of a composite membrane, which was made from GO, MoS₂ nanosheet, and polyvinyl alcohol, was used for NaCl rejection. It demonstrated an 89% rejection rate and 3.96 Lmh of water flux at a low pressure of 5 bar while using 2,000 mg/L NaCl [135]. Also, it was reported by Li *et al.* [48] that a RO membrane loaded with 0.01 Wt% MoS₂ into the PA matrix achieved the optimal water permeability of 6.2 Lmh/bar and salt rejection of 98.6% measured at the 2,000 mg/L NaCl solution at 15.5 bar and 25°C. In recent work, for instance, the desalination efficiency of a CVD-grown, near-atomic thickness MoS₂ membrane was assessed using real seawater from Atlantic Coast. Compared to traditional desalination membranes, a rejection rate of about 100% was attained [127]. Furthermore, the high-performance MoS₂ membranes developed by this research at a

Table 4: Summary of MoS₂-based membranes

	Method	Ion rejection	Water flux	Pore size	Ref.
MoS ₂ layers	CVD	99%	>322 Lmh/bar	~7 nm	[127]
Layer-stacked MoS ₂ nanosheet membranes	Solvent-assisted liquid exfoliation	~99%	0.033 Lmh/bar	5 µm	[128]
Layer-stacked MoS ₂ nanosheet membranes	Chemical exfoliation	~55–75%	50 Lmh/bar	~30 nm	[128]
Layer-stacked MoS ₂ nanosheet membranes	TA-assisted liquid exfoliation	97%	32 Lmh/bar	5 µm	[129]
Single-layer stacked MoS ₂ nanosheet membranes	Chemical liquid functionalized by organohalide reagent	87%	1.6 Lmh/bar	~0.12	[130]
Layer-stacked MoS ₂ nanosheet membranes	Solvent-assisted liquid exfoliation	96.85%-K ₃ Fe(CN) ₆ , 66.76%-Na ₂ SO ₄ , 58.31%-MgSO ₄ , 56.09%-NaCl	48.27 Lmh/bar	0.22 µm	[118]
Layer-stacked nanoporous MoS ₂ nanosheets	Solvent-assisted liquid exfoliation	>95%	5 Lmh/bar	32 nm	[67]
MoS ₂ nanosheet incorporated in Tfn Ro to form composite membrane	Solvent-assisted liquid exfoliation	98.6%	17 Lmh/bar	0.22 µm	[48]
MoS ₂ nanosheet-incorporated composite membrane	TA-assisted liquid exfoliation	98.5%	7.8 Lmh/bar		[40]
MoS ₂ nanosheet in Tfc to form incorporated composite membrane	Solvent-assisted liquid exfoliation	94.4%	7.8 Lmh/bar		[131]
MoS ₂ nanosheet-incorporated composite membrane	Hammer's	97.9%-NaSO ₄ , 92.9%-MgSO ₄ , 86.3%-NaCl	7.91 Lmh/bar	0.62 nm	[132]
FO membrane surface modified with MoS ₂	LbL deposition	16.42 gM/H	27.15 Lmh/bar	33.51 nm	[112]
TiO ₂ membrane surface coated with MoS ₂ nanosheets	Solvent-assisted liquid exfoliation	95.5%	4.6 Lmh/bar		[133]
PDDA membrane surface modified with MoS ₂ nanosheet to form hybrid membrane	LbL self-assembly	81.6%-NaSO ₄ , 51.5%-MgSO ₄ , 27.9%-NaCl, 16.1%-MgCl ₂	16 Lmh/bar	0.38 nm	[113]
MXene membrane surface modified with MoS ₂ nanosheet to form a composite membrane	Hummer's	90%	2-layer -378.9 Lmh/bar, 3-layer -243.3 Lmh/bar, 4-layer-169.4 Lmh/bar	9.5 Å	[45]
Multilayer composite MoS ₂ membrane	Ultrasound-assisted exfoliation	99%	245 Lmh/bar	30 nm	[67]
MoS ₂ nanosheet porous membrane	Chemical exfoliation	90%	182 Lmh/bar	0.1 µm	[134]
MoS ₂ nanosheet via covalent functionalization	Chemical exfoliation	87%	3 Lmh/bar	10 Å	[130]

centimeter scale hold significant promise for membrane testing in a bench-scale membrane system. There is still little work on fabrication methods such as CVD and ALD, which limits the surface behavior of MoS₂ experimental.

6.1 Problem association or current challenge of MoS₂ membrane

To comprehend the widespread application of 2D nanomaterials in water filtration, a number of issues must be resolved. Since 2D nanomaterials are still in the early stages of development, manufacturing issues and technological barriers make their incorporation into industrial processes expensive and restrict their use to small-scale structures. Many 2D nanomaterials still have manufacturing costs that are higher than those of conventional goods; therefore, significant cost savings are desired. Additionally, it is important to consider the 2D nanomaterial's long-term viability (both in terms of output and in terms of application).

Rapid water transport and high salt rejection qualities could be accomplished with nanoporous MoS₂ membranes, according to theoretical calculations and simulation studies, although most studies have concentrated on MD simulation rather than experimental research [70,128,136–138].

Furthermore, it appears that there may be some study results, which may be controversial, including theoretical predictions, experimental investigations, and variations in

experimental findings among different studies. For instance, fully hydrated MoS₂ membranes with 1.2 mm interlayer spacing displayed a moderate-to-high water permeability and ionic rejection [38]. In contrast, a different study found that MoS₂ nanosheet frameworks without tunability lacked water–salt selectivity in the separation layer [57]. In order to comprehend the mechanism of separation and enhance the performance of membranes for filtration and water treatment, it is critically necessary to summarize the important discoveries of MoS₂-based membranes and evaluate the state of the study.

As conventional 2D-based membranes, MoS₂-based membranes struggle with cost-effective scaling-up of production. Additionally, since they have high chemical activity, MoS₂-based membranes may not be suited for conventional cleaning methods and agents, unlike commercial polymeric membranes and inorganic ceramic membranes, even though pertinent details are rarely included in contemporary study reports [139].

As a result, new cleaning techniques must be suggested after unavoidable membrane fouling. The photochemical and electrochemical properties of MoS₂ nanoparticles may be fully used for membrane cleaning. For instance, light-induced ROS synthesis [140] and the production of free chlorine with electric help may improve the breakdown and release of membrane foulants, offering a fresh approach to cleaning MoS₂ membranes [139].

The significance of the possible environmental risk assessment of MoS₂ should be clearly understood when it

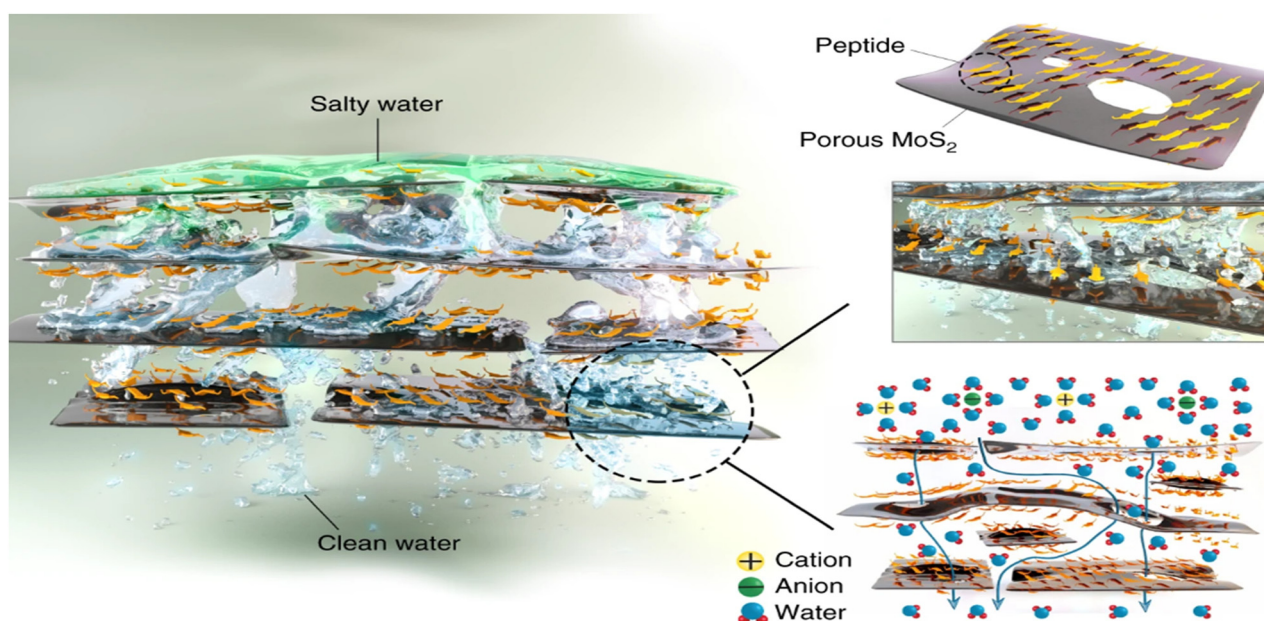


Figure 11: Ion rejection mechanism and membrane performance and schematic illustration of sub-nanosheet membrane pathways of water through the porous MoS₂ membrane [67].

has been discharged into the aquatic environment. The problem of fouling of MoS₂ membrane, particularly in seawater, is still seen as more real by the scientific community, which causes an increase in the maintenance cost and decreases the shelf life of the membrane. Hence, the main technical challenge with the fabrication of MoS₂ is the growth of 2D nanosheets in one direction while having little effect on growth in the other two directions. Although it has been recently reported that centimeter-scale MoS₂ nanosheets were successfully prepared using a bottom-up synthesis strategy, large-scale production of high-quality monolayer 2D nanosheet with large lateral size remains a significant challenge [19]. To choose the best synthesis method for 2D nanomaterials, we must consider the material properties as well as our application goals [19].

Some studies [138,141–143] did outline challenges as regards scalability. Although it has been particularly difficult to make large-scale continuous (>cm²) 2D MoS₂ layers with a thickness of ~1–10 nm. Although large area sizes are required in industrial membrane manufacturing, small-scale samples are typically sufficient for characterization to obtain data. With the advance of technology such as ALD, such characterization could be achieved [127].

The surface of the MoS₂ membrane fabrication still needs more analysis because the effect of coating techniques has not been fully elaborated on in the past research work.

The analysis of environmental and health risks is a crucial step in the manufacturing of MoS₂ membranes for water desalination. There are not enough studies pointing out that despite the significance of this material for desalination. Although research has indicated that MoS₂ is not toxic [138], the variability of MoS₂ nanosheets, including their thickness, phase, lateral size, and defects, may make it more difficult to understand the toxicity effects and necessitate further research on both the effects and the underlying mechanisms.

7 Conclusion

In conclusion, the most widely used water purification methods, including oxidation, distillation, boiling, sedimentation, and chemical and solar disinfection, are now unable to provide the world with a reliable and affordable water source. The inherent properties of 2D nanomaterials make them useful for integrated membrane operations and water filtration. Therefore, improved technology must be created and industrialized to provide clean drinking water. Using low-cost 2D material techniques that emphasize great scalability and processability may be advantageous.

MoS₂-based membranes have improved performance in recent years, including improved simultaneous permeability and selectivity, multifunctionality, and antifouling capacity. In light of recent advancements in MoS₂-based membrane technology, the design and development of three distinct membrane types (nanoporous membranes, layer-stacked membranes, and MoS₂ composite membranes), as well as their uses in water desalination, industrial wastewater treatment, and antifouling qualities, were investigated. Although theoretical calculations and simulation investigations have shown that nanoporous MoS₂ membranes can achieve high salt rejection and quick water transport capabilities, the majority of studies have focused on MD simulation, and there is currently a dearth of experimental investigations. Due to the technological challenges involved in the manufacture, the experimental measurement of the nanoscale thickness of MoS₂ has not been completely investigated.

With regard to the layer-stacked MoS₂ membranes, the interlayer spacing can be tuned depending on the target separation species and exhibits a remarkable stability in aqueous solutions. The layer-stacked membrane has an extreme advantage because of the interlayer spacing and vacancy defect when integrated with other membranes for water desalination. Further research still needs to be undertaken in examining several different directions, one of which is the development of multifunctional membranes.

The design of MoS₂-incorporated and MoS₂ surface modification membranes has recently attracted much attention due to their outstanding ability to remove contaminants in water desalination due to their stability, efficiency, facility, and scalability of these membranes. This combination of MoS₂ nanosheet with any of the commercial UR/NF/RO membranes will result in a polymeric membrane.

Hence, nanosheet MoS₂ can improve MoS₂ membranes for water desalination, and they also face similar challenges to other 2D materials in scaling-up manufacturing for useful applications. Monolayer MoS₂ has demonstrated to offer a significant promise for large-scale, defect-free manufacturing using CVD. Additionally, there is still a need to research how the fabrication procedure affects the wettability of MoS₂ for water desalination because different fabrication materials such as CVD, chemical exfoliation, and liquid exfoliation have been used, but there are limited studies on ALD. Therefore, novel fabrication of methods such as ALD needs to be investigated to examine the defect-free and integrate it on commercial UR/RO membranes. We hope this review contributes to understanding the design and production of MoS₂-based membranes for water application.

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