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Application of Semiconductor Nanomaterials in Water Treatment: A Study on MXene Membranes, α-MoO_3 Nanotubes, and MoS_2-Modified Ceramic Membranes

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Abstract. Global water pollution from industrial, agricultural, and domestic sources poses a serious threat to water security. Conventional treatment technologies face limitations such as secondary pollution, low efficiency, high cost, and membrane fouling. Semiconductor nanomaterials offer new solutions through quantum size effects, surface effects, and optoelectronic properties. This paper, through a systematic literature review, investigates three innovative processes: vacancy-engineered single-atom MXene membranes, α-MoO_3 nanotubes with a photocatalytic memory effect, and PEI-functionalized MoS_2-modified ceramic membranes. The results show that MXene membranes achieve an ultrahigh water flux of 2157 LMH and 98.7% TOC removal. α-MoO_3 nanotubes enable continuous purification in the dark with over 95% TOC removal. MoS_2-modified ceramic membranes provide nanofiltration-level separation for fluoride-containing wastewater. The paper concludes that deep integration of material properties and process design is key for future water treatment technologies.

Keywords: Semiconductor nanomaterials, Water treatment, MXene membrane, Photocatalytic memory effect, MoS_2 ceramic membrane

1. Introduction

Industrial emissions, agricultural runoff, and domestic sewage cause accumulation of persistent organic pollutants, heavy metals, and pathogens in water [1, 2]. Conventional treatments (coagulation, biological, adsorption, membrane) suffer from secondary pollution, low efficiency, and high costs [3]. Semiconductor nanomaterials like TiO_2 are limited by strong light dependence [4], but recent breakthroughs include MXene membranes with water permeance of 37–800 LMH/bar and >90% rejection [5], and α-MoO_3 nanotubes with a photocatalytic memory effect enabling dark degradation [6, 7]. This paper reviews three novel processes: vacancy-engineered single-atom MXene membranes, α-MoO_3 nanotubes, and PEI-functionalized MoS_2-modified ceramic membranes, to reveal material-process synergy rules for efficient water treatment.

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2. Literature review

2.1. MXene materials and their research progress in water treatment

Semiconductor nanomaterials exhibit three key effects. The quantum size effect (size decrease → bandgap increase) broadens light absorption and enhances redox capability [8]. The surface effect (higher surface area → more unsaturated surface atoms) provides abundant active sites for adsorption and catalysis [9]. Their optoelectronic properties enable light-induced electron-hole pairs to generate reactive oxygen species (·OH, $\cdot O_2^-$), mineralizing organic pollutants [4].

MXene is a new class of two-dimensional transition metal carbides/nitrides with the general formula $M_{n+1}X_nT_x$ (M = transition metal, X = carbon or nitrogen, T_x = surface functional groups). Due to their unique layered structure, high electrical conductivity, and abundant surface functional groups, MXene materials show great potential in adsorption, catalysis, and membrane separation.

In recent years, significant breakthroughs have been achieved in MXene-based membranes for water treatment. MXene-based membranes show water permeance of 37–800 LMH/bar (5× conventional) with >90% rejection [5]. Through carboxylation-induced hydrogen bonding, researchers constructed $Ti_3C_2T_x$ nanochannels achieving permeance of 1860 LMH/bar (13× improvement) and >96% removal of dyes and oils.

To overcome the "efficiency-flux-stability" trade-off, vacancy engineering and single-atom catalysis strategies have been introduced into the MXene system. The team of Professor Lingling Chen at Shenzhen Technology University and Professor Meng Zhang at Beijing Normal University constructed Co-N-$Ti_{3-x}C_2T$_y membranes with asymmetric Co-N_1C_2 sites on titanium-defective MXene through vacancy-mediated single-atom anchoring, achieving synergistic enhancement of asymmetric electronic structure, nanoconfinement effect, and hierarchical mass transfer [10]. This catalytic membrane reaches a water flux of 2157 LMH, an improvement of 2–3 orders of magnitude over conventional membranes. The reaction rate constant for ranitidine is 51420 min^{-1}, with TOC removal of 98.7% and cobalt leaching below 3% after 130 hours [10].

2.2. Photocatalytic properties and memory effect of α-MoO_3

α-MoO_3 nanotubes exhibit a "photocatalytic memory effect": under light, Mo^{6+} captures photogenerated electrons; in the dark, electrons are gradually released to generate free radicals, while internal electronic state changes improve charge separation and surface adsorption [6, 7].

The researchers verified the existence of the memory effect through three sets of control experiments: the no-sample group showed no degradation; the α-MoO_3 without pre-illumination group showed only adsorption equilibrium; and the α-MoO_3 with pre-illumination group showed continuous degradation in the dark [6]. Notably, after only 20 minutes of pre-illumination, the photocatalytic degradation and sterilization capability of α-MoO_3 nanotubes were significantly enhanced, achieving over 95% TOC removal of tetracycline within one hour, with stable performance over five light-dark cycles [7]. This "light-charge, dark-discharge, light-enhanced" continuous purification paradigm provides new materials and mechanistic support for sustainable water treatment in day-night alternating scenarios (Figure 1).

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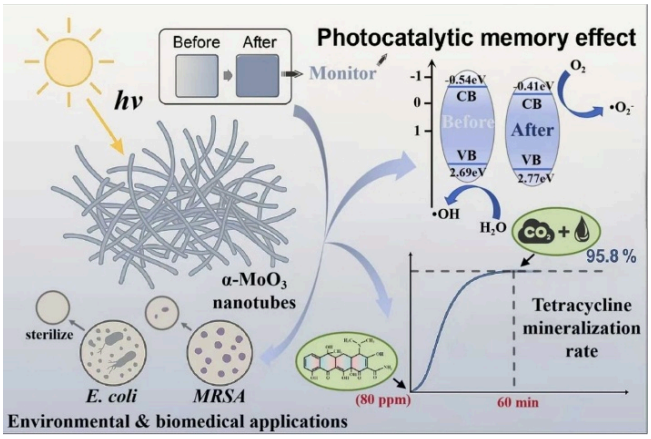

Figure 1. Schematic illustration of the photocatalytic memory effect mechanism of α-MoO_3 nanotubes [6]

2.3. MoS_2-modified membranes and their separation applications

MoS_2 is a two-dimensional material that is easy to exfoliate and form membranes [11]. However, the lack of oxygen-containing functional groups on the MoS_2 surface results in weak interfacial bonding when directly used for membrane modification, leading to limited separation selectivity. To address this issue, researchers have used polyethyleneimine (PEI) to functionalize MoS_2. PEI not only enhances the interfacial adhesion between MoS_2 and the substrate but also provides abundant amine reactive sites.

Researchers have developed hollow-fiber ceramic nanofiltration membranes containing functionalized MoS_2 nanomaterials for treating fluoride-containing wastewater from the semiconductor industry. Semiconductor manufacturing generates large amounts of fluoride-containing wastewater (500–2000 mg/L), and long-term exposure to high concentrations of fluoride can cause skeletal fluorosis and other health problems [12]. The results show that MoS_2-coated ceramic NF membranes exhibit significant removal capability for low-molecular-weight pollutants such as fluoride, achieving a fluoride removal rate of 20% (nearly 0% for pristine membranes), and $MgSO_4$ and $CaCl_2$ removal rates of approximately 14% and 12%, respectively [12].

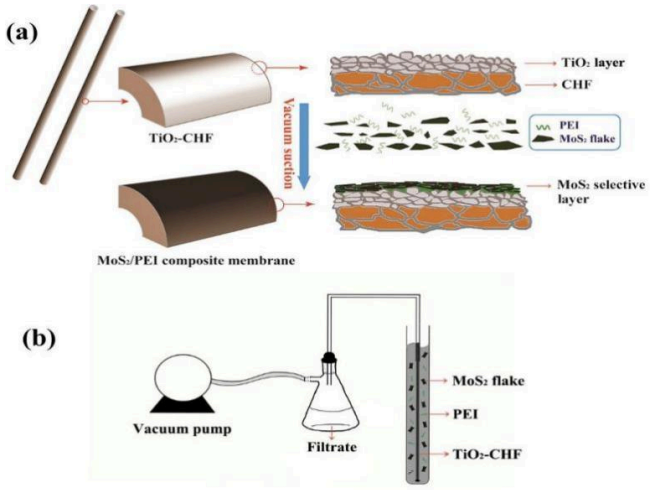

Figure 2. Schematic illustration of the preparation process and separation mechanism of PEI-functionalized MoS_2-modified ceramic membrane [11]

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The separation mechanism is mainly based on size sieving: the nanoscale channels (approximately 0.6–1.2 nm) formed by the stacked layered structure of MoS_2 enable selective separation based on the size exclusion principle, while the amine groups introduced by PEI functionalization provide electrostatic adsorption of negatively charged fluoride ions, further enhancing removal efficiency (Figure 2).

2.4. Limitations of existing research and the entry point of this study

Although the above studies have made important progress in the application of semiconductor nanomaterials in water treatment, several shortcomings remain. First, most studies focus only on a single material or process, lacking in-depth analysis of material-process synergy. Second, systematic comparison and commonality induction among the three novel processes (MXene membranes, α-MoO_3 memory effect, and MoS_2-modified membranes) are insufficient. Third, from an engineering application perspective, discussions on scale-up preparation, long-term stability, and nanomaterial safety are limited.

3. Case analysis

3.1. Case 1: vacancy-engineered single-atom MXene membrane

The core material of this process is $Ti_3C_2T_x$ MXene, using its titanium vacancies as "atomic traps" to anchor cobalt single atoms, forming an asymmetric Co-N_1C_2 coordination structure. This asymmetric electronic structure can modulate the d-band center position of cobalt atoms, thereby enhancing the adsorption and activation capability for peroxymonosulfate (PMS) [10]. The researchers regulated the layered structure (1.55 nm interlayer spacing, expanded external channels, reduced nanosheet size) to achieve a water flux of 2157 LMH.

This MXene membrane exhibits a reaction rate constant for ranitidine of 51420 min^{-1}, an improvement of 5–6 orders of magnitude over conventional systems; complete removal of pollutants within an extremely short residence time of 13.2 ms; removal rates for various organic micropollutants ranging from 92% to 100%; a TOC removal efficiency of 98.7%; and cobalt leaching below 3% after 130 hours of continuous operation in real water environments [10].

First,nanoconfinement-accelerated reaction—molecular dynamics simulations show that PMS decomposition within the confined channels takes only 135 femtoseconds, while under non-confined conditions it remains undecomposed after more than 1000 femtoseconds, achieving a reaction rate enhancement of 10^5–10^7 times. Second, multi-pathway synergy—the system contains two reactive species, singlet oxygen ($^1O_2$) and sulfate radical ($SO_4^{\bullet-}$), along with an electron transfer pathway mediated by metastable intermediates. The synergy of multiple mechanisms significantly enhances degradation efficiency [10].

3.2. Case 2: photocatalytic memory effect of α-MoO_3 nanotubes

α-MoO_3 nanotubes are synthesized by a hydrothermal method, possessing a one-dimensional nanotube morphology and layered crystal structure. Three sets of control experiments verified the existence of the memory effect: the no-sample group showed no degradation; the non-pre-illuminated group showed only adsorption equilibrium; and the pre-illuminated group showed continuous degradation in the dark [6].

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In the light-charge stage, photogenerated charge carriers are excited and stored in the material, with Mo^{6+} being reduced to $Mo^{(6-x)+}$. In the dark-discharge stage, the stored carriers are slowly released in the dark, continuously generating reactive species to degrade pollutants. The light-enhanced effect manifests as pre-illumination, improving the subsequent photocatalytic rate. This system is effective even for tetracycline at concentrations as low as 50 μg/L, achieving over 95% TOC removal with stable performance over five light-dark cycles [7].

This memory effect has significant engineering significance: it breaks the dependence on continuous illumination, reduces energy consumption, and simplifies system design by eliminating the need for artificial light sources.

3.3. Case 3: PEI-functionalized MoS_2-modified ceramic membrane

The pressure-assisted deposition method is used to coat PEI-functionalized MoS_2 nanosheets onto ceramic hollow-fiber ultrafiltration membrane substrates. PEI functionalization plays two key roles: first, introducing nitrogen-containing functional groups to enhance the interfacial adhesion between MoS_2 and the ceramic substrate; second, providing additional amine reactive sites to enhance electrostatic adsorption of negatively charged fluoride ions [11].

Under the optimal coating density of 20 mg/cm^2, the composite membrane achieves a fluoride removal rate of 20% (nearly 0% for the pristine membrane), and $MgSO_4$ and $CaCl_2$ removal rates of approximately 14% and 12%, respectively, reaching nanofiltration-level separation capability. The separation mechanism is primarily based on size sieving (0.6–1.2 nm channels formed by stacked MoS_2 layers) and electrostatic adsorption (interaction of PEI amine groups with fluoride ions) [12].

This process achieves a performance leap from microfiltration/ultrafiltration to nanofiltration. Compared with polymer-based nanofiltration membranes, MoS_2-modified ceramic membranes exhibit significant advantages in chemical corrosion resistance (tolerating pH 1–14), high-temperature resistance (up to 200°C), and biofouling resistance, making them particularly suitable for strongly corrosive wastewater treatment scenarios such as those containing fluoride/heavy metals in the semiconductor and electroplating industries.

4. Discussion

Although the three processes exhibit excellent performance at the laboratory scale, their engineering applications still face several major challenges. Maintaining the consistency of single-atom dispersion and defect engineering during scale-up is difficult, as precise control achieved in small-batch synthesis is often hard to replicate in large-scale production. Real wastewater contains complex components that may cause catalyst poisoning and membrane fouling, requiring thousands of hours of operational validation. The potential leaching of nanomaterials and their long-term ecotoxicity remain unclear, necessitating a full life-cycle risk assessment [13]. Additionally, atomic-level regulation and the use of precious metals increase material costs, so comprehensive economic comparison with conventional technologies is required.

Based on the analysis above, future research can focus on the following four directions.

First, multi-process coupling should be further explored. Integrating photocatalysis, membrane separation, and advanced oxidation could achieve synergistic pollutant removal.

Second, smart responsive materials (pH, temperature, electric fields) enable on-demand performance adjustment.

Third, shift from pollutant removal to resource recovery. Semiconductor nanomaterials with selective adsorption can recover valuable elements from industrial wastewater.

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Fourth, theoretical computation should guide experiments. DFT and molecular dynamics can accelerate material screening.

5. Conclusion

Through systematic analysis of three novel processes—vacancy-engineered single-atom MXene membranes, α-MoO_3 nanotubes, and PEI-functionalized MoS_2-modified ceramic membranes—it reveals the core rules of deep integration between material properties and process design.

The findings indicate that vacancy-engineered single-atom MXene membranes achieve a water flux of 2157 LMH and 98.7% TOC removal, breaking the efficiency-flux-stability trade-off. The photocatalytic memory effect of α-MoO_3 nanotubes creates a light-charge, dark-discharge, light-enhanced operation paradigm, breaking light dependence and maintaining over 95% TOC removal over five cycles. PEI-functionalized MoS_2-modified ceramic membranes provide nanofiltration-level separation for high-concentration fluoride-containing wastewater from the semiconductor industry.

This study has certain limitation. The performance data cited are mainly derived from laboratory-scale ideal condition tests with constant temperature, simple water quality, and no biological interference. The complexity of real wastewater—such as coexisting ions, natural organic matter, and microbial communities—may lead to performance degradation, poisoning, or membrane fouling. Future research should focus on pilot-scale validation in real wastewater scenarios, full life-cycle environmental risk assessment, and the establishment of multi-dimensional techno-economic evaluation models.

References

[1] Schwarzenbach R P, Escher B I, Fenner K, et al. The challenge of micropollutants in aquatic systems. Science, 2006, 313(5790): 1072-1077.
[2] Richardson S D, Kimura S Y. Water analysis: Emerging contaminants and current issues. Analytical Chemistry, 2020, 92(1): 473-505.
[3] Shannon M A, Bohn P W, Elimelech M, et al. Science and technology for water purification in the coming decades. Nature, 2008, 452(7185): 301-310.
[4] Hoffmann M R, Martin S T, Choi W, et al. Environmental applications of semiconductor photocatalysis. Chemical Reviews, 1995, 95(1): 69-96.
[5] Naguib M, Kurtoglu M, Presser V, et al. Two-dimensional nanocrystals produced by exfoliation of Ti_3AlC_2. Advanced Materials, 2011, 23(37): 4248-4253.
[6] Cai Q A, Chen Y, Lu L Z, et al. Effective dark activity and significantly enhanced photocatalytic detoxification of water by α-MoO_3 nanotubes from photocatalytic memory effect. Applied Catalysis B: Environment and Energy, 2026, 382: 125991.
[7] Chen Y, Wu Q, Li M, et al. Light-charge dark-discharge cycle of α-MoO_3 for continuous photocatalytic water purification. Environmental Science: Nano, 2026, 13(4): 1120-1130.
[8] Alivisatos A P. Semiconductor clusters, nanocrystals, and quantum dots. Science, 1996, 271(5251): 933-937.
[9] Burda C, Chen X, Narayanan R, et al. Chemistry and properties of nanocrystals of different shapes. Chemical Reviews, 2005, 105(4): 1025-1102.
[10] Meng C C, Chen L L, Zhang M, et al. Vacancy-engineered single-atom MXene membranes: A quantum leap in ultrahigh-flux nanoconfinement catalysis for robust water decontamination. Advanced Functional Materials, 2025.
[11] Zhang H, Taymazov D, Li M P, et al. Construction of MoS_2 composite membranes on ceramic hollow fibers for efficient water desalination. Journal of Membrane Science, 2019, 592: 117369.
[12] Li J, Kim S, Park J, et al. Development of ceramic hollow-fiber nanofiltration membranes containing a functionalized MoS_2 nanomaterial for semiconductor wastewater treatment. Separation and Purification Technology, 2025, 374: 133702.
[13] Nowack B, Bucheli T D. Occurrence, behavior and effects of nanoparticles in the environment. Environmental Pollution, 2007, 150(1): 5-22.