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Research on the Performance Optimization of Molybdenum Disulfide for Multifunctional Applications

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Abstract: Molybdenum disulfide (MoS_2), as a typical transition metal chalcogenide compound, has emerged as a research hotspot in nanomaterials due to its excellent electrochemical properties and catalytic activity. However, conventional MoS_2 exhibits certain limitations in terms of its catalytic performance, electrical conductivity, and cycling stability. To address these issues, this paper aims to explore the improvement of the multifunctional performance of MoS_2 via different performance optimisation strategies, such as heteroatom doping, semiconductor composites, as well as metallic and non-metallic loading. By reviewing and analyzing the relevant literature on the performance enhancement of MoS_2 in recent years, this paper summarizes the specific applications and effects of these optimization strategies, highlighting that they significantly improve the performance of MoS_2 in fields such as optics, electrochemical catalysis, lithium batteries, and supercapacitors, particularly in terms of catalytic activity, electrical conductivity, and cycling stability. The results indicate that the optimisation of MoS_2 performance provides an important theoretical basis and practical guidance for its application in energy storage and catalytic hydrogen evolution.

Keywords: Molybdenum Disulfide, Property Optimisation, Heteroatom Doping, Electrochemical Catalysis, Nanomaterials

1. Introduction

With the increasing global demand for energy, the development of efficient and sustainable energy technologies has become a critical research priority. Molybdenum disulfide (MoS_2) has shown promise due to its layered structure, high surface area, and good conductivity. Monolayer MoS_2, with a widened bandgap of ~1.9 eV, is suitable for optoelectronic devices [1,2]. Its edge sites and sulfur vacancies also make it effective for catalytic reactions, like CO_2 conversion to methanol [3]. However, MoS_2 has low catalytic activity and carrier mobility, especially in monolayer form. Strategies like doping, composites, and defect engineering aim to improve its performance, but their mechanisms are not fully understood [4]. To address these challenges, strategies like heteroatom doping, composite fabrication, and surface defect engineering have been explored to enhance conductivity, catalytic activity, and active site exposure. This paper reviews the main research progress in MoS_2 performance optimization, analyzing the mechanisms of different strategies and their effects on catalytic performance, conductivity, and stability. Moreover, it summarizes the practical applications of MoS_2 in photocatalysis and energy storage. Through an in-depth study of the mechanism and

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prospects of the optimization method, the paper aims to provide guidance and support for the efficient design and broad application of MoS_2.

2. Preparation Methods of Molybdenum Disulfide and its Process Analysis

2.1. Hydrothermal Synthesis

Hydrothermal synthesis is a widely used method for preparing MoS_2 films. In this process, molybdenum and sulfur precursors are dissolved in inorganic or organic solutions, and the resulting mixture is placed in a reaction vessel, where it undergoes synthesis under controlled temperature and time conditions. After the reaction, further operations such as centrifugation, purification, and drying are performed to obtain MoS_2. This method is simple, cost-effective, and highly versatile, allowing for the preparation of MoS_2 with various shapes and properties by adjusting key experimental parameters, such as temperature and reaction time. For instance, at 230°C, MoS_2 with high yield, excellent thermal stability, high purity, and superior crystallinity can be obtained. At 200°C for 24 hours, nanosheet MoS_2 with the highest photocatalytic degradation efficiency for methyl orange solution can be synthesized. The optimal reaction conditions for thiourea as both a sulfur source and reducing agent are 220°C for 24 hours. Temperature and reaction time significantly affect the material's crystallinity, purity, and photocatalytic performance.

Moreover, the introduction of gelatin during the hydrothermal synthesis process has been shown to improve the structure of MoS_2. The gelatin-assisted method leads to the formation of flower-like spherical MoS_2 nanosheets with a porous microstructure. This structure enhances the material's active surface area, facilitates electrode reactions, and creates multi-level channels for carrier diffusion, which helps mitigate volume expansion during cycling. The gelatin likely interacts with MoS_2 during synthesis, modifying its surface properties and creating defects or active sites that improve electrochemical performance. Further research is needed to fully understand how gelatin affects the layered structure of MoS_2 and its impact on the material's performance in energy storage and conversion applications [5].

2.2. Chemical Vapor Deposition

Chemical vapor deposition (CVD) is a widely used technique for the controlled fabrication of high-quality MoS_2 nanosheets, providing fine control over their morphology, crystallinity, and electronic properties, which are essential for a range of advanced applications. By precisely controlling reaction conditions such as temperature, pressure, and reaction time, CVD allows for effective control over the number of MoS_2 layers, morphology, and crystallinity, enabling fine-tuning of its electrical, optical, and catalytic properties. Compared to other synthesis methods, CVD can produce MoS_2 films with high purity, good uniformity, and strong tunability, making it suitable for large-scale production. For example, low-temperature CVD has been successfully used to synthesize monolayer MoS_2 films at 500°C, offering advantages in energy consumption and cost over high-temperature methods [6]. This method also prevents MoS_2 degradation, maintaining thermal stability and structural integrity, providing a more stable and controllable synthesis route for MoS_2 applications. It is important to further explore the impact of various CVD parameters such as temperature, pressure, and precursor concentration on the properties of MoS_2 films. Experimental data comparing different conditions would provide insights into how these factors affect MoS_2's morphology, crystallinity, and electronic properties, allowing for better optimization. Also, a comparison of low- and high-temperature CVD in terms of energy, cost, time, and film performance would help identify the most efficient methods for industrial-scale production.

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2.3. Mechanical Exfoliation

The mechanical exfoliation method is widely used to prepare monolayer or few-layer MoS_2 nanosheets, utilizing adhesive tape or friction-based techniques to shear thin layers from the bulk material. And this technique utilizes materials such as adhesive tape, silica gel, and double-sided tape, thus transferring the exfoliated MoS_2 onto substrates like SiO_2/Si. An environmentally friendly aqueous ultrasonic-assisted dispersion method has been employed to improve both exfoliation efficiency and MoS_2 dispersion quality [7]. The exfoliation efficiency is influenced by factors like the purity, crystallinity, and layer number of the raw MoS_2 material, where high-purity materials help minimize impurity impacts on the final product. Optimal layer numbers are key to producing high-quality nanosheets. Additionally, preparation time and particle size significantly affect the outcome. Excessively long preparation times can lead to larger MoS_2 fragments, which compromise uniformity, while short times may result in incomplete exfoliation. Particle size, in turn, affects the uniformity of MoS_2 sheets, which is critical for their performance in catalysis and electronics. In order to optimize this process, experimental data should explore the relationship between exfoliation efficiency, layer number, and particle size, as well as the impact of different starting materials on MoS_2 quality. By refining these parameters, the mechanical exfoliation method can be further enhanced to improve MoS_2quality and performance.

2.4. Lithium Intercalation

The lithium intercalation is an effective technique for interlayer exfoliation of MoS_2, where lithium ions are introduced into bulk MoS_2, forming $LixMoS_2$ intercalation compounds. These compounds then react with a protonic solvent (such as water), releasing a significant amount of hydrogen gas, which increases the interlayer spacing and reduces the van der Waals forces between layers. This allows for the extraction of thin or even monolayer MoS_2 via ultrasonic treatment. Though this method can efficiently exfoliate MoS_2, it requires high-temperature conditions and faces challenges such as lower electrode conductivity and efficiency. Fan et al. employed an ultrasonic-assisted rapid lithium intercalation method, combined with infrared laser-induced phase reduction, to successfully achieve complete intercalation of MoS_2 with butyllithium in just 1.5 hours [8]. By irradiating MoS_2 with an infrared laser from a DVD drive, they successfully reversed the phase transition from the 2H to the 1T phase during the lithium intercalation process. Figure 1 shows the reaction scheme for preparing and exfoliating 2H MoS_2 using this method [8]. Compared to the hydrothermal method, the CVD technique has higher equipment costs and more complex operations. However, it enables large-scale, high-quality MoS_2 production and can be combined with the mechanical exfoliation method to synthesize large-area films.

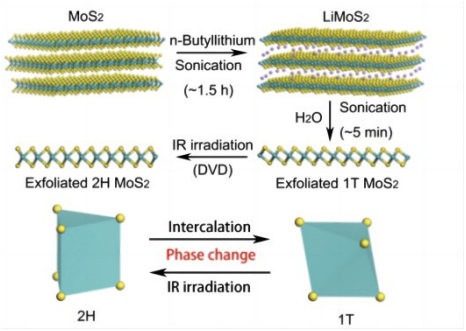


Figure 1: Reaction Scheme for the Preparation of Exfoliated 2HMoS_2

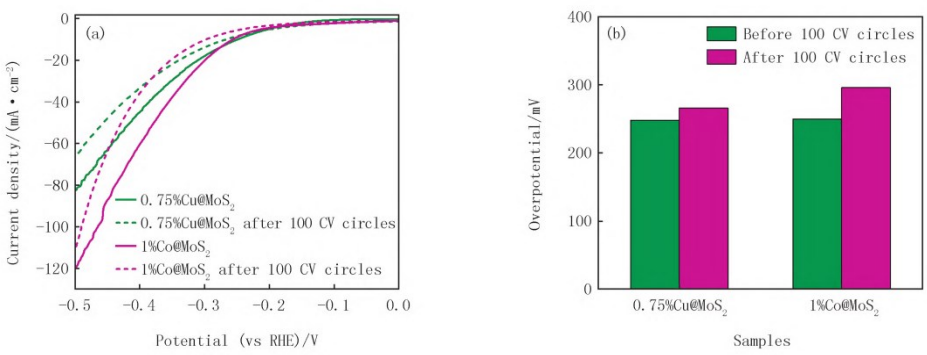
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3. MoS_2 Performance Enhancement Strategies

Due to its wide-band gap properties, traditional MoS_2 has weak electrical conductivity, which limits its activity and reaction speed in electrochemical catalysis. Therefore, the optimization of MoS_2 is necessary to adjust its band gap while improving its performance in optics, catalysis, and electrochemistry. It can be modified by doping of heteroatoms, preparation of semiconductor composites, and loading of metal and non-metal materials.

3.1. Heteroatom Doping Modification

In the synthesis of MoS_2, the incorporation of metal or non-metal elements significantly enhances its charge transfer efficiency and surface adsorption capacity, thereby optimizing its physical and chemical properties. Doping has become an effective modification technique widely applied in supercapacitors and electrocatalytic hydrogen evolution, where substantial performance improvements have been observed. For example, 5% Gd-doped MoS_2 exhibited higher conductivity and stability under high-power discharge conditions compared to undoped samples [9]. In electrocatalytic hydrogen evolution, doping with metal or non-metal elements can activate edge sites of MoS_2, optimize hydrogen adsorption free energy, and promote electron transfer, thereby enhancing its electrocatalytic performance [10,11]. Copper and cobalt doping significantly reduced the hydrogen evolution overpotential and Tafel slope, indicating that doping effectively reduces charge transfer resistance [12]. Figure 2 shows the good electrochemical stability of copper and cobalt-doped MoS_2 after 100 cycles.



(a) (b)

Figure 2: (a) Polarization curves of copper and cobalt-doped MoS_2; (b) Corresponding overpotentials

Nickel-doped MoS_2 (Ni@MoS_2) has exhibited superior hydrogen evolution activity and stability in photocatalytic applications. Table 1 compares the hydrogen production performance of Ni@MoS_2 with other photocatalytic materials, showing a higher hydrogen production rate [13].

Table 1: Comparison of Hydrogen Production Performance of Ni@MoS_2 with Various Photocatalytic Materials

Photocatalyst material	Hydrogen production rate (μmol h^{-1} g^{-1})	Light source	Sacrificial agent	Time(h)	Stability (cycles)
Ni@MoS_2	404.3	300W;Xe lamp(λ=420nm)	Lactic acid	5	6

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Table 1: (continued).

$MoS_2/Zn_3In_2S_6$	74.25	300W;Xe lamp(λ=420nm)	None	10	-
MoS_2/carbon dots/$ZnIn_2S_4$	150	300W;Xe lamp Simulated solar irradiation	Triethanolamine	8	3
CoS_2/carbon nitride	530	300W;Xe lamp	Lactic acid	-	3
MoS_2/CdS	250.8	300W;Xe lamp	Lactic acid	-	-
MoS_2/graphene	280.5	350W;Xe lamp	Formic acid	-	-

The introduction of silver (Ag) atoms into MoS_2 significantly improves its activity and stability as an electrocatalyst in water splitting. By controlling the amount of Ag doping, significant changes in the morphology of MoS_2 can be observed. Silver doping enhances electron transfer and catalysis performance [14]. Figure 3 shows the synthesis scheme and SEM images of Ag-doped MoS_2, with elemental mapping in Figure 3(g) confirming that Ag, Mo, and S are evenly distributed throughout the MoS_2 structure.

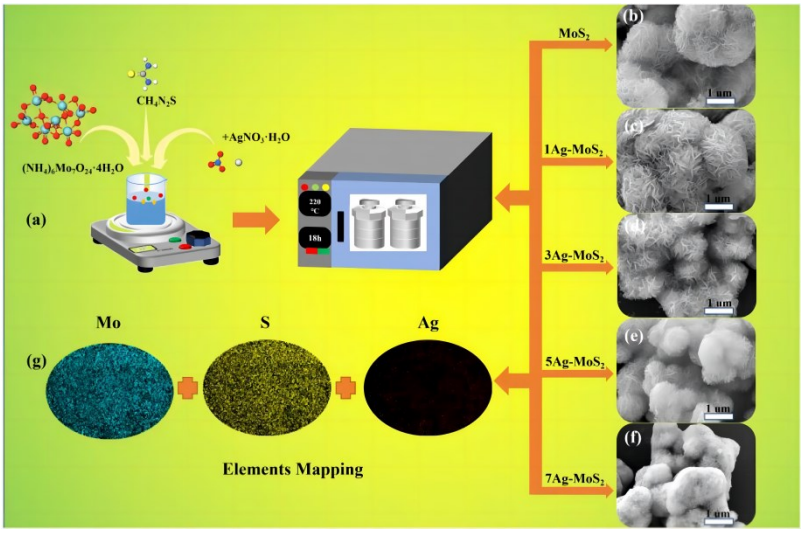


Figure 3: (a) Preparation scheme of Ag-doped MoS_2; SEM images of (b) pristine MoS_2; (c) 1Ag-MoS_2; (d) 3Ag-MoS_2; (e) 5Ag-MoS_2; (f) 7Ag-MoS_2; (g) corresponding elemental mapping images of Mo, S, and Ag.

Element doping greatly enhances the conductivity, catalytic activity, and stability of MoS_2. Doping with Gd improves the long-term charge and discharge capacity of supercapacitors, while copper and cobalt doping reduces charge transfer resistance, enhancing electrocatalytic performance. Nickel doping boosts hydrogen evolution capacity, and silver doping improves catalytic performance in water splitting. These studies highlight that heteroatom doping is a promising approach for tuning MoS_2's properties, thereby advancing its potential in energy storage and conversion technologies.

3.2. Semiconductor Composite Structures

Semiconductor composites, combining materials with different properties, are widely used to overcome the limitations of single semiconductors in electronic transport, stability, and catalytic

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performance. By combining semiconductors, multiple electron transport channels are created, enhancing charge migration efficiency while suppressing agglomeration and volume changes during electrochemical reactions. This strategy improves specific capacitance, cycle stability, and performance across various applications.

In photocatalysis, semiconductor composite structures can greatly improve the separation efficiency of photogenerated charge carriers, enhancing photocatalytic activity. When two semiconductor materials with well-matched band gaps are combined, their heterojunction structure can effectively promote the separation of electrons and holes, improving photocatalytic efficiency [15]. For MoS_2 materials, the common agglomeration phenomenon in electrode applications, especially during metal ion intercalation, can hinder charge diffusion and affect battery efficiency due to the stacking of the layered structure. Therefore, by fabricating MoS_2/C and other heterostructures, the structural stability can be effectively improved, alleviating agglomeration issues and enhancing overall performance [16].

For instance, MoS_2-C composite films, prepared using closed-field unbalanced magnetron sputtering, show excellent wear resistance, improving with temperature rise. At 50K, the composite's interlayer distance decreases, enhancing stability [17]. And the 2D-MoS_2/graphene nanocomposite synthesized by hydrothermal methods exhibits strong photoluminescence, surpassing pure MoS_2 [18]. MoS_2/GO composite films offer high stability and fast response times in humidity sensors (98% response, 1.3/12.1 seconds recovery) [19]. MoS_2-C composites can enhance conductivity, reduce volume effects during charge/discharge, and improve cycle stability [6]. In addition, $BiVO_4$ forms heterostructures with MoS_2, promoting charge transfer, reducing resistance, and improving electrochemical efficiency for NO_2-Tyr biomarker detection [20].

Moreover, MoS_2@$BiVO_4$ heterojunction materials synthesized by hydrothermal method exhibit excellent response range and detection limits in electrochemical sensors. The increased active surface area and reduced charge recombination increase the adsorption of analytes, significantly improving the selectivity and operational stability for biomarker detection [20]. By embedding nickel, manganese, and nickel-manganese Prussian blue analogs into MoS_2 as counter electrode materials, these modified MoS_2 materials demonstrate excellent catalytic activity in dye-sensitized solar cells, especially generating high reduction current density during the reaction process [21].

3.3. Metal and Non-metal Loading

Loading technology involves affixing metal or non-metal materials to the surface of MoS_2 or integrating them into its structure to enhance its performance. The loading of metals or non-metals can effectively modulate the electronic structure, conductivity, and catalytic activity of MoS_2, improving performance in energy storage, catalysis, and other fields.

For example, selenium-doped molybdenum disulfide (MoS_2-XSe_x) materials are uniformly coated with hollow carbon spheres (HCSs), which effectively mitigate the agglomeration of MoS_2 nanosheets and enhance the material's structural properties. Selenium doping increases the interlayer spacing of MoS_2, thereby facilitating charge transfer and improving catalytic efficiency. Under optimized conditions, the C@$MoS_{1.8}Se_{0.2}$ sample demonstrates excellent electrocatalytic performance, particularly in the oxygen reduction reaction, with an onset potential of 186 mV and a small overpotential required to achieve a current density of 10 mA/cm^2. Besides, after 1500 cycles, the material retains its catalytic performance, highlighting the beneficial effect of selenium on the electronic structure and catalytic activity of MoS_2. As shown in Figure 4, the coating of hollow carbon spheres significantly enhances the structural and catalytic properties of the C@$MoS_{2-2x}Se_{2x}$ sample [22].

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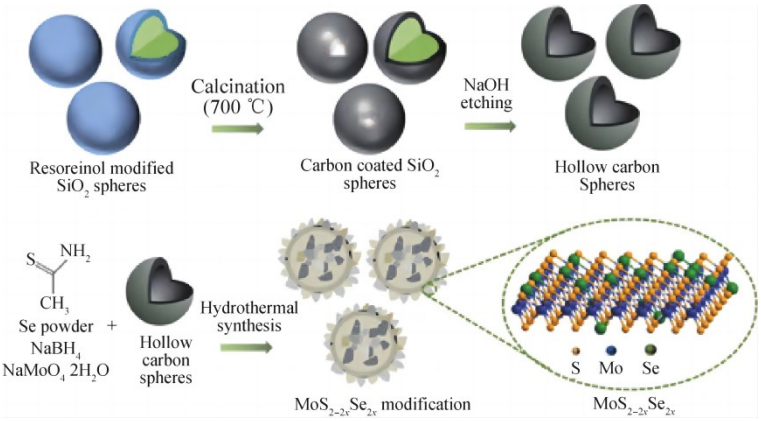


Figure 4: Schematic Diagram of the Formation Process of the C@MoS_2-2xSe_2x Sample

In contrast to non-metal doping, metal loading technology can notably enhance the electrocatalytic performance of MoS_2, particularly by improving the conductivity of catalysts with low conductivity in electrocatalytic applications. Atomic layer deposition (ALD) technology is used to modify the surface of ultrathin MoS_2 nanosheets, and studies show that this modification significantly reduces the overpotential in the hydrogen evolution reaction (HER). The MoS_2 material with metal loading exhibits significantly enhanced catalytic performance in the hydrogen evolution reaction [23]. From the experimental data, selenium-doped MoS_2 presents significant improvement in catalytic reactions compared to undoped materials, particularly in terms of overpotential and cycling stability. Moreover, metal loading technology improves the electrocatalytic performance of the material by enhancing the electron transfer rate. These studies indicate that metal and non-metal loading can not only optimize the catalytic efficiency of MoS_2 but also improve its stability in various electrochemical reactions. However, the effectiveness of different loading materials varies across different applications. Metal loadings, such as palladium, platinum, etc., typically provide higher electronic conductivity and catalytic activity but may introduce cost pressures. Non-metal loadings, such as selenium, nitrogen, and phosphorus, help enhance the electronic structure and stability of MoS_2 and are relatively more economical. Thus, the choice of appropriate loading materials needs to consider cost, performance enhancement, and specific requirements for the application field.

4. Conclusion

This paper focuses on the discovery of significant enhancement of MoS_2 under different performance optimization strategies, especially in heterogeneous atom doping, semiconductor composite preparation, and metallic and nonmetallic loading. Through these optimization methods, the performance of MoS_2 has been significantly improved in electrocatalysis, photocatalysis, lithium batteries and supercapacitors. Specifically, heterogeneous atom doping enhanced the electrical conductivity and catalytic activity of MoS_2, the semiconductor composite structure enhanced the photoelectrocatalytic efficiency, and the metallic and nonmetallic loading improved its electrocatalytic performance and stability. These findings provide strong support and practical basis for the wide application of MoS_2 in energy storage and catalytic reactions. However, despite the various optimization strategies analyzed in this study, there are limitations in experimental validation and practical applications. In particular, the precise control of heteroatom doping, including the effects of doping content and location, has not been fully explored. Furthermore, there are shortcomings in cost control and process simplification for large-scale production and practical applications. Future research could focus on fine-tuning the heteroatom doping process to investigate the impact of different doping levels and locations on the performance of MoS_2, as well as developing

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novel small molecule modifiers to enhance the interface properties of MoS_2 and carbon materials. Moreover, the preparation process of biomass carbon/MoS_2 composites must be further explored to reduce the cost and simplify the procedure to promote its practical feasibility in large-scale applications.

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