

Advancements in MoS₂-based Nanocomposites for Photothermal and Chemotherapy Applications: A Mini-Review

*Bello, Ismaila Taiwo; Adewumi, Hope Kofoworola; Ayanlola, Paul Sola; Aremu, Abraham Adewale; Oni, Emmanuel Abiodun and Amuda, Dauda Biodun

Department of Pure and Applied Physics, Ladoke Akintola University of Technology, Ogbomoso, Nigeria.

*Corresponding Author's Email: itbello@lautech.edu.ng; hkadewumi@lautech.edu.ng



ABSTRACT

Nanomaterials are recognized for their excellent properties and can be used in all areas of life. Nanomaterial-based drug delivery systems are increasingly promising and useful as tools in cancer therapy. Molybdenum sulfide (MoS₂), a 2D material, is extensively studied today due to its exceptional characteristics and wide range of applications. Due to its unique properties and versatility for numerous applications, MoS₂ has garnered considerable attention from researchers worldwide. MoS₂ has been extensively explored for biomedical applications due to its excellent photothermal conversion ability. Multiple research papers have explored the advancements and applications of MoS₂ materials, but this article aims to provide an overview of its photothermal and chemotherapy applications.

Keywords:

Nanocomposites,
MoS₂,
Photothermal,
Photodynamic,
Chemotherapy.

INTRODUCTION

Two-dimensional (2D) van der Waals materials have garnered significant attention from researchers due to their wide-ranging applications in optics, electronics, chemistry, and biology (Kabel et al., 2021; Mohammad-Andashti et al., 2022; Roy et al., 2019). Graphene was the first 2D material to be discovered, known for its exceptional properties and extensive applications. However, due to its inherent zero bandgap, scientists have been motivated to explore transition-metal dichalcogenides (TMDCs) as an alternative (Arul & Nithya, 2016). Zero bandgap materials, exemplified by graphene, present inherent limitations that restrict their applicability in nanoelectronic and optoelectronic devices. The absence of an energy bandgap results in continuous electronic states at the Fermi level, which inhibits effective current modulation and prevents the establishment of a clear on/off switching ratio in field-effect transistors. This characteristic also limits their performance in photodetectors, logic devices, and light-emitting systems, where controlled charge separation and selective optical absorption are required. Efforts to induce a practical bandgap often led to compromised carrier mobility or structural distortion, thereby limiting their technological utility (Hao et al., 2025; Toth & Velicky, 2017).

These challenges have stimulated significant interest in transition-metal dichalcogenides (TMDCs) as alternative

two-dimensional semiconductors. TMDCs possess intrinsic, layer-dependent band gaps within the visible to near-infrared spectrum, enabling efficient switching behavior and strong light-matter interactions. Their stable semiconducting nature, coupled with mechanical flexibility and chemical robustness, positions them as promising candidates for next-generation electronic and optoelectronic applications. This has led researchers to explore van der Waals 2D materials beyond graphene, such as hexagonal boron nitride (h-BN) and TMDCs. Unlike metallic graphene and electrically insulating h-BN, 2D TMDCs possess band gaps similar to that of silicon, which is crucial for field-effect transistors (FETs) (Bello et al., 2024; Weiss et al., 2012).

TMDCs have found applications due to their favorable electronic, optical, mechanical, chemical, and thermal properties. There is significant research interest in the transition from indirect band gaps in bulk TMDCs to direct band gaps in monolayer TMDCs (Kabel et al., 2021; Wang et al., 2012a). TMDCs have been widely explored in energy storage, sensors, catalysis, and biomedicine. Notably, chalcogenides such as MoS₂, WS₂, and WSe₂ have demonstrated lower toxicity compared to graphene, suggesting their potential for a range of biomedical applications (Bello et al., 2020a; Zhang, Wu, Williams, Niu, et al., 2019). Among all known TMDCs, MoS₂ has garnered significant attention since 2013 due to its direct bandgap and remarkable optoelectronic,

catalytic, energy, chemical, and biological properties, leading to widespread applications (Arul & Nithya, 2016; Chikukwa et al., 2021; Guo & Li, 2020; Kabel et al., 2021; Radhakrishnan et al., 2022; Tulsani et al., 2019; Yadav et al., 2019). The hexagonal layers of MoS₂ are held together by weak van der Waals forces, allowing it to be exfoliated into single-layer (2D) materials. In bulk MoS₂, indirect band gaps transition to direct band gaps in monolayers. 2D MoS₂ can be designed with controlled morphologies, including nano-flakes, nanoflowers, nanosheets, nanospheres, and quantum dots, for various applications (Pallikarathodi Mani et al., 2018; Xu et al., 2019). MoS₂ is a material with a double-layer structure known for its low cytotoxicity and genotoxicity.

Previous studies indicate that MoS₂ contains many unsaturated bonds, and reducing the number of layers transforms its structure from an indirect to a direct bandgap, thereby enhancing its photocatalytic performance (Cai et al., 2016; Liu et al., 2022). However, reducing the lamellar problem of MoS₂ has always been challenging. MoS₂ also features a larger specific surface area and stronger adsorption capacity, making it more likely to interact with other substances. Studies have shown that MoS₂ exhibits a better response to light, causing oxidative and membrane stress in organisms, which impedes their survival (Cao et al., 2017; Gao et al., 2015). Additionally, MoS₂ can produce hydroxyl free radicals that damage cell walls and membranes, achieving antibacterial effects. Thus, it is crucial to reduce the number of MoS₂ layers and improve the separation efficiency of photogenerated carriers through simple methods to achieve superior light-driven antibacterial activity. However, when MoS₂ is excited by light, the resulting electron-hole pairs quickly recombine, which limits its bactericidal efficacy (Alimohammadi et al., 2018; Liu et al., 2022).

MoS₂ has been investigated as a drug delivery carrier in numerous studies. It is particularly promising for photothermal therapy (PTT) treatments for cancer due to its high photothermal conversion efficiency in the near-infrared (NIR) region (Mou et al., 2015; Zhang et al., 2017). However, for clinical applications, MoS₂ needs to be modified to enhance its biocompatibility and colloidal stability. Modifications with poly(ethylene glycol), peptides, silica, and proteins have been employed to achieve this. Despite these pioneering studies, research on using MoS₂ for targeted drug delivery remains limited (Ariyasu et al., 2017; Lee et al., 2016; Liu et al., 2014; Wang et al., 2016). In this review, we examine the properties and applications of MoS₂ nanomaterials, including their use in photothermal and chemotherapy treatments. Recent progress shows that among the TMDC materials, MoS₂ has been showing outstanding results for the drug delivery system.

Overview of Molybdenum Sulfide (MoS₂)

Following the discovery of graphene in 2004 and subsequent advancements in graphene-like two-dimensional (2D) nanostructures, single-layered transition metal dichalcogenides, such as MoS₂ and WS₂, emerged as key materials for the next generation of 2D materials. Their large intrinsic band gaps make them ideal replacements for graphene, which lacks a band gap. Additionally, these materials possess narrow band gaps that are comparable to those of graphene (Coleman et al., 2011; Lee et al., 2012; Ramakrishna Matte et al., 2010; Wang et al., 2012b). MoS₂, often referred to as "moly," is an inorganic compound composed of molybdenum and sulfur. This compound belongs to the class of transition metal dichalcogenides. Molybdenum, a transition metal with a partially filled d-shell, contributes to the chemical stability and versatility of MoS₂ in compound synthesis. Metal disulfide compounds and nanocomposites are particularly attractive for a wide range of mechanical, electrical, and other applications due to the presence of strong S-S bonds (Bazaka et al., 2019; Gu et al., 2016). MoS₂ nanostructures have significantly improved due to their distinct physical and chemical characteristics. It has become a viable contender for sustainable applications that are both cost-effective and efficient (Zhang et al., 2016). MoS₂ has a layered structure resembling graphite, with Van der Waals forces holding together the S-Mo-S sandwiched layers. The spacing between adjacent Mo layers in MoS₂, which are sandwiched between sulfur layers, is 0.615 nm. This distance is nearly twice the spacing between graphite layers, which is 0.335 nm (Wu et al., 2015). Because of their atomic-layered thickness and 2D morphology, these features have led to a variety of applications, including energy storage, catalysis, light harvesting, gas sensors, biomedicine, etc. (Bello et al., 2020b; Huang et al., 2011, 2013; Novoselov et al., 2004, 2005; Zhang & Huang, 2017).

Occurrence of Molybdenum Sulfide (MoS₂)

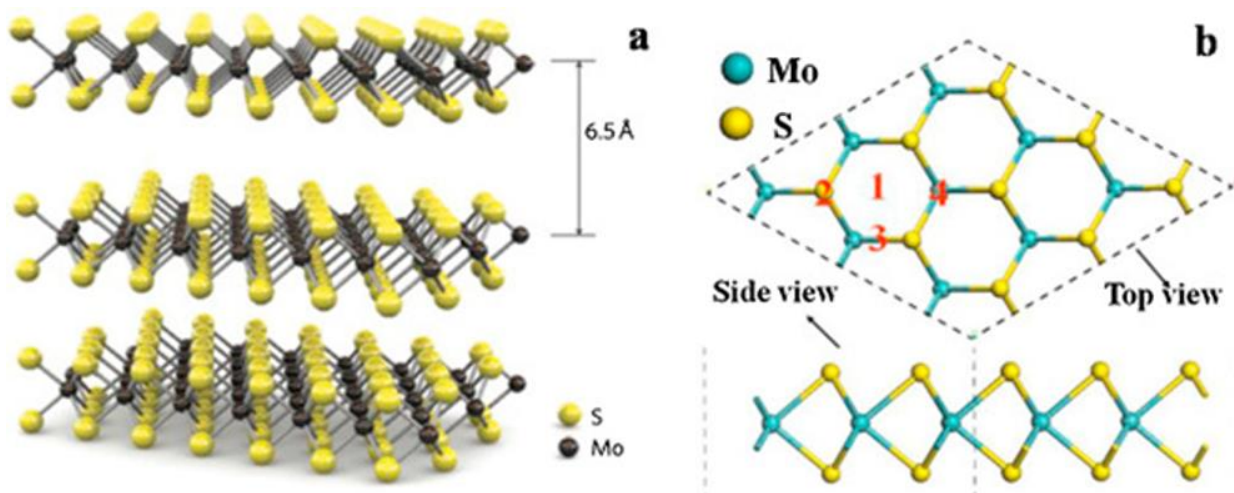
MoS₂ naturally occurs in 'molybdenite,' the primary source of molybdenum. It can be concentrated from its ores using foam flotation. Nowadays, molybdenite is predominantly obtained as a byproduct of copper mining (Benavente et al., 2002). MoS₂, a black solid with a bright sheen, is the primary ore of molybdenum. Its crystal structure consists of a hexagonal plane of sulfur (S) atoms on either side of a hexagonal plane of molybdenum (Mo) atoms. These three planes stack on top of each other, forming two-dimensional sheets of MoS₂, held together by strong covalent bonds between the Mo and S atoms (Mitchell et al., 2020; Rodriguez et al., 2021). The natural occurrence of MoS₂ is shown in Figure 1.



Figure 1: Naturally occurring crystal of Molybdenite (MoS₂). The crystals are approximately 2 cm across. Image adapted from Chianelli et al. (Chianelli et al., 2006), Copyright, Taylor & Francis Publishers, 2005.

The metal dichalcogenide layer comprises a plane of hexagonally packed metal atoms sandwiched between two planes of chalcogenide atoms. In these layers, the chalcogen atoms surrounding each metal atom typically form an octahedral or trigonal prismatic arrangement. Because of their extremely anisotropic characteristics, Molybdenum (Mo) is one of the transition metals of groups IVb, Vb, and VIb that are part of the layered dichalcogenides (Wilson & Yoffe, 1969). MoS₂ is a polytypic material since it can be found in three different crystalline structures: hexagonal (2H), trigonal (3R), and synthetic octahedral (1T). The 2H structure belongs to the

P6₃/mmc space group ($a = b = 3.16 \text{ \AA}$, $c = 12.29 \text{ \AA}$) (Benavente et al., 2002), while the 3R structure is part of the R3m space group ($a = b = 3.16 \text{ \AA}$, $c = 18.37 \text{ \AA}$) (SCHONFELD et al., 1983). The metastable 1T-MoS₂ structure falls under the P1 space group ($a = b = 3.36 \text{ \AA}$, $c = 6.29 \text{ \AA}$) (Py & Haering, 1983). Additionally, the point groups of D_{6h}, C_{3v}, and D_{6d} in the structures (2H, 3R, and 1T) have semiconductor, metal, and semiconductor electronic behavior, respectively (Mouloua et al., 2021). The three structures of the MoS₂ polymorphs are depicted in Figure 2(a-c).



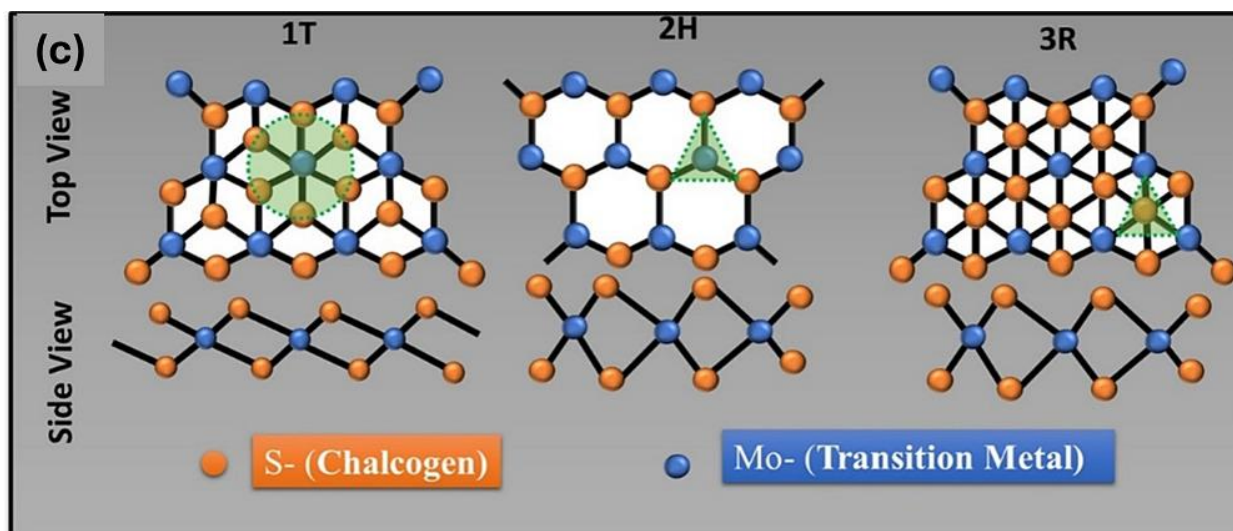


Figure 2: (a) Three-dimensional representation of the structure of MoS₂. Single layers, 6.5 Å thick, can be extracted using scotch tape-based micromechanical cleavage. Image reproduced from Radisavljevic et al. (Radisavljevic et al., 2011), Copyright, Macmillan Publishers, 2011. (b) Optimized structures of MoS₂ monolayer with four adsorption sites: (1) hollow site, (2) top site of the S atom, (3) Mo–S bridge site, and (4) top site of the Mo atom. Image reprinted from Chen et al. (Chen et al., 2013), Copyright, Elsevier Publishers, 2011. (c) Representation of the 3 polytype structures 1T, 2H, and 3R MoS₂ from both (Top and side views). [images reproduced from Molybdenum Disulfide (MoS₂): Theory & Applications].

In these polymorphs, the first digit indicates the number of monolayers in a unit cell, while the letters T, H, and R represent the structural symmetries: trigonal, hexagonal, and rhombohedral, respectively (He & Que, 2016; Jaleel UC et al., 2022). These phases are distinguished by their unique features resulting from changes in layer symmetry. The 1T trigonal phase, with its deformed octahedral symmetry, is known for its metallic behavior and effective electrical conductivity. The hexagonal 2H phase, characterized by a band gap, exhibits semiconducting properties. The 3R phase, with

rhombohedral symmetry and rotational stacking, also demonstrates semiconductor capabilities, but its specific properties differ due to the unique layer arrangement. These structural variations not only influence electrical conductivity but also affect the piezoelectric characteristics of MoS₂, impacting its ability to generate electric charge in response to mechanical stress (Ataca et al., 2011; Lin et al., 2014; Song et al., 2015). The distinctive properties of the three polytype structures of MoS₂ are represented in Table 1 (Srivastava et al., 2024).

Table 1: Distinctive properties among the three polytype structures of MoS₂ (Srivastava et al., 2024)

MoS ₂ Properties	Trigonal (1T)	Hexagonal (2H)	Rhombohedral (3R)
Coordination	Octahedral	Trigonal Prismatic	Trigonal Prismatic
Space Group	P3m1	P6 ₃ /mmc	R3m
Lattice Parameters	a=5.60 Å, c=5.99 Å, & edge-sharing octahedral	a=3.15 Å, c=12.30 Å	a=3.17 Å, c=18.38 Å
Property	Paramagnetic & Metallic	Semiconducting	Semiconducting
Electrical Conductivity	10 ⁵ times higher than the 2H phase	Low (~0.1 S m ⁻¹)	Low (~0.1 S m ⁻¹)
Band Gap	1.8-2.1 eV	1.2-1.3 eV	1.416
Absorption Peak	No peak at 604 nm & 667 nm	Showed peaks at 604 nm & 667 nm	Showed peaks at 604 nm & 667 nm
Symmetry	Octahedral	Hexagonal	Rhombohedral
Stacking	AbC	AbABaB	AbABcBCaC
Application	Intercalation Chemistry	Dry lubricants	Dry lubricants & non-linear optical devices

Photothermal and Chemotherapy Applications

In recent years, there has been significant research interest in the biomedical applications of MoS₂ nanosheets, marking them as a highly promising and innovative area of study (Lu et al., 2020). These nanosheets offer notable advantages such as polymer functionalization capability and high load-carrying capacity, owing to their expansive surface area, distinctive band gap, and atomically thin planar structures (Li et al., 2018). Leveraging their high sensitivity, MoS₂ nanosheets serve as excellent nanoprobe for applications including cancer therapy, optical sensing, and biomedical imaging (Li et al., 2019; Liu et al., 2018; Zhang et al., 2018). MoS₂ nanosheets exhibit remarkable photothermal conversion efficiency within the near-infrared (NIR) region and possess strong absorption capabilities, addressing the challenge of low NIR radiation absorbance in biological tissues. These properties make MoS₂ nanosheets ideal candidates as NIR conversion agents for tumor photothermal therapy (PTT), known for their minimal invasiveness and high selectivity.

Moreover, the exceptional photothermal conversion efficiency and high biocompatibility of MoS₂ nanosheets further enhance their suitability for PTT applications (Li et al., 2019; Zhang, Wu, Williams, Niu, et al., 2019). Photothermal therapy (PTT) serves as an alternative to chemotherapy by converting near-infrared (NIR) light into heat. This heat is absorbed by a photothermal platform within the tumor and induces thermal ablation, effectively destroying the tumor without the need for chemical interventions. PTT offers advantages such as enhanced local treatment efficacy and reduced systemic side effects compared to chemotherapy. However, challenges such as limited tissue penetration by NIR irradiation, the potential for uneven heat distribution, and the risk of tumor cells developing heat resistance remain drawbacks of PTT (Chen et al., 2018; Chen et al., 2017). To address these limitations, extensive research has focused on nanoscale platforms, with particular attention to materials capable of effective absorption of near-infrared (NIR) light. These materials include copper chalcogenides, carbon nanotubes, gold nanostructures, graphene, and MoS₂, among others (Yan et al., 2017; Zhang et al., 2017).

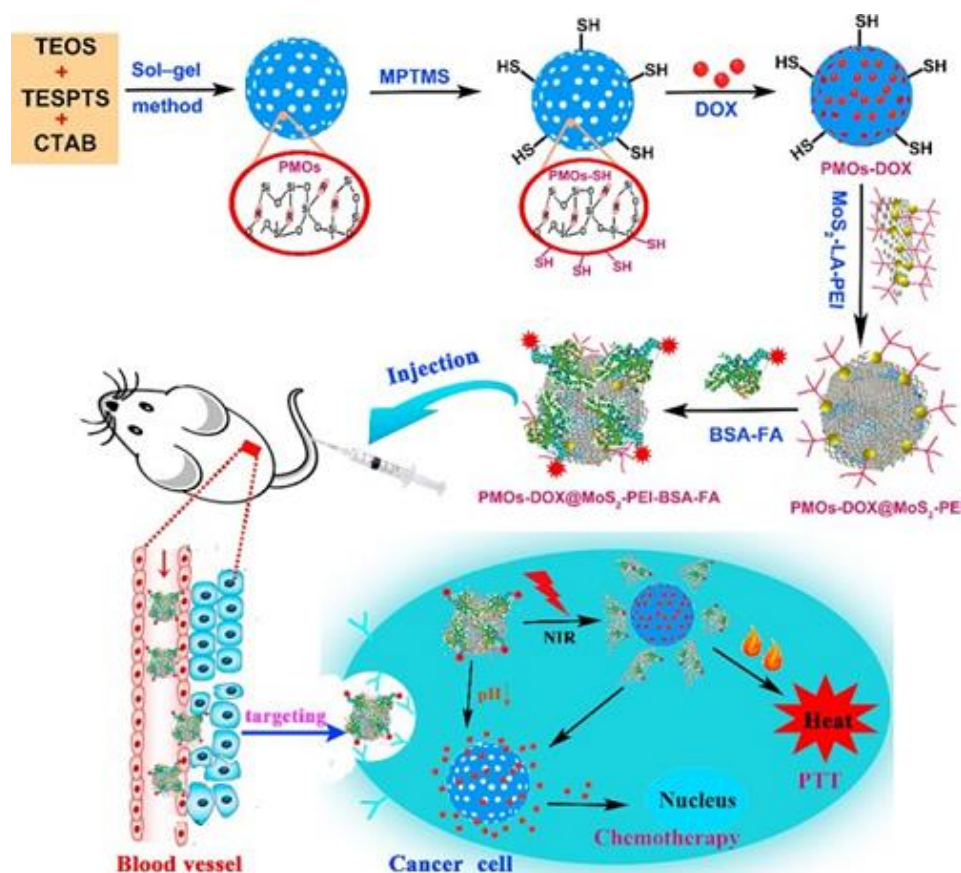


Figure 3: Schematic illustration for the synthesis and preparation of PMOs-DOX@MoS₂-LA-PEI-BSA-FA composite as a multifunctional drug delivery system for synergistic chemo-photothermal targeted therapy of tumors. Image adapted from Wu et al. (Wu et al., 2018), Copyright, Elsevier Publisher, 2018.

The concept of chemo-photothermal therapy, which combines photothermal therapy (PTT) with chemotherapy, has gained increasing recognition due to the potential synergistic effects of materials possessing both PTT properties. This approach involves raising local temperatures to directly ablate tumor cells, while the elevated temperature promotes drug release from carriers and enhances uptake by increasing cellular membrane permeability (Dong et al., 2013; Liu et al., 2014). Chemo-photothermal therapy offers the possibility of delivering chemotherapy directly to tumors, significantly reducing systemic side effects. Several studies have demonstrated that chemo-photothermal therapy improves therapeutic efficacy compared to either photothermal therapy or chemotherapy alone (Duan et al., 2017; Wu et al., 2018). Zhang and colleagues introduced a versatile nanoplatform consisting of MoS₂ nanosheets decorated with copper sulfide and functionalized with polyethylene glycol (PEG). The platform exhibited an average particle size of 115 nm and a loading capacity of 162.3 mg of doxorubicin per gram of carrier. Controlled drug release was achieved through near-infrared irradiation and pH stimuli, ensuring excellent colloidal stability. Compared to pure MoS₂ nanosheets, the MoS₂/CuS composite demonstrated higher photothermal conversion efficiency. In vitro studies confirmed the biocompatibility of the blank carrier (CuS-MoS₂-SH-PEG), and its application in synergistic chemo-photothermal therapy induced greater cell death compared to photothermal therapy or chemotherapy alone.

Furthermore, the nanoplatforms exhibited effective cellular uptake by tumor cells, with enhanced uptake observed under NIR irradiation, highlighting their potential as an advanced nanoplatform for synergistic chemo-photothermal therapy and responsive drug delivery systems (Zhang, Wu, Williams, Yang, et al., 2019). MoS₂/C@SiO₂ nanospheres were synthesized via hydrothermal methods for the in vitro ablation of MCF-7 cancer cells, employing a combination of synergistic chemotherapy and photothermal approaches. The study evaluated the photothermal effect induced by near-infrared (NIR) light, as well as the drug loading and release behaviors of the model drug DOX, to assess the antitumor capabilities of both MoS₂/C@SiO₂ and C@SiO₂ nanospheres. Results indicated a significant photothermal effect with a 42.5% conversion efficiency for MoS₂/C@SiO₂, surpassing the 34.7% efficiency observed for C@SiO₂. Additionally, the drug loading capacity of MoS₂/C@SiO₂ (46.5%) was notably higher than that of C@SiO₂ (12.4%). Under simulated acidic tumor conditions and NIR irradiation, MoS₂/C@SiO₂ exhibited a higher aggregate drug release of 58.9%, compared to 27.29% for C@SiO₂ (Zhao et al., 2022). A straightforward hydrothermal method was employed to fabricate porous MoS₂ nanoflowers intended for a multifunctional theranostic platform capable of

integrating sensitive photoacoustic (PA) imaging, enhanced photothermal therapy (PTT), photodynamic therapy (PDT), and nano-enzyme activated chemodynamic therapy (CDT). The porous structure of the MoS₂ nanoflowers facilitated improved photothermal conversion efficiency by enhancing light trapping and peroxidase (POD)-like activity via exposure of active defects. This enhancement was attributed to the abundance of active pore sites and the large surface area of the assembled 3D-stacked MoS₂ nanosheets.

To encapsulate the 3D-MoS₂ nanostructure, a polyethylene glycol-polyethylenimine polymer modified with the nucleolar translocation signal sequence of the LIM Kinase 2 protein (LNP) was utilized, forming a stable complex via strong electrostatic interaction. This complex efficiently delivered the anticancer drug doxorubicin (DOX) into tumor cells for pH/NIR-responsive chemotherapy. Additionally, the complex exhibited strong photoacoustic and photothermal performances and stimulated the generation of reactive oxygen species (ROS) for imaging-guided PTT/PDT/CDT combined therapy (Jiang et al., 2020). In 2021, Zhou and colleagues introduced a novel single-pot bottom-up hydrothermal synthesis method to produce Eu³⁺-doped MoS₂ nanoflowers for effective photothermal/photodynamic synergistic therapy in breast cancer treatment. The photothermal conversion efficiency of the MoS₂:5%Eu³⁺ photothermal agents was notably enhanced to 49.05%, surpassing that of pure MoS₂, when subjected to 808 nm NIR laser irradiation. Moreover, MoS₂:5%Eu³⁺ exhibited potent photodynamic therapy (PDT) capabilities by inducing the generation of cytotoxic reactive oxygen species (ROS) under similar 808 nm NIR laser irradiation conditions. These multifunctional nanoprobe demonstrated promising potential in improving in vitro breast cancer therapy through the combined modalities of photothermal therapy (PTT) and photodynamic therapy (PDT) (Zhou et al., 2021).

Cao and colleagues engineered a photodynamic antibacterial system based on chlorin e6 (Ce6) stacked chitosan-functionalized MoS₂ nanocomposites (M-CS-Ce6). This innovative nanocomposite facilitated the penetration of Ce6 into the cells of Gram-positive bacteria while disrupting the cell wall permeability of Gram-negative bacteria, thereby enhancing the photo-antibacterial efficacy. Remarkably increased photo-antibacterial performance was observed against both Gram-positive and Gram-negative bacteria when 10 µg/mL of M-CS-Ce6 was irradiated by a 660 nm laser for 5 minutes, effectively eliminating the target pathogens. M-CS-Ce6 demonstrated superior and broader-spectrum photo-antibacterial effects compared to other cationic photodynamic composites (Cao et al., 2022). In a similar study, Yang and colleagues explored a multifunctional nanoplatform based on MoS₂ nanosheets for drug

delivery and chemo-photothermal therapy, specifically targeting CD44 receptor-positive MCF-7 cells with hyaluronic acid (HA) targeted dual-stimulation-responsive MoS₂ nanosheets (HA-PEI-LA-MoS₂-PEG, HPMP). The developed HPMP nanocomposite exhibited exceptional photothermal conversion efficiency of 55.3% and remarkable biocompatibility, characterized by a uniform hydrodynamic diameter of 104 nm and a higher drug loading capacity of 944.3 mg/g HPMP. The dual stimuli of the acidic tumor microenvironment and external laser irradiation enabled precise control over drug release from the HPMP@(DOX/Mel) composite, while the photothermal effect of the MoS₂ nanosheets was enhanced by loading Melanin (Mel) onto the surface. This multifaceted MoS₂ nanosheet-based nanoplatform holds significant promise for targeted drug delivery responsive to pH and NIR stimuli, enabling synergistic chemo-photothermal therapy for tumors (Yang et al., 2020).

A hydrothermal method was employed to synthesize a three-dimensional (3D) urchin-like MoS₂@C nanocomposite, which exhibited impressive characteristics, including a high photothermal conversion capacity of 40.8%, substantial drug loading capacity for doxorubicin (52.34%), robust absorption properties, and excellent biocompatibility. In vitro studies demonstrated a pH, temperature, and near-infrared laser-triggered release profile for doxorubicin-hydro, enhancing its therapeutic efficacy against cancer. Systemic in vitro experiments utilizing the DOX-loaded nanoplatforms further underscored its potential for synergistic photothermal therapy against cancer (Zhang et al., 2020). In 2022, Wan and colleagues introduced a versatile Z-scheme nanocomposite composed of Fe₂O₃@MoS₂@SDS, achieved by modifying sodium dodecyl sulfate (SDS) onto the surface of Fe₂O₃@MoS₂ via ultrasonic treatment. This innovative composite demonstrated dual functionalities: efficient antibiotic degradation and suppression of antibiotic resistance gene (ARG) dissemination. Under near-infrared (NIR) irradiation, the Fe₂O₃@MoS₂@SDS nanocomposite exhibited a notable photothermal conversion efficiency of 45.96% and generated abundant reactive oxygen species (ROS). Through synergistic photothermal and photodynamic mechanisms, the nanocomposite displayed remarkable antibacterial efficacy, achieving eradication rates of 99.95%, 99.97%, and 99.58% against *E. coli*, MRSA, and *P. aeruginosa*, respectively, showcasing its exceptional photothermal-photodynamic therapy (PPT) capabilities (Wang et al., 2022).

A novel nanocomposite, MoS₂/PDA-TPP, was designed for dual-responsive drug delivery and synergistic chemo-photothermal therapy targeting tumor acidity and near-infrared radiation. Loaded with doxorubicin (DOX), this nanoplatform takes advantage of the tumor-specific mitochondria accumulation ability and photothermal

therapy (PTT) for enhanced anti-tumor efficacy. The pH-responsive dissociation of MoS₂/PDA-TPP triggers rapid DOX release in the acidic tumor microenvironment (TME), amplifying the effectiveness of PTT. Furthermore, the mechanism involves MoS₂/PDA-TPP inducing mitochondrial-dependent apoptosis by generating reactive oxygen species (ROS) and reducing mitochondrial membrane potential (MMP) (Zhang et al., 2022). Saravanan and colleagues investigated enhanced cytotoxicity in cancer chemo-photothermal therapy using MoS₂ nanoflowers decorated with CeO₂ nanoparticles as nanozyme-controlled photothermal agents. They found that nanoflowers decorated with long-chain PEI molecules exhibited superior photothermal heat generation compared to those decorated with low molecular weight PEI. Factors such as the concentration of nanozymes, duration of near-infrared (NIR) light exposure, power density of NIR light, and folic acid (FA) conjugation significantly influenced the biocompatibility, photothermal heat generation, and anti-cancer activity of the nanozymes. This study underscores the potential of nanozymes as promising candidates for nanophotothermal agents in cancer photothermal therapy (Saravanan et al., 2023).

A confined solvothermal technique was utilized to fabricate a porous silica nanosystem loaded with MoS₂. The ultrasmall MoS₂ nanoclusters and abundant porous sites contributed to the maximum photothermal efficiency of 79.5% exhibited by the MoS₂@P-SiO₂ nanosystem. In vitro and in vivo studies of glucose oxidase (GOD) loaded onto the cascade hybrid system (MoS₂/GOD@P-SiO₂) demonstrated a remarkable tumor-suppressive effect and excellent biosafety through the combined impacts of photothermal and enzyme-mediated cascade catalytic therapy. The integration of a hybrid porous network system, an in situ solvothermal approach for inorganic functional components, and effective encapsulation of organic enzyme macromolecules offer a promising approach for the construction of synergistic agents for the efficient and safe treatment of tumors (Song et al., 2022). Recently, Dual tumor and subcellular-target photodynamic therapy were reported by Xu et al., using glucose-functionalized MoS₂ nanoflakes to combat multidrug-resistant (MDR) cancer. The MoS₂ nanoflakes were functionalized with glucose-modified hyperbranched polyglycerol (hpG) to construct the nanoplatforms and thereafter loaded with organelle-targeting PDT agents. The resultant nanoplatforms significantly enhance internalization within multidrug-resistant (MDR) cells and precisely localize PDT agents subcellularly. This facilitates in situ near-infrared (NIR)-triggered reactive oxygen species (ROS) generation, augmenting photodynamic therapy (PDT) and reversing MDR. The approach has demonstrated impressive tumor shrinkage in a HeLa multidrug-resistant tumor mouse model. This

nanoplatfrom, with its NIR-responsive properties and ability to target tumors and subcellular organelles, presents a promising strategy for the effective treatment of multidrug-resistant (MDR) cancer (Xu et al., 2022).

In a light-driven antibacterial activity, Liu et al., reported a facile hydrothermal technique to synthesize silver sulfide/molybdenum disulfide/palygorskite (Ag₂S/MoS₂/Pal) nanocomposites for light-driven antibacterial study. The Ag₂S/MoS₂/Pal nanocomposites demonstrated excellent antibacterial activity under various lighting conditions. The minimum inhibitory concentrations (MICs) of these nanocomposites against *Escherichia coli* (*E. coli*) and *Staphylococcus aureus* (*S. aureus*) were 0.3 mg/mL and 0.5 mg/mL, respectively. Additionally, Ag₂S/MoS₂/Pal nanocomposites exhibit an exceptional photothermal effect. The synergistic combination of physical puncture, photodynamic, and photothermal effects results in rapid bacterial death. The enhanced antibacterial performance is attributed to the increased active centers and efficient interfacial carrier transfer. This study opens new avenues for the development of advanced functional clay materials to address the growing bacterial resistance issue (Liu et al., 2022).

In a related study, Lai et al. utilized a hydrothermal method to synthesize a silver indium sulfide/nickel molybdenum sulfide (AgInS₂/NiMoS₄) nanostructure, which was then decorated on Palygorskite (Plg) to achieve synergistic light-driven antibacterial performance. The composite (AgInS₂/NiMoS₄/Plg) was evaluated for its antibacterial activity under light exposure and its ability to detect uric acid in biological samples. The results showed that AgInS₂/NiMoS₄/Plg exhibited the highest antibacterial activity with minimum inhibitory concentrations of approximately 0.2–0.3 mg/mL. Additionally, the composite demonstrated enhanced peroxidase-like activity for uric acid detection, with a detection limit of around 26.1 nM. These findings suggest that AgInS₂/NiMoS₄/Plg composites have potential applications in bactericidal processes and sensing in complex biological systems (Lai et al., 2022). Owing to its outstanding photothermal conversion ability, functionalized MoS₂-nanosheets were reported for targeted drug delivery and chemo-photothermal treatment by Zhang et al., 2019. A nanoplatfrom-based folic acid (FA) targeted dual-stimuli responsive MoS₂ was employed for the FA-receptor positive human breast cancer therapy. The obtained nanocomposites had a uniform diameter (ca. 133 nm) and could be easily loaded with the anti-cancer drug doxorubicin (DOX) to a high capacity of 151.4 mg/g. It was found that drug release is enhanced under near-infrared (NIR) laser irradiation, demonstrating that the composites can be used as dual-responsive systems, with DOX release controllable through pH changes or NIR irradiation. The platform also enabled the combination of chemotherapy and

photothermal therapy, resulting in synergistic effects superior to monotherapy alone. The functionalized MoS₂ nanoplatforms developed could thus be a potent system for targeted drug delivery and synergistic chemo-photothermal cancer therapy (Zhang, Wu, Williams, Niu, et al., 2019).

In search of a multifunctional platform for synergistic targeted chemo-photothermal treatment, a functionalized MoS₂ nanosheet-capped periodic mesoporous organosilica was used as a capping agent to block PMOs to control the drug release and to investigate their potential in near-infrared photothermal therapy. The resulting PMOs-DOX@MoS₂-PEI-BSA-FA complexes exhibited a uniform diameter of 196 nm, a high DOX loading capacity of 185 mg/g PMOs-SH, excellent photothermal conversion efficiency, and good biocompatibility under physiological conditions. In vitro, experimental results confirmed that the material exhibits excellent photothermal conversion ability, outstanding tumor-killing efficiency, and specific targeting of tumor cells via an FA-receptor-mediated endocytosis process. In vivo experiments further demonstrated that the platform for synergistic chemo-photothermal therapy significantly inhibits tumor growth, outperforming any monotherapy (Wu et al., 2018). In a separate study, Lei et al. proposed a photothermal-enhanced photo-Fenton pollutant degradation approach to address the limitations of relatively low catalytic activity and cycling stability in the Fenton reaction. They developed hybrids of magnetically recyclable 1T-2H MoS₂/Fe₃O₄, which exhibited excellent photothermal conversion efficiency. These hybrids not only increased the reaction temperature of the Fenton reaction on the material surface but also demonstrated effective interfacial photothermal water evaporation efficiency. Due to the synergistic effect of photocatalysis and the photo-Fenton catalytic reaction, simulated pollutants were rapidly degraded within 5 minutes, achieving a 98.3% degradation rate, which could be further improved to 99% with photothermal promotion. The 1T-2H MoS₂/Fe₃O₄ hybrids also showed good magnetic recyclability, cyclic stability, and photothermal performance, making them promising for applications in environmental remediation and photothermal interface water evaporation (Lei et al., 2023).

The study investigated multifunctional MoS₂-based nanoplatforms designed for the co-delivery of erlotinib (Er) and doxorubicin (DOX), enabling controlled drug release for effective synergistic photothermal chemotherapy. Initially, Er was loaded onto MoS₂ nanosheets through click chemistry with a PEG linker, followed by incorporation with DOX. The resulting MoS₂-PEG-Er/DOX nanocomposite converted absorbed near-infrared (NIR) light into heat, facilitating the controlled release of DOX and inducing photothermal ablation of cancer cells. Notably, upon NIR irradiation,

MoS₂-PEG-Er/DOX achieved synergistic photothermal chemotherapy, significantly inhibiting tumor growth in lung cancer cell-bearing mice. This study highlights the excellent antitumor efficacy of MoS₂-PEG-Er/DOX, offering a promising strategy for clinical cancer treatment (Liu et al., 2020).

To enhance cancer photothermal therapy (PTT), Rajasekar et al. reported on the development of a 2D nanomaterial specifically designed for targeted photothermal treatment, which efficiently kills cancer cells while sparing normal cells. They prepared chitosan-coated MoS₂ nanosheets combined with tantalum oxide nanomaterials through electrostatic interactions to improve PTT efficacy. Detailed studies showed that the TaO₂-CS-MoS₂ nanomaterial exhibited no toxicity, excellent photostability, and an increase in photothermal conversion efficiency (PCE) from 26°C to 47.2°C under 808 nm irradiation for 5 minutes. The deposition of TaO₂ significantly enhanced the photostability, biocompatibility, and PCE of the MoS₂ nanosheets. This innovative approach is highly anticipated to improve the biological features of cancer PTT (Rajasekar et al., 2020). Various studies have demonstrated that the transdermal drug delivery system (TDDS) is an effective non-invasive method with numerous advantages. Zhang et al. first reported using CPAM-MoS₂ nanoparticles (NPs) as drug carriers in TDDS. They employed a simple hydrothermal technique to develop polyacrylamide-modified MoS₂ nanoparticles (CPAM-MoS₂ NPs) for controlled drug release and prolonged treatment duration via light stimulation. An *in vivo* skin erythema study confirmed the biocompatibility and skin safety of the colloid-stable CPAM-MoS₂ NPs, showing a high drug load efficiency of 87.2% and excellent photothermal conversion efficiency, successfully applied in TDDS with an enhancement ratio of 1.82. The *in vitro* skin penetration test demonstrated the controlled release capacity, with no drug depletion observed during the 8-hour study under light stimulation (Zhang et al., 2020).

A traceable and pH-responsive drug delivery system based on PEGylated MoS₂ quantum dots (QDs) was successfully developed, incorporating the fluorescent antineoplastic anthracycline drug, doxorubicin (DOX). The functionalized PEGylated MoS₂ QDs endowed the nanocomposite with strong blue photoluminescence, low cytotoxicity, and excellent physiological stability. It was observed that the MoS₂-PEG-DOX nano-assembly could be efficiently taken up by U251 cells, with accelerated DOX release triggered by intracellular acidic conditions. This targeted release diminishes the unwanted side effects of DOX on healthy cells. The findings suggest that MoS₂-PEG-DOX has the potential for high treatment efficacy with minimal side effects in future therapies (Liu et al., 2020). In another development, a regenerated silk fibroin/molybdenum disulfide (RSF/MoS₂) nanoparticle hybrid fiber was prepared via wet spinning with varying

concentrations of MoS₂ nanoparticles. The 2wt% RSF/MoS₂ nanoparticle hybrid fibers demonstrated a temperature increase from 20.0°C to 81.0°C in 1 minute and to 98.6°C in 10 minutes under simulated sunlight. This indicates good thermal stability and excellent photothermal properties for fabrics created through manual blending. This novel approach presents a method for preparing high-toughness, photothermal property fibers suitable for multifunctional applications (Guo et al., 2021).

Prospects and Challenges

MoS₂ demonstrates broad applicability across electronics, biomedicine, catalysis, and environmental remediation due to its versatile structural, optical, and photothermal properties. Its effectiveness in drug delivery, photothermal therapy, imaging, and antibacterial applications highlights its value as a multifunctional nanomaterial. These advantages underscore MoS₂'s strong potential for next-generation biomedical and environmental technologies.

However, several gaps remain in the literature. Scalable synthesis methods capable of producing uniform MoS₂ structures with consistent properties are still underdeveloped. The long-term stability, toxicity, and biodegradation pathways of MoS₂ nanomaterials in physiological and ecological environments require deeper investigation. In addition, translational studies evaluating pharmacokinetics, biodistribution, and clinical safety remain limited. Comparative studies with other emerging 2D materials are also needed to clarify unique advantages and optimize MoS₂-based architectures. Addressing these gaps will be essential to fully realize the practical and clinical potential of MoS₂ in advanced technological applications.

CONCLUSION

MoS₂ has been shown to have applications across various disciplines, including electronics, enzymes, biomedicine (such as patchable and implantable devices), and energy. It also holds potential for environmental applications. Historically, bulk MoS₂ has been recognized for its utility as an environmental catalyst and adsorbent, occurring naturally as the abundant mineral molybdenite. Although current publications indicate that the synthetic routes for MoS₂ are simple and cost-efficient, more innovative approaches are needed to scale up synthesis techniques for real-world applications. Studies have shown that the synthesis and assembly processes significantly influence the structure, properties, and potential applications of MoS₂-based nanocomposites. Efficient, reliable, and affordable anti-cancer therapy approaches are crucial for improving the quality of life and extending the lifespan of people worldwide. Nanoparticle-based techniques, including those utilizing nanostructured MoS₂, offer

promising methods for targeting cancer cells and could be applied in various environments.

The unique mechanical and photothermal properties of MoS₂ enhance functionality in drug delivery systems. MoS₂ quantum dots (QDs) exhibit a direct bandgap and high biocompatibility, leading to diverse applications. MoS₂'s versatility extends to its use as an antibacterial agent, in photodynamic therapy, and synergistic chemophotothermal activities. MoS₂ nanosheets demonstrate remarkable photothermal conversion efficiency within the near-infrared (NIR) region and strong absorption capabilities, addressing the challenge of low NIR radiation absorbance in biological tissues. These properties make MoS₂ nanosheets ideal candidates for tumor photothermal therapy (PTT), known for their minimal invasiveness and high selectivity. Furthermore, MoS₂ nanocomposites show promise for high treatment efficacy with minimal side effects in anti-cancer therapy, drug delivery, and medical imaging, offering key advantages and opportunities over other similar materials and nano-architectures.

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