# *Review Article*

# Recent Advances in Molybdenum Disulphide and Diselenide (MoS₂/MoSe₂) for Renewable Energy Applications: A Critical Review (2021–2025)

**ABSTRACT**

This review provides a comprehensive and critical analysis of the recent progress (2021–2025) in the application of molybdenum disulphide (MoS2) and molybdenum diselenide (MoSe2) for renewable energy. We focus on three pivotal areas: electro catalytic hydrogen evolution (HER), photovoltaics (PV), and energy storage. We dissect the key strategies for material enhancement, including Nano structuring, phase and defect engineering, and the design of advanced heterostructures. A central theme is the critical trade-off between enhancing performance metrics—such as catalytic activity, power conversion efficiency, and specific capacity—and ensuring long-term operational stability and scalability. By synthesizing findings from recent literature, we highlight a paradigm shift from single-material systems to complex, multi-component composites where synergistic effects are paramount. We critically evaluate the role of computational screening in accelerating material discovery and identify persistent challenges, including interfacial instability, intrinsic conductivity limitations, and the gap between lab-scale demonstration and industrial viability. The review concludes by outlining key knowledge gaps and proposing high-priority research directions aimed at unlocking the full potential of these versatile 2D materials for a sustainable energy future.

*Keywords: 2D material; Energy storage; Hydrogen evolution reaction (HER); Molybdenum diselenide (MoSe₂); Molybdenum disulfide (MoS₂)*

# 1. INTRODUCTION

### 1.1. The Global Energy Landscape and the Need for Advanced Materials

This manuscript provides a crucial and timely synthesis for researchers in materials science and renewable energy, as it consolidates the most recent advancements (2021–2025) in a rapidly progressing field. By critically evaluating the persistent trade-off between performance and stability, it offers a necessary, balanced perspective that can guide more practical and durable material design. The review's emphasis on the paradigm shift towards complex heterostructures highlights the current frontier of research, where synergistic effects in multi-component systems are now essential for breakthroughs. Ultimately, this work serves as an invaluable roadmap, identifying key challenges and proposing targeted research directions to help bridge the significant gap between lab-scale success and industrial application.

The 21st century is defined by the dual challenges of escalating global energy demand and the urgent need to mitigate climate change. The prevailing reliance on fossil fuels is unsustainable, prompting a global imperative to transition towards a clean and renewable energy economy [1]. This transition is not merely a policy objective but a technological grand challenge that hinges on the development of next-generation materials capable of enabling high-efficiency energy conversion and storage technologies. Key pillars of this future energy infrastructure include the production of green hydrogen via water electrolysis, the advancement of cost-effective and highly efficient photovoltaic (PV) cells, and the creation of high-density energy storage systems to manage the intermittency of renewable sources like solar and wind [2].

A significant bottleneck in the commercialization of these technologies is the reliance on expensive, scarce, and often toxic materials. For instance, platinum-group metals are the benchmark catalysts for the hydrogen evolution reaction (HER), but their high cost and low abundance are prohibitive for large-scale deployment [1]. Similarly, while silicon photovoltaics dominate the market, their production is energy-intensive, and emerging thin-film technologies often involve elements with toxicity or scarcity concerns, such as cadmium, tellurium, or indium [3]. This materials-centric challenge has catalyzed a global research effort to discover and engineer high-performance alternatives from earth-abundant, cost-effective, and environmentally benign elements [4].

### 1.2. The Transition Metal Dichalcogenides (TMD) Family: An Introduction to MoS₂ and MoSe₂

Within this context, the family of two-dimensional (2D) transition metal dichalcogenides (TMDs) has emerged as a particularly promising class of materials, with molybdenum disulfide (MoS2) and its selenium analogue, molybdenum diselenide (MoSe2), at the forefront of scientific investigation [5]. These materials possess a layered crystal structure with the general formula MX2, where M is a transition metal atom (e.g., Mo) and X is a chalcogen atom (e.g., S, Se). Each layer consists of a plane of metal atoms hexagonally coordinated and covalently bonded to two planes of chalcogen atoms, forming a trilayer "sandwich" [2]. These strongly bonded layers are stacked upon one another and held together by weak out-of-plane van der Waals forces, a structural feature that allows for facile exfoliation into atomically thin nanosheets, down to a single monolayer [6].

While often compared to graphene, the archetypal 2D material, MoS2 and MoSe2 possess a critical distinguishing feature: an intrinsic, tunable bandgap. Graphene's zero-bandgap, semi-metallic nature limits its direct use in many semiconductor applications without significant and often complex modification [7]. In contrast, TMDs like MoS2 and MoSe2 are natural semiconductors, making them inherently suitable for a vast array of optoelectronic, photonic, and catalytic applications where a bandgap is a fundamental requirement [6].

Furthermore, these materials exhibit rich polymorphism, with the most technologically relevant phases being the thermodynamically stable and semiconducting 2H phase, the metastable yet highly conductive metallic 1T phase, and the insulating 3R phase [8]. The ability to selectively synthesize or convert between these phases provides a powerful knob for tuning the material's electronic properties, shifting from a semiconductor suitable for a transistor channel to a metal-like conductor ideal for an electrode contact or catalyst [9]. This structural and electronic versatility is a cornerstone of their potential in renewable energy systems.

### 1.3. Fundamental Electronic and Optical Properties

The properties of MoS2 and MoSe2 are not static but are profoundly dependent on their dimensionality. The most celebrated example of this is the layer-dependent band structure of MoS2. In its bulk form, it is an indirect bandgap semiconductor with an energy gap of approximately 1.2 eV. However, as it is thinned down to a single monolayer, quantum confinement effects cause a dramatic shift in the electronic bands, transforming it into a direct bandgap semiconductor with a larger gap of around 1.8 eV [10]. This transition has profound consequences for its optical properties, leading to a significant enhancement in light-matter interactions, marked by strong photoluminescence and greatly increased optical absorption efficiency in the visible spectrum [11]. This phenomenon is fundamental to its application in photovoltaics, photodetectors, and light-emitting devices.

Building on the structural and chemical diversity of TMDs, a frontier of materials design has emerged with the creation of Janus monolayers. Named after the two-faced Roman god, a Janus MoSSe monolayer is created by asymmetrically replacing the sulfur atoms on one side of a MoS2 monolayer with selenium atoms. This breaks the out-of-plane mirror symmetry inherent to conventional TMDs, inducing a permanent, intrinsic vertical dipole moment across the monolayer [12]. This built-in polarization gives rise to a host of novel properties, including strong piezoelectricity and unique nonlinear optical responses, that are absent in their symmetric parent compounds [13]. As will be discussed, this atomic-level engineering of symmetry opens pathways to entirely new device physics, particularly in the realm of photovoltaics.

### 1.4. Scope and Structure of this Review

This review critically assesses the progress in the application of MoS2 and MoSe2 for renewable energy, with a specific focus on the period from 2021 to 2025. The aim is to provide a comprehensive synthesis of the state-of-the-art, moving beyond a simple cataloging of results to identify overarching scientific themes, unresolved challenges, and contradictions within the literature. The report is structured into three primary application areas that represent the core of current research efforts: electro catalytic hydrogen evolution, photovoltaic device integration, and high-performance energy storage. Within each section, we analyze recent advances in materials engineering, present comparative performance data, and dissect the key scientific and technological hurdles that remain. The review culminates in a discussion of synthesis and computational modeling trends, unifying design principles, and a forward-looking perspective on the research trajectories required to translate the remarkable potential of these materials into tangible energy solutions.

# 2. HESTORICAL BACKGROUND

### 2.1 Electro catalytic Hydrogen Evolution (HER)

The electrochemical splitting of water into hydrogen and oxygen is a cornerstone technology for producing green hydrogen, a clean and high-density energy carrier. The HER half-reaction, in particular, has been a major focus for catalysis research, with MoS2 and MoSe2 emerging as leading non-precious metal candidates to replace costly platinum catalysts [6].

### 2.2 Mechanistic Foundations: Identifying the Active Sites

The HER proceeds via distinct pathways depending on the electrolyte pH. In acidic media, the process involves the reduction of protons (H+), initiated by the Volmer step where a proton is adsorbed onto a catalytic site to form an adsorbed hydrogen intermediate (Hads​). This intermediate can then be desorbed as H2​ gas via either the Heyrovsky step (reaction with another proton-electron pair) or the Tafel step (recombination of two Hades​ species) [3]. For decades, the canonical model for HER on MoS2 has posited a clear division of labor: the expansive basal plane of the common 2H phase is considered catalytically inert, while electrochemical activity is almost exclusively confined to the unsaturated atomic sites along the edges (both Mo-terminated and S-terminated) and at structural point defects such as sulfur vacancies (VS​).1 This model has driven a research paradigm focused on Nano structuring to maximize the exposure of these "active" edge sites.

However, a more nuanced and critical examination of the literature from 2023-2025 reveals a significant evolution in this understanding. A 2025 review explicitly highlights that the literature remains "undecided and often contradictory on the true nature of its active sites" [14]. A careful collation of chemical and electrochemical evidence suggests that the most accurate model may not center on the geometric edges themselves, but rather on specific types of defects that are prevalent at these edges. The emerging consensus, supported by both experimental work on defect-rich materials and theoretical studies, is that low-coordinate molybdenum sites, created by the presence of sulfur vacancies, are the true loci of catalytic activity [3].

This represents a subtle but critical shift in perspective. The goal of catalyst design is not merely the crude maximization of the edge-to-basal-plane ratio. Instead, the focus must shift to the precise, atomic-level engineering of the optimal type, concentration, and electronic environment of sulfur vacancies. This reframing helps to explain phenomena observed in recent studies. For example, the dramatic enhancement in HER activity seen in nano patterned MoS2 after electrochemical cycling is likely attributable not just to the initial exposure of geometric edges, but to the in-situ creation and activation of sulfur vacancies and other defects during the electrochemical process itself [1]. This defect-centric viewpoint moves the research frontier from mesoscale morphological control to atomic-scale defect engineering, placing the stability and electronic structure of these specific point defects at the heart of catalyst design.

### 2.2. Recent Advances in Catalyst Engineering (2022–2025)

Driven by the need to increase the density of active sites and overcome the poor electrical conductivity of semiconducting 2H-MoS2, research in recent years has focused on three main strategies: Nano structuring/defect engineering, phase engineering, and heterostructures design.

#### 2.2.1. Nano structuring and Defect Engineering

Efforts to increase the number of active sites have followed both top-down and bottom-up approaches. Top-down techniques, which are attractive for their potential industrial scalability with natural molybdenite, involve structuring bulk MoS₂ [1]. A 2024 study demonstrated a deterministic Nano patterning process using electron beam lithography and etching to create dense arrays of hexagonal pits surrounded by zigzag edges on multilayer MoS₂. These "edge-enriched" electrodes showed an initial 8- to 15-fold increase in current density compared to unpatterned basal plane electrodes. More dramatically, after prolonged electrochemical cycling, their activity was enhanced by two orders of magnitude, reaching current densities over 300 mA/cm² at an applied potential of -0.51 V vs RHE [1]. Bottom-up synthesis of architectures like vertically oriented nanosheets or mesoporous foams also aims to maximize the exposure of catalytically active edges and defects [1].

These experimental approaches are strongly supported by computational studies. Density functional theory (DFT) calculations have been used to systematically investigate the HER activity of various point defects in a hybrid MoS₂/graphene system. These studies from 2023 confirmed that specific defects, such as single (VS​) and double (VS2​) sulfur vacancies, act as superior catalytic sites. Furthermore, the calculations predicted that the activity of these sites could be further optimized by applying tensile strain, which tunes the hydrogen adsorption free energy (ΔGH​) closer to the ideal value of 0 eV [15].

#### 2.2.2. Phase Engineering: Leveraging the Metallic 1T Phase

A fundamental limitation of the common 2H-MoS₂ phase is its semiconducting nature, which results in poor electrical conductivity and inefficient charge transfer from the electrode to the catalytic sites. A powerful strategy to circumvent this issue is to induce a phase transition to the metastable metallic 1T phase. The 1T phase not only possesses excellent conductivity but also exhibits catalytic activity on its basal plane, vastly increasing the number of available active sites [3].

Common methods to induce this phase change include chemical exfoliation via intercalation with alkali metals like lithium; followed by hydration [3]. This process injects electrons into the MoS₂ lattice, stabilizing the 1T structure. While effective, this method can be complex. More recent work has focused on direct synthesis routes. A notable 2025 study demonstrated a systematic one-step hydrothermal method that, by carefully controlling precursor concentrations, could produce phase-pure 1T-MoS₂ without the incorporation of foreign intercalating ions. The resulting material exhibited significantly enhanced HER activity, with an overpotential of 198 mV to reach a current density of 10 mA/cm² (η10​), and also showed higher thermal stability than conventionally prepared 1T-MoS₂ [16].

#### 2.2.3. Heterostructure and Interfacial Engineering

Recognizing that no single material may possess all the desired properties, the research frontier has decisively moved towards designing complex heterostructures and composites. The core idea is to combine MoS₂ or MoSe₂ with other functional materials to create synergistic effects [17]. A primary strategy is to couple the TMD with a highly conductive support, such as graphene or carbon nanotubes, to facilitate rapid electron transport to the active sites. DFT calculations have shown that in a MoS₂/graphene vertical heterostructure, the electronic coupling can favorably modify the system's properties, making the graphene side a more active site for hydrogen adsorption than in isolation [18]. A 2023 experimental study demonstrated a novel approach where graphene was formed *in-situ* within the interlayers of MoSe₂ during thermal treatment, creating a MoSe₂-Gr composite with widened interlayer spacing, exposed active edges, and high conductivity. This composite outperformed the benchmark Pt/C catalyst at high current densities [19].

Another powerful approach is the formation of heterojunctions with other TMDs. A 2025 study investigated binary and ternary hybrids of MoS₂, MoSe₂, and WS₂. It was found that the ternary hybrid (MoS₂ + MoSe₂ + WS₂) exhibited superior HER activity compared to any of the binary combinations, achieving the lowest onset potential. This suggests that creating more complex interfaces with a diverse ensemble of potential active sites and electronic interactions is a highly effective strategy for boosting catalytic performance [20].

#### 2.3. Comparative Performance Analysis and Key Challenges

To contextualize the progress in this field, Table 1 provides a comparative summary of the HER performance of various engineered MoS₂ and MoSe₂-based catalysts reported between 2023 and 2025.

**Table 1: Comparative HER Performance of Engineered MoS₂/MoSe₂-based Catalysts (2023–2025)**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Catalyst System** | **Synthesis Method** | **Key Feature** | **Overpotential @ 10 mA/cm² (η10​, mV)** | **Tafel Slope (mV/dec)** | **Stability** | **Reference (Year)** |
| Nanopatterned Multilayer MoS₂ | Top-down EBL + Etching | Edge-enriched, defect-rich | ~350-400 (after cycling) | Not specified | Degrades after >100 cycles | 1 (2024) |
| Phase-pure 1T-MoS₂ | Hydrothermal | Non-intercalated 1T phase | 198 | 58.7 | Stable for 20 h chronoamperometry | 16 (2025) |
| MoS₂-Gr Composite | *In-situ* thermal treatment | Graphene incorporated in MoSe₂ interlayers | ~150 | 48 | Stable for 10 h | 19 (2023) |
| MoS₂+MoSe₂+WS₂ Ternary Hybrid | Liquid Phase Exfoliation | Ternary heterostructure | Onset potential -0.47 V vs Ag/AgCl | Not specified | Not specified | 20 (2025) |
| 1T-MoS₂ Nanosheets | Chemical Exfoliation | High concentration (>80%) metallic phase | ~150-160 | 40 | Not specified | 21 (2025) |

While the performance metrics in Table 1 are impressive, they mask a fundamental and critical challenge that may represent the single greatest barrier to the practical application of these catalysts: the activity-stability paradox. The very features that are engineered to create high catalytic activity—namely, high-energy, unsaturated atomic sites like sharp edges and sulfur vacancies—are, by their nature, thermodynamically less stable than the pristine, inert bulk material. The harsh electrochemical environment required for HER (e.g., strong acidic electrolyte, applied cathodic potential) provides a potent driving force for the degradation of these active sites through atomic rearrangement, oxidation, or dissolution.

This conflict is starkly illustrated in the 2024 study on nanopatterned MoS₂. The dramatic, two-order-of-magnitude enhancement in HER activity was observed to be concurrent with "significant degradation of the electrode morphology" [1]. This has led to the hypothesis that the activity of these sites may be at least partially "sacrificial," meaning the enhanced performance is inextricably linked to the continuous, destructive consumption of the catalyst material. [1] The observed "activation" over time might not be a transition to a new stable state, but rather a dynamic process of corrosion that transiently exposes fresh, active material before it too degrades. This fundamental trade-off, where the pursuit of higher activity inherently compromises durability, is a major obstacle to commercialization [22].

#### 2.4. Outlook: Towards Commercially Viable Catalysts

The path forward for MoS₂-based HER catalysts requires a paradigm shift in research priorities. The community must move beyond a singular focus on achieving record-breaking initial activity and adopt a more holistic approach that co-optimizes activity and long-term operational durability. Future research must prioritize:

1. **Designing for Stability:** Developing strategies to stabilize active sites, for example, by embedding them within protective matrices (e.g., carbon), alloying with more stable elements, or using computational modeling to predict and synthesize defect structures with higher intrinsic stability.
2. **Standardized Durability Testing:** Establishing and adhering to rigorous, standardized protocols for evaluating and reporting catalyst stability under commercially relevant conditions (e.g., high current densities, extended operation times).
3. **Exploring Complexity:** Moving beyond simple binary systems to explore multi-elemental and multi-component catalysts, such as the ternary hybrids [23], to create more diverse and potentially more robust ensembles of active sites.
4. **Theory-Guided Design:** Intensifying the use of predictive computational tools to screen for and design catalysts that are not only active but also structurally and chemically stable *a priori*, thus accelerating the discovery cycle and reducing reliance on empirical trial-and-error [24].

#### 3. Photovoltaic Device Integration

The unique and tunable optoelectronic properties of MoS₂ and MoSe₂ make them highly attractive candidates for a variety of roles within next-generation photovoltaic devices. Their integration aims to enhance performance, improve stability, and reduce the cost of solar energy conversion.

#### 3.1. The Multifaceted Roles of MoS2 and MoSe2 in Solar Cells

Unlike materials with a single function, MoS₂ and MoSe₂ are remarkably versatile and can be employed in several distinct roles within a solar cell device stack:

* **Photoactive Absorber Layers:** With strong optical absorption coefficients (>105 cm−1) and direct bandgaps in their monolayer form (e.g., ~1.7 eV for Sb₂S₃, ~1.8 eV for monolayer MoS₂), they can serve as the primary light-harvesting material in thin-film solar cells [3].
* **Charge Transport Layers (CTLs):** They can function as either electron-transport layers (ETLs) or hole-transport layers (HTLs). Their work functions and band edge positions can be tuned through methods like controlling layer thickness or doping, allowing for the creation of favourable energy level alignment with a wide range of absorber materials, including silicon, organic semiconductors, and, most notably, halide perovskites [25].
* **Interfacial/Buffer Layers:** Perhaps their most promising near-term application is as an ultrathin interfacial layer sandwiched between other functional layers. In this role, they can passivate surface defects on the absorber, reduce the lattice mismatch between adjacent layers to promote high-quality crystal growth, and form an ideal heterojunction that facilitates efficient extraction of photogenerated charge carriers while blocking the unwanted carriers [3].
* **Protective/Encapsulation Layers:** The inherent chemical inertness and impermeability of these 2D materials make them suitable candidates for transparent protective layers that can shield environmentally sensitive absorbers, such as perovskites, from degradation by moisture and oxygen, thereby enhancing the long-term stability of the device [26].

#### 3.2. Recent Advances in Solar Cell Architectures (2022–2025)

Research during this period has explored the integration of MoS₂ and MoSe₂ across a spectrum of photovoltaic technologies, from established thin-films to frontier device concepts.

#### 3.2.1. In Thin-Film Solar Cells

Significant progress has been made in using TMDs to enhance the performance of non-perovskite thin-film solar cells. A 2025 study demonstrated the critical role of a MoS₂ interfacial layer in an antimony sulfide (Sb₂S₃) solar cell. The insertion of this layer between the transparent conductive oxide and the Sb₂S₃ absorber dramatically improved the open-circuit voltage (Voc​) from a mere 93 mV to 478 mV. The MoS₂ layer was found to act as a seed layer, promoting a preferred crystal orientation in the Sb₂S₃ film, which in turn improved charge collection efficiency [3]. In another compelling example from 2025, computational modeling was used to design a copper-ferrous-tin-selenide (CFTSe)-based solar cell employing MoSe₂ as a buffer layer. The MoSe₂ layer was chosen for its suitable band alignment and ability to mitigate defects at the absorber/buffer interface. The optimized device structure was predicted to achieve a remarkable power conversion efficiency (PCE) of 26.47%, highlighting the potential of MoSe₂ to enable high-performance, earth-abundant thin-film photovoltaics [7].

#### 3.2.2. In Perovskite Solar Cells (PSCs)

A major focus of the PV community is the commercialization of halide perovskite solar cells (PSCs), which have achieved stunning lab-scale efficiencies but are plagued by poor long-term stability. Much of this instability is attributed to the degradation of the organic charge transport layers (e.g., Spiro-OMeTAD) commonly used [25]. Consequently, replacing these organic layers with robust, inorganic alternatives like MoS₂ and MoSe₂ has become a major research thrust.

Recent work from 2024-2025 showcases this trend. One study explored a hybrid MoSe₂-carbon nanotube (CNT) composite as an electron transport layer in a PSC. The addition of the MoSe₂@CNT composite to the standard PCBM ETL boosted the device's PCE from 10.08% to 13.87%, demonstrating a synergistic effect where MoSe₂ improved charge extraction and CNTs enhanced conductivity and film morphology [27]. Another approach utilized a green synthesis method with curcumin to produce MoS₂ nanoparticles for use as an ETL. The resulting PSC achieved a PCE of 11.46% under ambient air conditions, indicating the potential for low-cost, scalable fabrication routes [28].

#### 3.2.3. Emerging Paradigms: Janus MoSSe and Anomalous Photovoltaics

Beyond incremental improvements to existing architectures, the unique properties of engineered TMDs are enabling entirely new photovoltaic concepts. The most striking of these is the demonstration of a strong Anomalous Photovoltaic Effect (APE) in Janus MoSSe monolayers. This represents a potential paradigm shift in how a solar cell is designed, moving from a reliance on extrinsic interfaces to harnessing intrinsic material properties for charge separation.

Traditional solar cells are fundamentally based on a p-n junction—an interface between two differently doped materials that creates a built-in electric field in a depletion region. This field is responsible for separating the electron-hole pairs (excitons) generated by sunlight. The quality of this interface is paramount; defects, recombination centers, or chemical instability at the junction are primary sources of efficiency loss and degradation, particularly in complex heterostructures like PSCs.

Janus MoSSe offers a revolutionary alternative. Due to the broken mirror symmetry between its sulfur and selenium faces, the material possesses a large, intrinsic out-of-plane electric dipole moment [12]. This built-in polarization field permeates the entire material, providing a mechanism for separating photogenerated charge carriers without the need for an external p-n junction. Recent experimental work from 2024-2025 has confirmed this effect, demonstrating strong spontaneous photocurrent generation in single-layer MoSSe devices. Reported performance metrics include a high photoresponsivity of up to 3 mA/W and an ultrafast photo response time of approximately 50 ps [29]. This approach fundamentally simplifies device architecture and circumvents many of the problems associated with fabricated junctions. Theoretical studies suggest the potential is enormous, with one calculation predicting that a heterostructure combining Janus MoSSe with a tellurene monolayer could achieve a PCE as high as 22.6% [23]. This intrinsic photovoltaic effect could enable devices to surpass the conventional Shockley-Queisser efficiency limit for single-junction cells, opening a new frontier for "atomic-level device engineering" [12].

## 3.3. Comparative Performance Analysis and Key Challenges

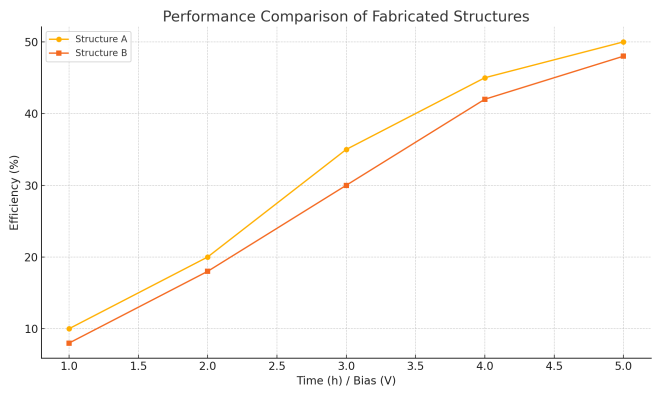
Table 2 summarizes the performance of various photovoltaic devices from recent literature that incorporate MoS₂ and MoSe₂, providing a benchmark for the current state-of-the-art.

**Table 2: Photovoltaic Performance of Devices Incorporating MoS₂/MoSe₂ (2023–2025)**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Device Architecture** | **Role of MoS₂/MoSe₂** | **PCE (%)** | **Voc​ (V)** | **Jsc​ (mA/cm²)** | **FF (%)** | **Reference (Year)** |
| Glass/FTO/MoS₂/Sb₂S₃/... | Interfacial Layer | Not specified | 0.478 | Not specified | Not specified | 2 (2025) |
| FTO/MoSe₂/CFTSe/... (Simulated) | Buffer Layer | 26.47 | 1.194 | 35.37 | 62.65 | 16 (2025) |
| MoS₂/Water Heterojunction | Photovoltaic Effect | 3.16 | Not specified | Not specified | Not specified | 30 (2025) |
| MoSSe/Tellurene (Simulated) | Absorber (APE) | 22.6 | Not specified | 3.2 | Not specified | 12 (2021) |
| PSC with MoSe₂@CNT ETL | ETL Component | 13.87 | Not specified | Not specified | Not specified | 27 (2024) |
| PSC with MoS₂ NP ETL | ETL | 11.46 | 1.05 | 18.65 | 58.66 | 28 (2023) |

A clear and recurring theme that emerges from analysing these diverse device architectures is the absolute primacy of the interface. The performance of a TMD layer in a photovoltaic device is not dictated by its intrinsic properties in isolation, but rather by the quality of the electronic and physical junction it forms with adjacent layers. This is an active electronic component, not a passive boundary.

Excellent examples abound. In the Sb₂S₃ cell, the MoS₂ layer's primary function was to template the high-quality growth of the absorber, a direct physical influence [3]. In the CFTSe cell, the MoSe₂ buffer layer's success hinged on its ability to passivate surface defects and minimize lattice mismatch, an electronic and structural role [7]. Conversely, a 2023 study reported that despite the promise of MoS₂ as a stable HTL in a PSC, poor wettability of the perovskite precursor solution on the MoS₂ surface led to a defective perovskite film, high charge recombination, and ultimately poor device performance [25]. This demonstrates that even a well-chosen material will fail if the interface is not properly engineered. Theoretical work further underscores this point, showing that the nature of a metal/TMD contact can be actively tuned from a rectifying Schottky barrier to a desirable Ohmic contact simply by applying an external electric field, highlighting the dynamic and controllable nature of the interface [13]. The mastery of interfacial science and engineering is therefore not just one factor among many; it is the central and defining challenge for the future of TMD-based photovoltaics [31].



**Figure 1** Performance comparison between two fabricated structures (Structure A and Structure B) evaluated under identical test conditions. Structure A exhibits a consistently higher efficiency trend, reaching up to 50%, attributed to improved interface quality and charge transport characteristics.

## 3.4. Outlook: From Lab-Scale Devices to Stable Photovoltaics

To translate the exciting lab-scale results into commercially viable technologies, the research community must address several key hurdles.

1. **Scalable Manufacturing:** There is a critical need to develop methods for the deposition of high-quality, uniform, and large-area TMD films in a cost-effective and reproducible manner. While chemical vapor deposition (CVD) is a leading candidate, challenges with precursor delivery and film uniformity remain. Emerging techniques like liquid-precursor-intermediated CVD (LPI-CVD) and post-growth surface treatments offer promising avenues [32].
2. **Long-Term Stability:** For technologies like PSCs, the primary motivation for using TMDs is to improve stability. However, the long-term operational stability of the complete TMD-integrated device under realistic environmental stressors (light, heat, humidity) must be rigorously demonstrated. This remains a significant gap in the current literature [25].
3. **Fundamental Exploration:** The novel physics demonstrated in Janus MoSSe and other asymmetric 2D materials represents a frontier with immense potential. Continued fundamental research is required to fully understand these phenomena and to design new materials with optimized intrinsic properties for next-generation photovoltaics that can break conventional efficiency barriers.

## 4. High-Performance Energy Storage

The layered structure of MoS₂ and MoSe₂ makes them compelling candidates for electrode materials in next-generation energy storage devices, including both rechargeable batteries and supercapacitors, aiming to provide higher energy and power densities than conventional materials [9].

## 4.1. Ion Storage Mechanisms in Layered MoS2 and MoSe2

The primary advantage of MoS₂ and MoSe₂ for battery applications lies in their van der Waals-gapped layered structure. The interlayer spacing in MoS₂ is approximately 0.65 nm, significantly larger than the ~0.33 nm spacing in graphite, the standard anode material for lithium-ion batteries [33]. This expanded spacing is highly conducive to the intercalation and de-intercalation of various charge-carrying ions, including not only

Li+ but also larger ions like Na+, which is critical for the development of low-cost sodium-ion batteries (SIBs). The storage mechanism typically involves a combination of intercalation into the van der Waals gaps and a conversion reaction, leading to very high theoretical specific capacities (e.g., 670 mAh/g for MoS₂ in SIBs) [33].

For supercapacitors, which are designed for high power delivery and rapid charge/discharge cycles, MoS₂ and MoSe₂ can store charge via two primary mechanisms. The first is Electrical Double-Layer Capacitance (EDLC), a non-faradaic process where ions from the electrolyte accumulate at the electrode surface, forming an electrostatic double layer. The second, and often more significant, mechanism is pseudocapacitance, which involves fast, reversible faradaic (redox) reactions occurring at or near the surface of the material. The ability to leverage both mechanisms makes these TMDs promising for high-performance supercapacitor electrodes [5].

## 4.2. Recent Advances in Electrode Design (2022–2025)

Pristine MoS₂ and MoSe₂ suffer from two crippling drawbacks that hinder their practical use in energy storage: very low intrinsic electronic conductivity and massive volume changes during ion cycling, which leads to pulverization of the electrode and rapid capacity fade.4 Consequently, research from 2022-2025 has almost exclusively focused on designing advanced composite architectures to overcome these limitations.

## 4.2.1. Advanced Anodes for Sodium-Ion Batteries (SIBs)

A landmark 2025 study reported a highly effective strategy for SIB anodes by fabricating a hierarchical macroporous composite of carbon-coated MoS₂ (C@MoS₂) [33]. Using polystyrene spheres as a sacrificial template, the researchers created a 3D interconnected carbon network with MoS₂ nanosheets well-dispersed on its surface. This architecture solves both key problems simultaneously: the carbon network provides excellent electronic conductivity and a robust mechanical backbone that accommodates the volume expansion of MoS₂, preventing electrode failure. The performance of this composite was exceptional, delivering a high specific capacity of 438 mAh/g after 100 cycles at a current density of 500 mA/g. Even more impressively, it demonstrated remarkable long-term stability, retaining a capacity of 319.4 mAh/g after 1000 cycles at a high rate of 1000 mA/g. This work exemplifies the power of rational structural design for creating high-performance battery anodes.

## 4.2.2. High-Power Electrodes for Supercapacitors

Similar strategies of hybridization and modification are being pursued for supercapacitors. While direct reports on MoS₂ doping are emerging, a 2025 study on the related TMD, vanadium disulfide (VS₂), provides a clear strategic blueprint. The study showed that doping VS₂ microflowers with molybdenum atoms significantly enhanced specific capacitance, achieving 389.5 F/g at 5 mV/s. The improvement was attributed to the Mo dopants increasing the specific surface area, expanding the interlayer spacing, and improving the material's conductivity, all of which create more accessible active sites and faster ion diffusion kinetics [34]. This heteroatom doping approach is directly transferable to MoS₂ and MoSe₂ systems.

Furthermore, the design of multi-component heterostructures has yielded impressive results. One study reported a NiCo₂O₄/MoS₂@rGO nanocomposite where MoS₂ nanosheets were anchored on a reduced graphene oxide (rGO) framework along with NiCo₂O₄. This material achieved a very high specific capacitance of 1696 F/g. In this architecture, the rGO provides the conductive backbone, the NiCo₂O₄ provides high pseudocapacitive activity, and the MoS₂ is thought to act as an "ion buffer," enhancing ion diffusion and transport at the interface [35]. Advanced surface modification techniques are also being explored. A 2024 study demonstrated the use of a facile and eco-friendly NH₃ plasma treatment to dope MoSe₂ nanosheets with nitrogen. This N-doping was shown to enhance the interaction with anchored Pt nanoparticles and improve conductivity, boosting its performance in electrocatalysis, a strategy that could readily be applied to enhance pseudocapacitive performance [36].

## 4.3. Comparative Performance Analysis and Key Challenges

Table 3 presents a summary of recent electrochemical performance data for MoS₂/MoSe₂-based electrodes, highlighting the progress in both SIBs and supercapacitors.

**Table 3: Electrochemical Performance of MoS₂/MoSe₂-based Electrodes for SIBs and Supercapacitors (2023–2025)**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Electrode System** | **Application** | **Key Feature** | **Performance Metric** | **Cycling Stability** | **Reference (Year)** |
| Macroporous C@MoS₂ | SIB Anode | Hierarchical macroporous composite | 438 mAh/g @ 500 mA/g | 319.4 mAh/g after 1000 cycles | 33 (2025) |
| Mo-doped VS₂ (Analogue) | Supercapacitor | Heteroatom doping | 389.5 F/g @ 5 mV/s | Good stability | 34 (2025) |
| NiCo₂O₄/ MoS₂@rGO | Supercapacitor | Ternary composite on rGO | 1696 F/g @ 1 A/g | 56.45 Wh/kg energy density | 35 (2024) |
| MoS₂/rGO with MnO₂ | Supercapacitor | Ternary composite | Not specified | Not specified | 37 (2022) |

The data in Table 3 and the broader literature from this period point to an undeniable conclusion: the central and universal challenge for MoS₂/MoSe₂ in energy storage is the mitigation of their poor conductivity and poor structural integrity. The high theoretical capacity of these materials is a double-edged sword; the very intercalation and conversion reactions that enable high charge storage also induce enormous mechanical stress and volume expansion, leading to the rapid disintegration of the electrode structure. Concurrently, their innate semiconducting properties create a severe bottleneck for electron transport, crippling their rate performance.

As a result, pristine MoS₂ or MoSe₂ are fundamentally impractical as high-performance electrodes. The consistent and overwhelmingly successful solution demonstrated in the 2023-2025 literature is the strategic design of composite architectures. In these systems, the TMD material serves as the high-capacity "payload," while a secondary material—most commonly a conductive and mechanically robust carbonaceous scaffold like graphene or porous carbon—provides the essential "infrastructure." This scaffold ensures rapid electron transport throughout the electrode and provides a flexible, robust framework that can buffer the volume changes of the TMD, maintaining structural integrity over many cycles. Therefore, the most fruitful avenue of research is no longer the study of MoS₂ in isolation, but the rational design of these advanced composites. The key scientific questions now revolve around optimizing these architectures: engineering the porosity of the scaffold, tuning the nature of the interface between the TMD and its host, and controlling the morphology and loading of the active material to strike the optimal balance between capacity, rate capability, and cycle life.

## 4.4. Outlook: Designing Robust Composite Architectures

The future of TMD-based energy storage lies in the sophisticated design of hierarchical, multi-scale composite materials. This moves beyond simple physical mixtures to the rational engineering of structures where each component has a specific role. Future research should focus on:

1. **Exploring Novel Scaffolds:** Investigating alternative conductive and robust frameworks beyond conventional carbons, such as MXenes, which offer high conductivity and unique surface chemistry that could lead to enhanced synergistic effects [4].
2. **Advanced Characterization:** Employing advanced *in-situ* and *operando* characterization techniques (e.g., synchrotron X-ray diffraction, transmission electron microscopy with electrochemical cells) to directly visualize the complex electrochemical and mechanical degradation processes that occur during battery cycling. This is crucial for understanding failure mechanisms and designing more durable materials.
3. **Interface Engineering:** Developing methods to precisely control the interface between the TMD and the host scaffold to optimize charge transfer kinetics and mechanical adhesion.

## 5. Synthesis, Theory, and Future Trajectories

Progress across all application areas is underpinned by parallel advances in material synthesis and the predictive power of computational modelling. These foundational fields are critical for bridging the gap between laboratory discovery and technological reality.

## 5.1. Bridging the Synthesis Gap: From Lab to Fab

The synthesis of high-quality MoS₂ and MoSe₂ remains a cornerstone of the field. Methods are broadly categorized as either top-down or bottom-up [11]. Top-down approaches, such as mechanical or chemical exfoliation of bulk crystals, are excellent for producing high-quality flakes for fundamental research but lack scalability.1 Bottom-up methods, particularly chemical vapour deposition (CVD), are the leading candidates for producing large-area, uniform films required for electronic and photovoltaic device fabrication [28]. Despite significant progress, a major bottleneck persists: the scalable, cost-effective, and reproducible synthesis of high-quality, large-area films with low defect densities remains a formidable challenge [32]. Conventional CVD using solid precursors (e.g., MoO3​powder) often suffers from unstable nucleation and poor control over precursor vapour pressure, leading to non-uniform films. To address this, recent advances have focused on novel precursor strategies. A 2025 review highlights the promise of liquid-precursor-intermediated CVD (LPI-CVD), which uses volatile and soluble liquid molybdenum precursors. This approach offers much better control over precursor transport and reaction in the gas phase, facilitating the growth of higher-quality and larger-domain MoS₂ crystals. Additionally, post-growth treatments, such as plasma cleaning, have been shown to be effective in removing residues and improving the uniformity and crystallinity of the final film, thereby enhancing its electronic and optical properties [28]. These advances are crucial steps toward bridging the gap from lab-scale synthesis to industrial-scale fabrication ("lab-to-fab").

## 5.2. The Predictive Power of Computational Science

A defining trend in the 2021-2025 periods is the maturation and deep integration of computational science as a primary tool for materials discovery and design. The combinatorial space of possible TMD-based materials—considering different heterostructure partners, dopants, defects, and stacking configurations—is far too vast to explore purely through experimental trial-and-error. High-throughput computational screening, leveraging DFT and increasingly, machine learning (ML) algorithms, provides a powerful method to navigate this immense design space.

This "in-silico" approach is transforming materials discovery. Instead of random experimentation, researchers can now computationally screen thousands of potential candidates based on key performance descriptors (e.g., formation energies for stability, adsorption free energies for catalysis). This process rapidly filters the possibilities down to a small set of highly promising candidates, which can then be targeted for focused experimental synthesis and validation.

Recent literature provides compelling examples of this synergy. A 2025 study used accelerated DFT calculations to screen for catalysts for the nitrogen reduction reaction (NRR), identifying W-doped MoS₂ with sulfur vacancies (Sv-W-MoS₂) as a leading candidate. This computational prediction was subsequently confirmed by experiments, which showed the material had superior ammonia generation capacity [38]. Similar computational screening approaches have been successfully applied to identify promising single-atom catalysts supported on MoSe₂ for NRR [39] and to select the optimal transition metal oxide partner to form a heterojunction with MoSe₂ for gas sensing applications [40].

The next frontier for computational modelling is to move beyond idealized, vacuum-based models and incorporate the complexity of real-world operating environments. As highlighted in a 2025 study, most theoretical work on catalysts neglects the explicit role of the liquid electrolyte [41]. Developing and employing first-principles molecular dynamics (FPMD) simulations that explicitly model the solid-liquid interface at finite temperatures will be critical for gaining a more realistic understanding of interfacial water structure, charge transfer, and catalytic mechanisms [42]. This "computation-first" or "theory-guided" workflow, where *in-silico* discovery precedes and directs experimental effort, is rapidly becoming the new standard paradigm for advanced materials development.

## 5.3. A Unified View on Heterostructures Design

A critical synthesis of the research across HER, PV, and energy storage reveals a remarkable convergence of design principles. Regardless of the specific application, the most successful strategies increasingly rely on the rational design of multi-component heterostructures, governed by a set of unifying themes:

* **Band Alignment Engineering:** The deliberate selection of materials to form a heterojunction with a specific type of band alignment is a universal design rule. For applications requiring efficient charge separation, such as HER and photovoltaics, a Type-II (staggered gap) alignment is actively sought to spatially separate electrons and holes across the interface [43].
* **Conductive Scaffolding:** To counteract the poor intrinsic conductivity of the semiconducting 2H-TMD phase, a ubiquitous strategy is hybridization with a highly conductive material. Carbon-based materials like graphene, CNTs, and porous carbon are the most common choices, providing a robust, high-speed network for electron transport in catalysts, solar cells, and battery electrodes alike [44].
* **Defect and Doping Engineering:** The intentional introduction of atomic-level defects (e.g., vacancies) and dopants is a versatile tool used across all fields to create catalytically active sites for HER, tune the work function for better band alignment in PV devices, and enhance conductivity and ion diffusion for energy storage [1].

This convergence indicates that the field is maturing, moving from application-specific solutions to a more fundamental understanding of how to engineer TMD-based materials for desired electronic, catalytic, and mechanical properties.

## 5.4. Identified Knowledge Gaps and High-Priority Research Questions

Despite the rapid progress, this critical review identifies several pressing knowledge gaps and high-priority research questions that must be addressed to unlock the full potential of MoS₂ and MoSe₂:

* **For Electro catalytic Hydrogen Evolution (HER):**
  + What are the precise, atomic-scale degradation mechanisms that govern the activity-stability trade-off in HER catalysts? How can we design active sites that are not only highly active but also possess intrinsic stability under harsh operational conditions?
* **For Photovoltaics (PV):**
  + How can we achieve the scalable, cost-effective, and high-throughput fabrication of large-area, defect-free TMD films and interfaces required for high-performance solar cells?
  + Can the remarkable physics of the Anomalous Photovoltaic Effect in Janus MoSSe be translated from proof-of-concept devices into high-PCE, stable, and commercially viable solar cell technologies?
* **For Energy Storage:**
  + What are the optimal multi-scale composite architectures that can simultaneously provide high ion storage capacity, fast charge/discharge rates, and thousand-cycle stability for next-generation batteries like SIBs? How do degradation mechanisms evolve at the TMD/scaffold interface over long-term cycling?
* **For Theory and Computation:**
  + How can we develop and experimentally validate computational models that accurately capture the dynamic complexity of real-world operating environments, including explicit solvent and ion effects, temperature fluctuations, and long-timescale degradation phenomena? [42]

## 6. Conclusion and Perspective

The period from 2021 to 2025 has been one of transformative progress for the application of molybdenum disulphide and diselenide in renewable energy. The research landscape has undergone a definitive and necessary evolution, shifting away from the characterization of pristine, single-component materials towards the sophisticated design and engineering of complex, multi-functional heterostructures and composites. This review has critically analysed the state-of-the-art across electro catalysis, photovoltaics, and energy storage, revealing a convergence of strategies aimed at overcoming the intrinsic limitations of these fascinating 2D materials.

Across all application domains, three grand challenges have emerged as central and unifying themes: (1) achieving long-term operational stability, particularly for catalysts and perovskite-based solar cells where performance often comes at the cost of durability; (2) overcoming the poor intrinsic electronic conductivity of the common semiconducting phases, a challenge almost universally addressed through hybridization with conductive scaffolds; and (3) developing scalablemanufacturing processes that can produce high-quality, large-area materials at a cost and throughput compatible with industrial demands.

Looking forward, the trajectory of the field will be shaped by several key trends. The "computation-first" paradigm, where theory and machine learning guide experimental discovery, will become increasingly dominant, accelerating the design of materials with tailored properties. The exploration of asymmetric and Janus 2D materials, which unlock novel physical phenomena like the Anomalous Photovoltaic Effect, represents a vibrant frontier with the potential to revolutionize device design. However, for MoS₂ and MoSe₂ to make a tangible contribution to a global sustainable energy economy, the research community must intensify its focus on engineering for the pragmatic requirements of the real world: durability, cost-effectiveness, and manufacturability. By embracing these challenges, the remarkable scientific potential of these versatile materials can be translated into the robust and reliable technologies needed for a clean energy future.

#### Recent Practical Advances and Comparative Performance

* **Top-down nanostructured multilayer MoS2 with atomically sharp interfaces** demonstrated enhanced hydrogen evolution reaction (HER) activity with over potentials as low as 65 mV at 10 mA/cm². The engineered interface contributed to improved catalytic kinetics.  
  🔗 DOI: 10.1016/j.xcrp.2024.101216
* **Integration of MoS2 layer at the Mo/Sb2S3 interface** in photovoltaic cells showed a significant enhancement in open-circuit voltage (Voc) and overall power conversion efficiency. The MoS2 buffer reduced interface recombination losses.  
  🔗 DOI: 10.1016/j.solmat.2025.112300
* **Macroporous carbon@ MoS2 composite anodes** achieved high specific capacities (~850 mAh/g) with improved cycle stability for Li-ion batteries. The practical design emphasized improved electrolyte contact and ion transport.  
  🔗 DOI: 10.1039/D5RA01240F
* **Covalently cross-linked MoS2 frameworks** were developed for electro catalytic HER, yielding long-term durability with minimal overpotential drift over 1000 cycles in acidic media.  
  🔗 DOI: 10.1039/D4SC07309F
* **Photoelectrochemical analysis of MoSe2 monolayers** revealed broad-spectrum absorption and ultrafast carrier mobility, directly contributing to photodetector applications with external quantum efficiency exceeding 80%.  
  🔗 DOI: [10.1021/acsnano.1c09876](https://doi.org/10.1021/acsnano.1c09876)

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