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Review

Synergistic hybrid systems of 2D-MOFs and TMDs for advanced energy harvesting

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ABSTRACT

The globally trending move towards renewable energy sources requires materials capable of harvesting, storing, and converting energy in a competent fashion and yet scalable, robust, and affordable. Two-dimensional metal-organic frameworks (2D-MOFs) and transition metal dichalcogenides (TMDs) have been promising materials for photovoltaics, thermoelectrics, piezoelectrics, and triboelectrics, respectively, but both material families are plagued by intrinsic drawbacks. MOFs have high area and chemical tailoring but are hampered by low conductivity, and TMDs have robust electronic and catalytic functionality but are plagued by stability and scalability issues. Recent developments indicate hybrid 2D-MOF/TMD systems are capable of offsetting failings by encapsulating complementary properties, facilitating superior charge separation, band alignment engineering, and enhancement in environmental tolerance. This review critically examines the structural, electronic, and functional synergies of 2D-MOF/TMD hybrids with emphasis on synthesis strategies, interface engineering, defect modulation, and emerging applications in diverse energy harvesting platforms. Comparative analyses of existing studies highlight how hybrid architectures deliver higher power densities, longer cycling stability, and superior device integration relative to their parent materials. Critical issues such as scalable synthesis, long-term stability under operating conditions, and reproducible device-level integration are also mentioned as hurdles in commercialization. Experimental design, computational modeling, and machine learning are envisaged in the future to accelerate discovery and optimization of high-performance hybrids. Bridging the gap between applied engineering and basic research, 2D-MOF/TMD hybrids are a paradigm shift in multifunctional materials and a promising avenue towards next-generation sustainable energy technology.

1. Introduction

The growing global energy demand, in addition to the depletion of non-renewable sources, poses significant challenges in energy production. Resource availability, especially oil, coal, and gas, poses challenges in long-term energy sustainability, while environmental issues like greenhouse gas emissions emphasize the need for cleaner energy production (Chauhan et al., 2025). Additionally, energy security faces a greater threat as a result of geopolitical and economic instability, making it increasingly difficult to achieve a stable supply of energy (Khan et al., 2023). To counteract these challenges, renewable energy generators like solar, wind, and hydropower are gaining importance. These are important sources in lessening the dependence on fossil fuels and combating climate change (Kovalskyi et al., 2024). In this context, energy harvesting technology that harvests ambient energy from sources like solar radiation, wind, and mechanical vibrations are promising solutions in powering low-energy applications like sensors and MEMS (Ali et al., 2025). Even with the promising nature of energy harvesting systems, their efficacy, scalability, and cost-effectiveness are problematic. For instance, mechanical vibration energy harvesting typically produces low power outputs, and it remains difficult to upscore these systems in order to obtain higher power outputs (Mehta et al., 2023). To eliminate these challenges, new materials in the form of two-dimensional metal-organic frameworks (2D-MOFs) and transition metal dichalcogenides (TMDs) have gained potential as solutions. These materials achieve improved efficacy, scalability, and cost-effectiveness in energy

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harvesting systems by increasing charge storage capacity, energy conversion, and systemic workability (Choudhary et al., 2018; Muzaffar et al., 2023). Incorporation of these materials into energy harvesting systems can potentially eliminate existing challenges and lead to more sustainable solutions in energy.

Advanced functional materials, 2D-MOFs and TMDs, are fundamental in addressing the main challenges facing energy harvesting systems through their unique properties and versatility (Roy et al., 2024). 2D-MOFs are characterized by extensive porosity and structural features that are critical in effective charge storage and electrochemical function in energy devices (Muzaffar et al., 2023). These properties enable 2D-MOFs to boost energy storage capacity and power density, making them ideal for supercapacitors and other energy storage devices (Zeggai et al., 2025). TMDs, including MoS_2 and WSe_2, are also known for their high porosity and impressive electronic conductivity, which ensure rapid charge transfer and enhance energy conversion efficiencies in electrochemical devices (Roy et al., 2024). The tunability in 2D-MOFs, as well as potential in altering their conductivity and stability, also broadens their potential applications in energy harvesting systems (Zeggai et al., 2025). Correspondingly, TMDs offer adjustable electronic properties, namely bandgap tunability, which is particularly beneficial in solar cells and light-energy harvesting devices generally (Sivan et al., 2023). 2D-MOF and TMD hybrid systems increase the general performance yet farther. Correspondingly, composites made up of MOF-5 and WSe_2, among others, exhibit exemplary electrochemical properties (Imran et al., 2024). Such materials are scalable in synthesis and are thus useable in large systems at lower costs, thereby offering a pathway towards low-cost and efficient energy harvesting systems (Dong et al., 2026). Engineering the materials as composites and through methods such as doping and intercalation are capable of significantly boosting their catalytic activity and electrochemical properties and are thus serious contestants in future energy harvesting systems (Panchu et al., 2024).

2D-MOFs and TMDs are two promising material classes with different yet complementary structural and electronic properties well-suited for energy harvesting applications. 2D-MOFs are characterized by their high porosity, large specific surface area (SSA), and tunability in structure, which are desirable in ions accommodation and improved electrochemical activity in supercapacitors and other storage devices (Lu et al., 2023). These scaffolds exhibit good thermal stability by virtue of robust metal-ligand coordination and π-conjugation, and their tailorable electronic structures make it possible to design tailored conductivity and catalytic activities necessary for hydrogen and oxygen evolution processes (Li et al., 2022). Unlike 2D-MOFs, TMDs like MoS_2 and WSe_2 have layered geometries with robust in-plane covalent linkage and weak interplanar van der Waals attractions, facilitating exfoliation into atomically thin sheets that are useful in high-efficiency photovoltaics and optoelectronics devices (Farris et al., 2024). Their ultra-thin aspect, in combination with a large fraction of exposed surface atoms, gives rise to increased catalytic active sites and accelerated charge transfer and ionic diffusion, both important in energy storage and conversion processes (Rawat et al., 2018). More, the electronic properties in TMDs are amenable through phase, composition, and defect engineering, and thus there are possible transitions among semiconducting, metallic, and superconducting behaviors depending on application destinies (de Carvalho et al., 2023). Such distinctive characteristics render both 2D-MOFs and TMDs amenable as materials in next-generation energy harvesting platforms, where material design

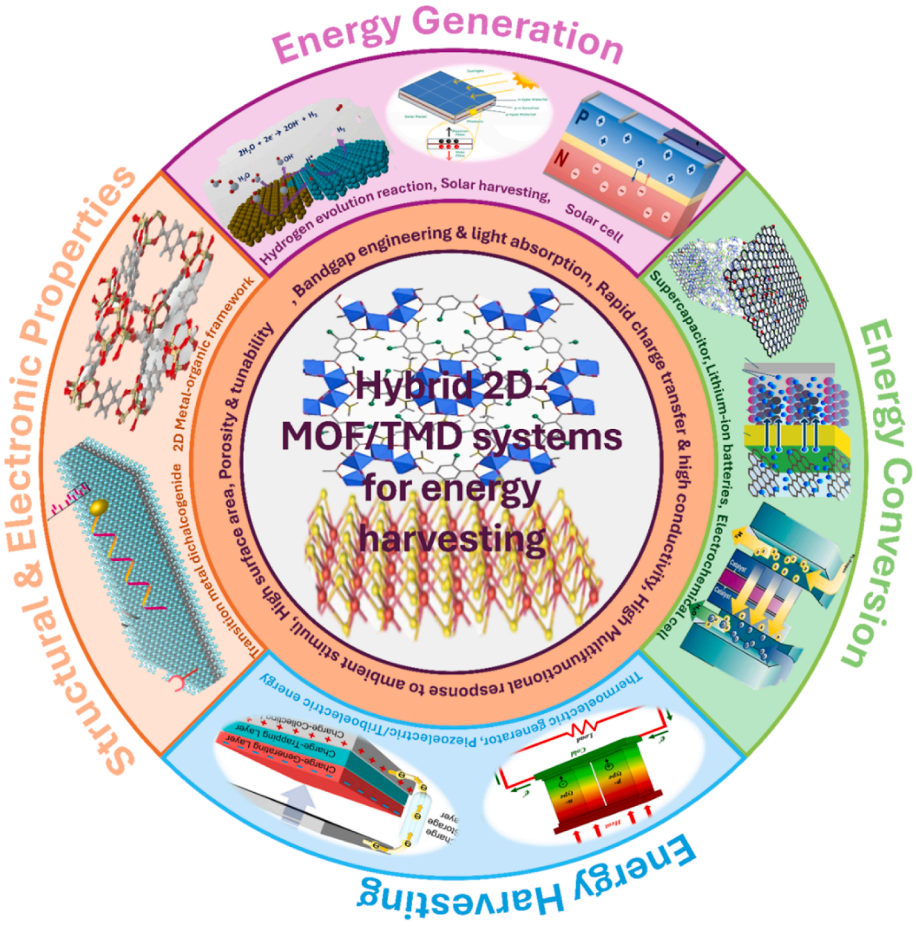


Fig. 1. Schematic diagram of hybrid 2D-MOF/TMD materials emphasizing their architectural attributes (surface area, tunability, layered nature) and multifunctional activity in energy production, interconversion, and harvesting.

specific to certain functional requirements is necessary. Fig. 1 depicts the application scope of materials in energy production, transformation, and storage processes.

The hybridization of 2D-MOFs and TMDs can significantly increase the efficiency of energy harvesting devices by overcoming individual material limitations. The resulting hybrid material benefits from multiple mechanisms that enhance its function, creating complementary effects. First, charge transfer efficiency is improved through the development of heterojunctions between 2D-MOFs and TMDs, facilitating efficient charge separation and minimizing recombination losses, a prerequisite in photocatalytic and electrochemical applications (Hosseini and Safarifard, 2024). Furthermore, bandgap engineering through hybridizing 2D-MOFs and TMDs tailors the electronic characteristics of the hybrid material, ensuring efficient charge transport and obtaining maximum energy conversion efficiency (Yu et al., 2017). Interface engineering, both in structure and chemical composition, additionally enhances the electrochemical and catalytic characteristics, leading to improved energy storage and conversion functions (Roy et al., 2024). The combination of 2D-MOFs extensive porosity and TMDs excellent conductivity and catalytic properties, along with enhanced stability and conductivity, significantly increases energy conversion efficiency, making the hybrid material an ideal candidate for a broad range of energy applications (Ashraf et al., 2026). Furthermore, interactions among 2D-MOFs and TMDs increase long-term stability and cyclic stability in energy harvesting devices, as structural stability in MOFs upholds hybrid material integrity, and efficient charge transport mediated through TMDs guarantees a steady function in a long-term capability (Mohamed et al., 2020).

Previous reviews have highlighted the promise of 2D-MOFs, TMDs, and related hybrids for energy conversion and storage, but their coverage is often separated by material class or restricted to specific device families. As summarized in Table 1, this leaves an unmet need for a dedicated synthesis of 2D-MOF/TMD hybrids for energy harvesting that connects interface design choices to device-level performance, stability, and scalability requirements.

Despite the growing number of reports on hybrid 2D-MOF/TMD systems, key barriers to practical deployment remain insufficiently resolved, including scalable synthesis with controlled thickness and defect density, interfacial reproducibility across batches, and stability under realistic operating stresses (illumination, humidity, bias, and repeated mechanical loading). Prior reviews acknowledge parts of these issues but typically treat material chemistry, synthesis, and device performance in parallel rather than through a unified interface-to-device lens that enables like-for-like comparison and actionable design choices. Accordingly, this review goes beyond recent surveys on MOF-based hybrids and TMD-based energy materials by concentrating on four key contributions:

- Interface mechanisms are explored, linking material properties (heterojunctions, band alignment, and defect engineering) to charge transport and recombination in energy harvesting applications.
- The connection between processing and structure is established, explaining how synthesis methods influence material properties such as thickness, morphology, and defect density.
- Performance metrics are analyzed, with an emphasis on durability and the impact of long-term stability on device efficiency.
- Insights into device integration are provided, highlighting scalability, reproducibility, and stability as critical challenges.

2. Fundamentals of 2D materials

2.1. Overview of 2D materials

The properties of 2D materials, including their extensive porosity, electrical conductivity, and mechanical flexibility, are crucial for their functionality in energy harvesting processes. This increased porosity enhances charge storage in batteries and supercapacitors, light absorption in photovoltaics, and electrochemical activity in catalytic processes. For instance, graphene, with a theoretical SSA of 2630 m^2/g, facilitates rapid ion adsorption and desorption, boosting energy and power densities in supercapacitors (Zhang et al., 2020). MOFs, with surface areas ranging from 4500 to 6000 m^2/g, provide numerous active sites for energy storage and catalysis, making them effective in processes like oxygen evolution reactions (OER) (Holst and Cooper, 2010). TMDs,

Table 1
Comparison of previous reviews on energy harvesting materials and the role of hybrid 2D-MOF/TMD systems.

Author, Ref.	Study Type	Materials	Focus	Key results/findings	Gaps identified
Imran et al. (2024)	Review	2D MOFs/ TMDs	Energy storage devices	High electrical conductivity, wide surface area, effective as anode materials for supercapacitors	Need for further research into composite materials doped with 2D MOFs/TMDs
Chen et al. (2022)	Review	2D MOFs	Scalable synthesis	Overview of synthetic approaches and advances in scalable synthesis	Challenges in scalable synthesis limiting commercialization
Zhao et al. (2020)	Review	2D MOFs	Energy storage and electrocatalysis	Synthetic strategies and application progress in batteries and supercapacitors	Challenges in synthesis and application for future development
Priyadarshini and Parida (2024)	Review	MOFs, COFs	Energy harvesting (PENGs, TENGs)	Structural diversity and optimization for efficient energy conversion	Stability, scalability, and performance improvements needed
Choudhary et al. (2018)	Review	MOFs	Energy harvesting	Structural diversity and optimization for efficient energy conversion	Stability, scalability, and performance improvements needed
Gonçalves et al. (2021)	Review	MOFs	Electrochemical sensors	Potential of MOF-derived structures for sensors	Need for enhanced electrochemical properties
Ashraf et al. (2026)	Research	MOF-5/ WSe_2/g-C_3N_4	Hydrogen evolution reaction (HER)	Superior electrochemical performance with high energy and power densities	Further exploration of composite materials for enhanced catalytic performance
Xu et al. (2023)	Review	MOFs, MXenes	Electrochemical energy storage	Structure and properties of MXenes@MOFs hybrids	Challenges in developing and applying MXenes@MOFs hybrids
Roy et al. (2024)	Review	TMDs	Energy conversion and storage	TMDs offer significant catalytic activity, improving energy conversion efficiency	Need for optimization of TMDs for large-scale energy storage
Present Review	Review	2D-MOFs and TMDs	Hybrid 2D-MOF/TMD systems for energy harvesting	Links interface mechanisms (heterojunctions, band alignment, and defect/phase engineering) to transport and recombination across PV, thermoelectric, piezoelectric, and triboelectric harvesting; relates synthesis/processing to thickness, morphology, and defect control; summarizes platform-specific performance metrics together with durability considerations.	Highlights scalability, reproducibility, and environmental/mechanical stability as key barriers and outlines prioritized directions for device-level integration.

including MoS_2, and MXenes, known for their high porosity and active sites, improve electrochemical activity for energy storage and catalysis (Panda et al., 2021).

The electrical conductivity is another significant parameter, and 2D materials, which include graphene, have exemplary conductivity, ideally well adapted to the application in energy harvesting in supercapacitors and flexible electronics (Fan and Wu, 2019). MoS_2 and the rest of the TMDs are semiconducting and are tunable and thus applicable in thermoelectric and piezoelectric devices (Zhang et al., 2024). Furthermore, the mechanical flexibility in 2D materials drastically increases the functionality in the devices, particularly in devices subjected to mechanical strains, such as, triboelectric or piezoelectric nanogenerators (Khan et al., 2025). The flexibility in $CuInP_2S_6$-based piezoelectric nanogenerators, as an example, enhances the output currents by enhancing the energy conversion efficiency (Zhang et al., 2023). Accordingly, it is pertinent that the most essential properties, namely surface area, conductivity, and flexibility, are tailored in a way as to increase the efficacy and shelf life in 2D material-based energy harvesting systems.

2.2. Two-dimensional metal-organic frameworks (2D-MOFs)

2D-MOFs are a class of materials that have attracted widespread interest due to their distinctive properties and broad potential applications in fields, especially in energy harvesting and storage applications (Zhao et al., 2023). 2D-MOFs are comprised of metal ions or clusters coordinated by organic ligands, presenting a two-dimensional porous material. The architectural design of 2D-MOFs provides large surface areas, adjustable pore sizes, and flexibility in the accommodation of numerous centers of metals, all directly impacting their electrochemical, catalytic, and mechanical properties (Muzaffar et al., 2023; Zeggai et al., 2025). Fig. 2 shows the variable attributes and important features of 2D-MOFs, highlighting their superiority in energy applications.

The most important advantages of 2D-MOFs are their porosity and tunability in the structure, enabling them to find application in various storage applications in energy, e.g., in supercapacitors, batteries, and in storage systems for hydrogen, as well as in catalysis and sensors (Priyadarshini and Parida, 2024). The materials are most efficient in virtue of their capability to offer a large number of active sites, greater accessibility of ions, and higher charge transport abilities. 2D-MOFs can also be designed in a way that they are highly thermally and chemically stable, and that is a fundamental aspect in ensuring long-term functionality in applications in energy storage (Yusuf et al., 2022).

The ability to integrate metal ions from various transformation metals, including copper (Cu), zinc (Zn), and cobalt (Co), into 2D-MOFs allows for the tailoring of their electronic structure, making them promising candidates for electrocatalysis applications such as OER, hydrogen evolution reactions (HER), and supercapacitors (Xing et al., 2023). Their mechanical properties, particularly flexibility, also enhance their functionality in energy harvesting devices subjected to mechanical stresses, such as triboelectric and piezoelectric systems. With their structural flexibility and ability to incorporate diverse metal centers, 2D-MOFs hold great potential for next-generation energy storage and transformation systems, making them valuable contributors to energy harvesting and renewable energy technologies.

2.2.1. Properties and characteristics of 2D-MOFs

2D-MOFs are well known for having high SSA and tunable pore sizes, thus making them highly effective in both catalytic and energy storage applications, which usually in the range 1000-5000 m^2/g and 0.7-2.5 c/g in pore volumes. They can be finely adjusted using synthetical

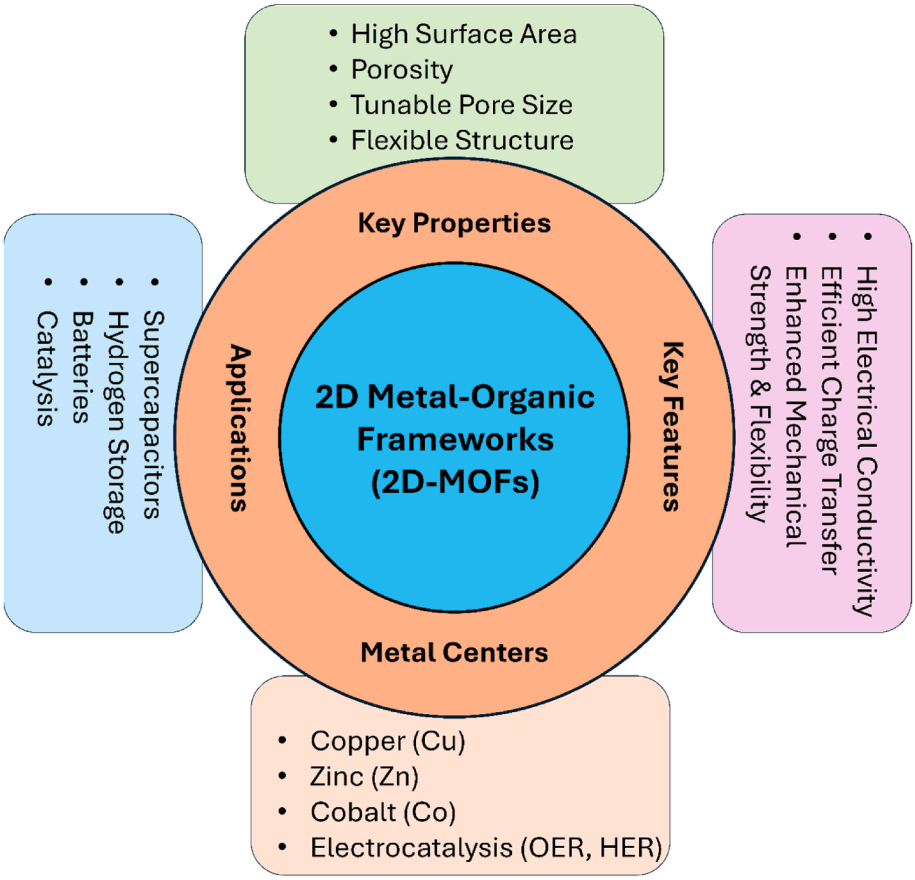


Fig. 2. Overview of the properties, features, and applications of 2D-MOFs, highlighting key advantages in energy storage and catalysis.

conditions in order to maximize their functionality in specific applications, namely energy storage and catalyzing.

The role of pore size, surface area, and performance in energy storage and catalytic application has been established well in literature. High porosity and large surface area in 2D-MOFs contribute towards efficient storage of ions, contributing significantly towards improved supercapacitor and battery performance. As a case in point, Iqbal et al. (2023) demonstrated that a copper-based 2D conductive MOF exhibited a specific capacitance and energy density of 135 c/g and 32 Wh/kg, respectively, highlighting how increased porosity leads to improved energy storage capabilities. As seen in Fig. 3(a), specific capacitance decreases as a function of increasing current density, as tested by cyclic voltammetry and galvanostatic charge-discharge, respectively. Furthermore, Fig. 3(b) shows energy and power density trends in the $Cu_3(HHTP)_2$//AC hybrid supercapattery device, which exhibited 32 Wh/kg and 2100 W/kg, respectively, revealing the superior energy storage ability of the material. Correspondingly, Lee et al. (2024) showed a 2D conductive MOF, $Cu_3(HHTATP)_2$, reached 340 ± 15 F/g at 0.2 A/g specific capacitance and established the relationship between surface area, porosity, and improved capacitance, respectively. The material possessed impressive cycle stability as well and showed 94% retention in its capacitance after 7000 cycles at a 5 A/g density, respectively. As evidenced by Fig. 3(c)–(d), Fig. 3(f), and Fig. 3(g), the corresponding results emphasize the superior electrochemical characteristics and long cycle stability in $Cu_3(HHTATP)_2$ in a supercapacitor application, respectively.

Recent studies have further explored the electrochemical performance of 2D-MOF-based supercapacitors, focusing on specific capacitance, cycling stability, and energy/power density. Zhang et al. (2018) synthesized a two-dimensional Ni-MOF via a solvothermal method, which exhibited a high specific capacitance of 1668.7 F/g at 2 A/g (Fig. 4(a)) and retained 90.3% of its capacitance after 5000 cycles at 5 A/g (Fig. 4(b)). The Ni-MOF//AC hybrid supercapacitor device achieved an energy density of 57.29 Wh/kg at a power density of 160 W/kg, as shown in (Fig. 4(c)). The material's exceptional electrochemical performance is attributed to its favorable pore structure and surface characteristics, confirmed by BET analysis (Fig. 4(d)). Charge-discharge behavior shown in Fig. 4(e) further highlights the stability and efficiency of the material across different current densities, confirming its pseudocapacitive nature. These results underscore the potential of 2D-MOFs for high-performance, long-cycle, and high-energy-density supercapacitors. Similarly, Azadfalah et al. (2019) reported that a Cu-MOF/graphene composite achieved a specific capacitance of 482 F/g at a scan rate of 10 mV/s and demonstrated 93.8% capacitance retention after 1000 cycles at 0.3 A/g. As shown in (Fig. 4(f)), the charge-discharge curves at different current densities reveal the material's excellent electrochemical performance.

Tuning pore size is crucial for optimizing electrochemical behavior. Miao et al. (2022) demonstrated that adjusting the ethanol content in the solvent when modifying Zn-MOF-derived carbon improved its pore hierarchy, rate performance, and electrochemical stability. The optimal material, with a SSA of 1930 m^2/g and an average pore size of 2.9 nm, showed 78.8% capacitance retention from 1 to 100 A/g and 2.2% capacitance loss after 200000 cycles at 50 A/g. The symmetrical capacitor also achieved 16.09 Wh/kg at 698 Wh/kg and 11.89 W h/kg at 41.56 Wh/kg, demonstrating its high performance. Adjusting pore size in 2D-MOFs improves ion transport and electrochemical performance. Zhang et al. (2022) showed that larger pores reduce pore blocking, enhancing ionic conductivity. This is seen in Fig. 5(a), where IL conductivity increases with pore size in UiO MOFs, and in Fig. 5(b), which

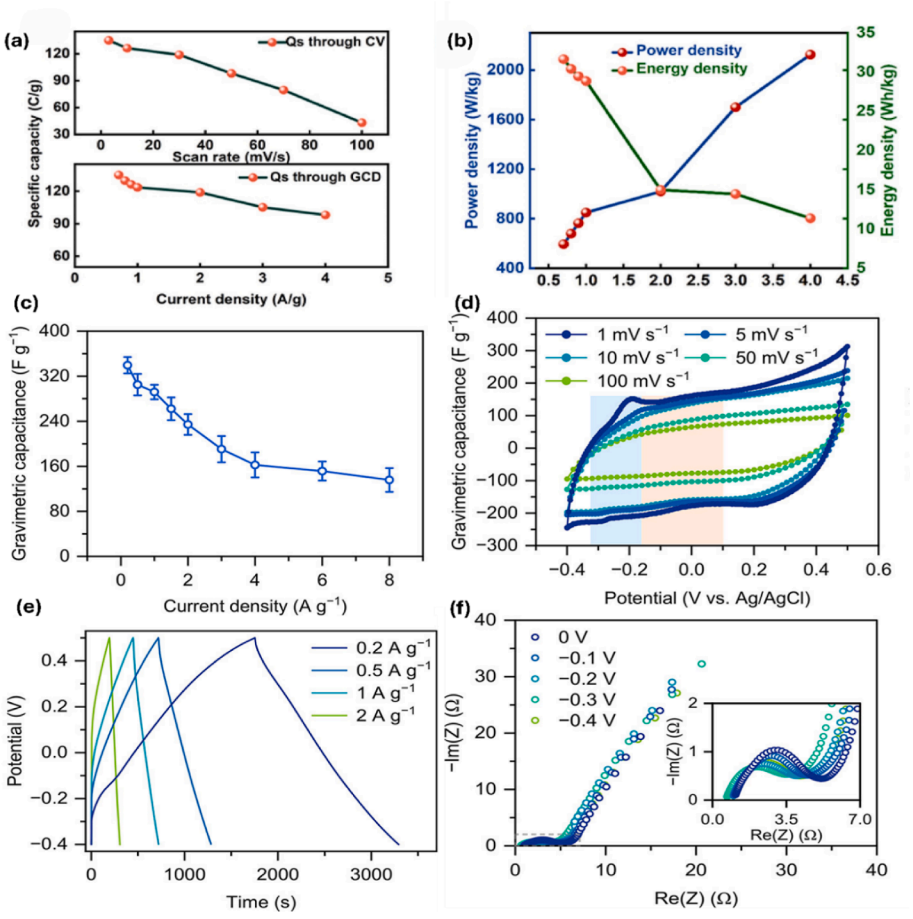


Fig. 3. (a) Specific capacitance vs current density measured through CV and GCD; (b) Energy and power density trends for $Cu_3(HHTP)_2$//AC hybrid supercapattery (Reproduced from Ref. (Iqbal et al., 2023)); (c) Gravimetric capacitance vs current density; (d) Scan rate vs capacitance contributions (PC vs EDL); (e) Galvanostatic charge-discharge curves at different current densities; (f) Galvanostatic charge-discharge curves at different current densities; (Reproduced from Ref. (Lee et al., 2024)).

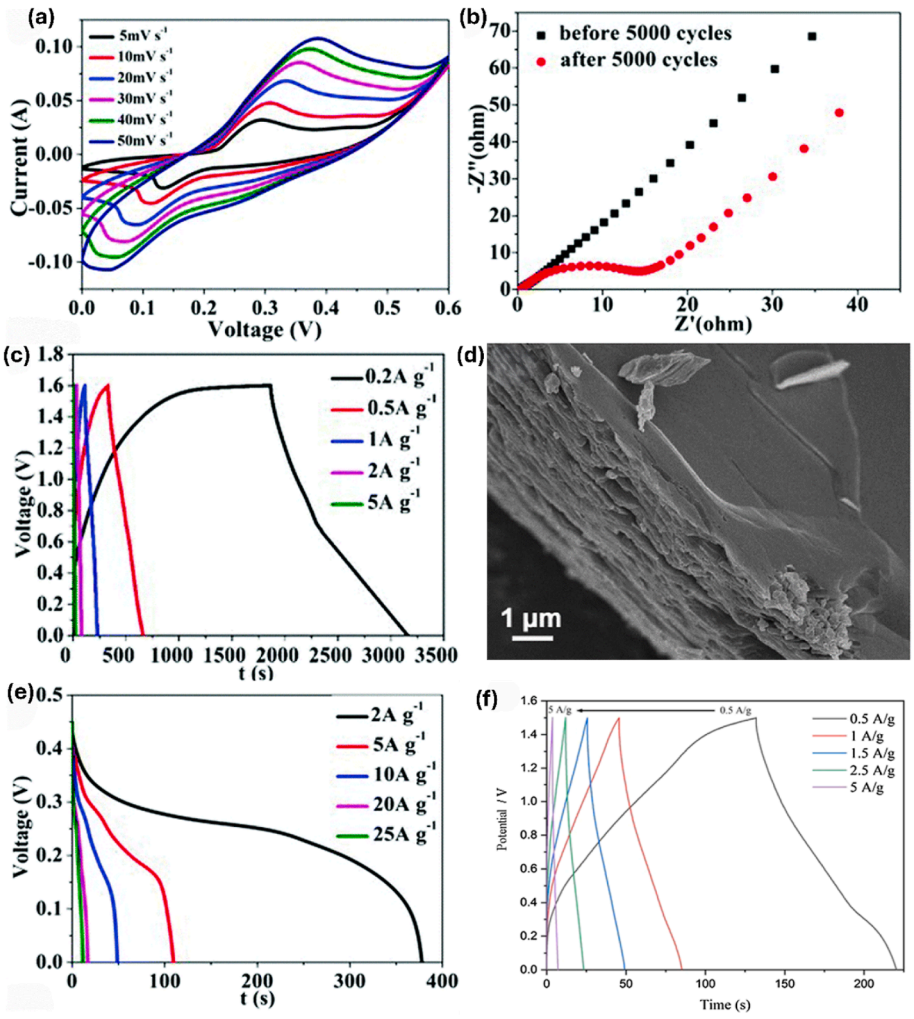


Fig. 4. (a) Cyclic voltammetry curves for different scan rates, (b) Impedance data before and after 5000 cycles; (c) Charge-discharge behavior of the Ni-MOF//AC hybrid supercapattery at different current densities; (d) BET surface area analysis, (e) Charge-discharge curves at different current densities (Reproduced from Ref. (Zhang et al., 2018)); and (f) Charge-discharge curves of the Cu-MOF/graphene composite at different current densities (Reproduced from Ref. (Azadfalah et al., 2019)).

shows higher simulated IL conductivity with larger pores, highlighting the importance of pore size tuning. Liu et al. (2022) showed that optimizing micropore size enhances ion transport and electrochemical performance, especially at low temperatures. Their optimized carbon electrode achieved 200 F/g at −40°C and 245 F/g at 60°C, with an energy density of 63.4 Wh/kg at −40°C, demonstrating excellent low-temperature performance and fast charge/discharge capability, as shown in Fig. 5(c) and (d). These studies collectively underscore the importance of pore size engineering and current density optimization in enhancing the electrochemical behavior and long-term performance of 2D-MOFs for both energy storage and catalytic applications.

However, the tunable properties of 2D-MOFs, particularly their surface characteristics and adjustable pore sizes, are essential for optimizing their performance in energy storage and harvesting systems. As demonstrated in the studies discussed, precise control over these structural features can significantly enhance electrochemical behavior, cycling stability, and efficiency. The ability to manipulate these properties through synthetic strategies not only improves the functionality of 2D-MOFs but also expands their potential for integration into next-generation energy storage devices and harvesting technologies.

2.2.2. *Synthesis and functionalization of 2D-MOFs*

The synthesis and post-synthetic functionalization of 2D-MOFs are critical for enhancing their electrochemical properties in energy storage applications. Common synthesis techniques include solvothermal, hydrothermal, microwave-assisted, and mechanochemical methods. These approaches allow fine-tuning of morphology, porosity, and crystal structure, which directly influence conductivity, ion diffusion, and surface reactivity. Among the most notable functionalization strategies are doping, ligand modification, and hybridization with conductive materials such as graphene or carbon nanotubes. For example, phosphate-ion doping in Ni-Co layered double hydroxide nanosheets derived from MOFs significantly enhances SSA and conductivity, resulting in a 49.7% increase in specific capacitance and an energy density of 64.89 Wh/kg (Li et al., 2023).

Ligand engineering, such as the incorporation of ethylenediamine (ED) or missing-linker strategies (e.g., IPA embedding in Ni-BTC), improves redox site exposure and optimizes pore distribution, enhancing electrochemical performance (Kalyon et al., 2024). Hybridization strategies, particularly with reduced graphene oxide (rGO), have yielded supercapacitor materials with improved capacitance and durability. For example, Ni-MOF/graphene hybrids demonstrate excellent cyclic stability with 97.7% capacitance retention over 10000 cycles (Biji et al., 2024). In addition to capacitance and cycle life, energy and power densities are also critical metrics. Materials such as 2DNi-GA achieve high gravimetric (71 Wh/kg) and volumetric energy densities, thanks to interfacial coordination between MOF metal nodes and carboxyl groups on functionalized graphene (Sundriyal et al., 2025). Similarly, hybrid

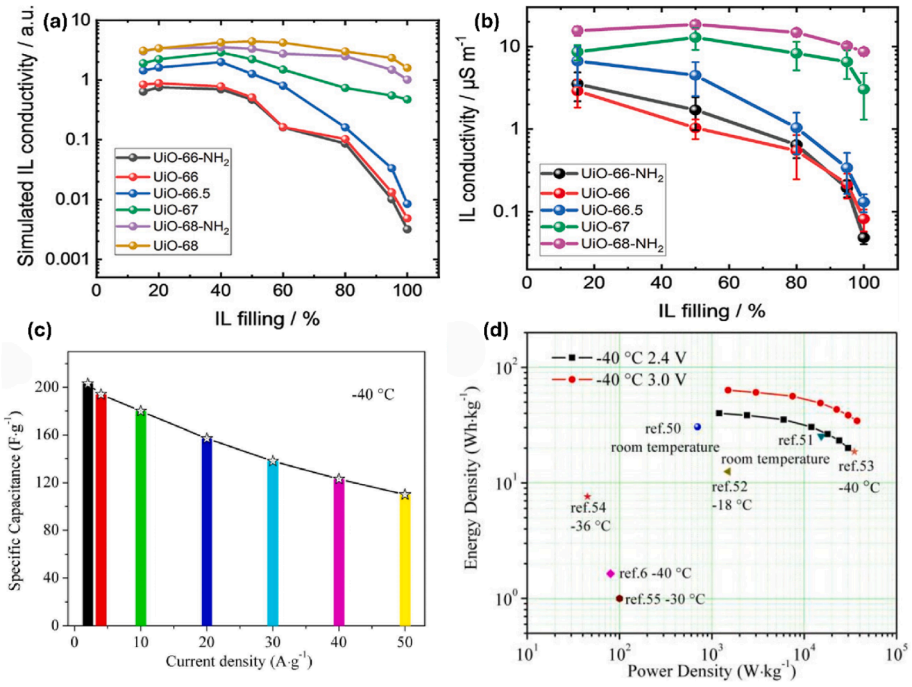


Fig. 5. Impact of pore size tuning on electrochemical performance and ion transport properties of 2D-MOFs. (a) IL conductivity vs. IL filling in UiO MOFs; (b) Simulated IL conductivity with varying pore sizes (Reproduced from Ref. (Zhang et al., 2022)); (c) Specific capacitance at different current densities at −40°C; (d) Energy density vs. power density of the optimized carbon electrode (Reproduced from Ref. (Liu et al., 2022)).

Table 2
Summary of synthesis methods, functionalization strategies, and electrochemical performance metrics of selected 2D-MOFs for energy storage applications.

2D-MOF System	Synthesis Method	Functionalization Strategy	Specific Capacitance (F/g)	Cycling Stability (%)	Energy Density (Wh/kg)	Power Density (W/kg)	Ref.
CoNi(1:6)-MOF	Stirring reaction (solvent-based)	Co/Ni co-doping	455	90% after 5000 cycles	38.8	263.3	Hang et al. (2023)
$Cu_3(HHTP)_2$	Solvothermal	None (pristine)	135	99% after 1000 cycles	32	2100	Iqbal et al. (2023)
Ni-MOF/ graphene	Solvothermal	Hybridization with graphene	111.68	97.70% after 10000 cycles	14.68	291.82	Qiang et al. (2022)
C-Co@MOF	Stirring reaction (solvent-based)	Co nanoparticle doping	1201.6	45% capacitance retention at 30× current density	37.0	2250.2	Tian et al. (2021)
Ni-MOF	Solvothermal	-	198	84 % after 3000 cycles	44	3663	Iqbal et al. (2023)
Cu-MOF	Solvothermal	-	138	95% after 3000 cycles	39	3298	
Cu-MOF/ graphene	One-step solvothermal	Hybridization with graphene	482	93.8% after 1000 cycles	34.5	1350	Azadfalah et al. (2019)
$Ni_2[CuPc(NH)_8]$	Ball milling exfoliation	Hybridization with exfoliated graphene	18.9 mF/cm^2	91.4% after 5000 cycles	-	168	Wang et al. (2020)
Fe/Zn-BDC, Fe/ Ni-BDC	Solvothermal, Exfoliation	Bimetallic (Fe/Ni, Fe/Zn)	633.21 (Fe/Zn), 1190.88 (Fe/Ni)	83.5 (Fe/Zn), 93.7 (Fe/Ni) after 5000 cycles	-	-	Nivetha et al. (2023)
Mo_2N (Molybdenum Nitride)	Nitridation of Mo-complex	Phase-pure 2D Mo_2N	248	98% after 10000 cycles	23.39	1829.6	Palraj and Therese (2025)
Ni-BTC/IPA-x (Defective)	Solvothermal, embedding IPA as linkers	Missing-linker defects for enhanced electrochemical properties	1209	-	30	1775.8	Zhang et al. (2024)
2DNiMOF/ Graphene (2DNiGA)	Low-temperature synthesis	Coordination of Ni nodes with carboxyl groups of graphene (GA)	>100% improvement (compared to unfunctionalized graphene)	>94% after 10000 cycles	71	800	Sundriyal et al. (2025)
Meso-Zn-MOF@rGO-PBA	Hybrid synthesis of mesopores in Zn-MOF sheets	Hybridization with rGO-PBA	292.8	83.2% after 2000 cycles	19.5	818	Li et al. (2023)

heterostructures like Meso-Zn-MOF@rGO-PBA exhibit well-balanced electrochemical properties, with a specific capacitance of 292.8 F/g and an energy density of 19.5 Wh/kg. These enhancements are linked to the introduction of mesopores, which facilitate both pseudocapacitive and double-layer charge storage mechanism (Li et al., 2023).

However, it is important to note that the specific electrolyte used in these studies significantly influences the performance metrics reported, especially when comparing capacitance and energy density. For example, aqueous electrolytes often exhibit lower performance than non-aqueous systems due to differences in ionic conductivity. The type of electrolyte should be consistently reported in studies to allow better comparisons of the data. Additionally, electrode mass loading plays a critical role in the performance, as higher mass loading can reduce capacitance per unit mass of material, thereby impacting the energy density. It is crucial to normalize current density across different studies to ensure that comparisons of capacitance, energy density, and other metrics are fair and meaningful. Table 2 presents an overview of selected functionalized 2D-MOFs and their electrochemical performance, highlighting recent advancements achieved through different synthesis methods and functionalization strategies.

The sustained evolution of synthesis and functionalization methodologies of 2D-MOFs has allowed impressive breakthroughs in tailoring their structural and electrochemical characteristics towards energy storage applications. The challenges faced by poor intrinsic conductivity and low cycling stability have been overcome by the introduction of hierarchical porosities, redox-active groups, and conducting hybrid scaffolds. Through methodologies involving metal doping, ligand tailoring, defect introduction, and carbon-based materials hybridization, 2D-MOFs now offer improved specific capacitance, energy and power densities, and long-cycle stability. These customized modifications demonstrate the versatility of 2D-MOFs and confirm their capability as high-efficiency materials in next-generation energy storage devices. Through scalable and controllable synthesis methodologies, 2D-MOFs are poised to contribute substantially toward meeting the requirements of efficient and sustainable energy systems.

2.3. Transition metal dichalcogenides (TMDs)

TMDs are a family of two-dimensional materials with the general formula MX_2, where M is a transition metal (Mo, W, Ti) and X is a chalcogen (S, Se, or Te) (Han et al., 2018; Vogel and Robinson, 2015). These materials consist of covalently bonded X–M–X layers held together by weak van der Waals forces, allowing for exfoliation into monolayers (Fig. 6(a)) (Luxa et al., 2022). Unlike graphene, which is a zero-bandgap semimetal, TMDs such as MoS_2 and WS_2 exhibit semiconducting behavior. Their band gaps are thickness-dependent; for example, MoS_2 transitions from an indirect band gap of approximately 1.2 eV in the bulk to a direct band gap of around 1.8 eV in the monolayer form, enhancing its optoelectronic capabilities (Fig. 6(b)) (Lv et al., 2015; Martini et al., 2023). These features, along with tunability through doping, strain, or phase engineering, contribute to their versatility for energy applications (Kumar et al., 2022; Voiry et al., 2015).

TMDs are particularly promising for energy harvesting and conversion due to their favorable electrical conductivity, chemical stability, and elemental abundance. Their catalytic activity is enhanced by the presence of active edge sites that facilitate electrochemical reactions such as the hydrogen evolution reaction (HER) (Samy and El Moutaouakil, 2021). Various exfoliation techniques such as liquid-phase exfoliation (LPE), mechanical exfoliation, and chemical vapor deposition (CVD) provide scalable routes for monolayer production and defect

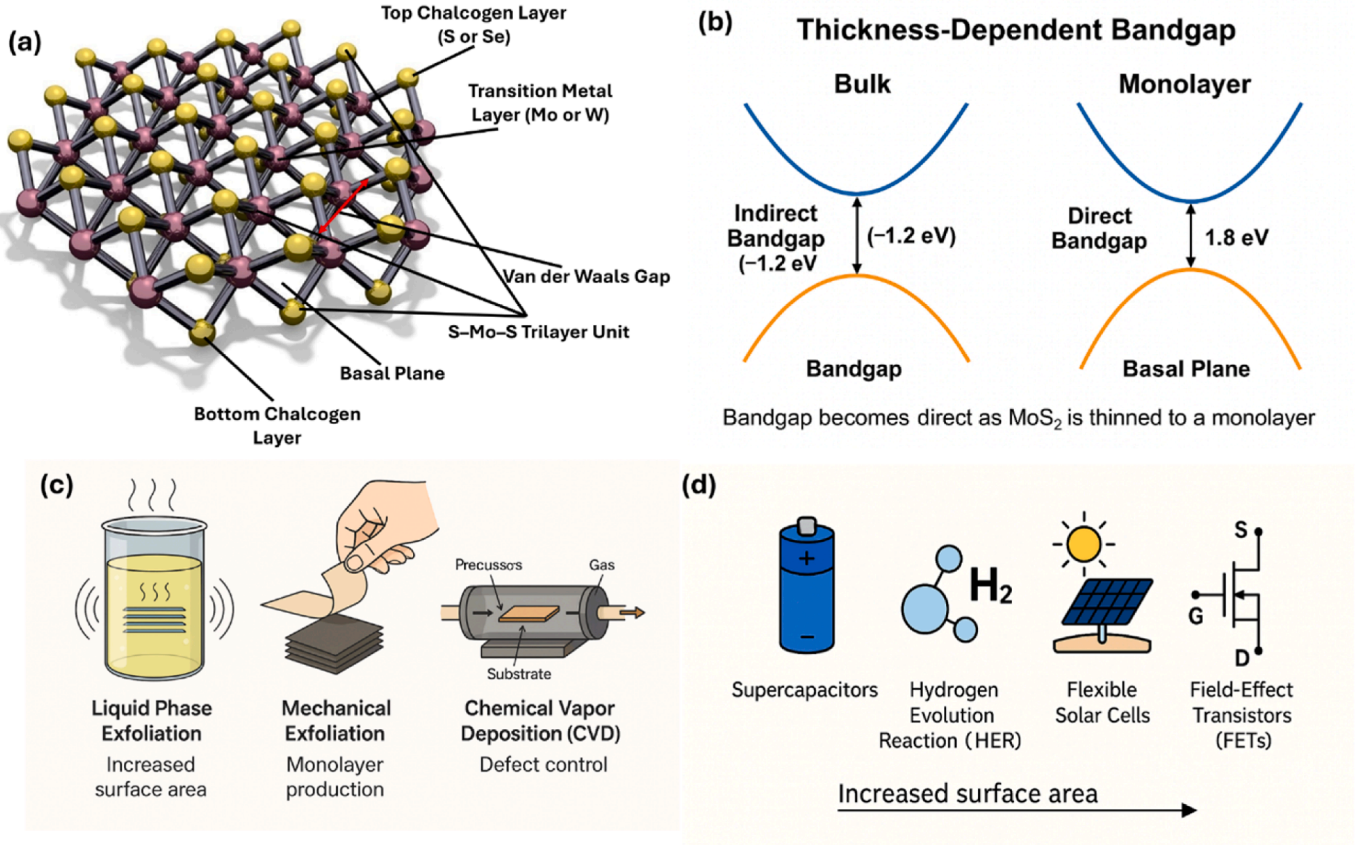


Fig. 6. (a) Crystal structure of MoS_2 with layered Mo–S arrangement and van der Waals gap; (b) Thickness-dependent bandgap transition from bulk indirect (~1.2 eV) to monolayer direct (1.8 eV); (c) Exfoliation methods for 2D TMDs including liquid-phase, mechanical, and CVD; (d) Energy applications such as supercapacitors, HER, solar cells, and FETs.

control (Fig. 6(c)). TMDs like MoS_2 and WS_2 are highly effective in supercapacitors and batteries, offering excellent charge–discharge performance (Alam et al., 2025), while $MoSe_2$ and WSe_2 are utilized in flexible electronics and thin-film solar cells (Nazif et al., 2023; Rawat et al., 2019). These materials, combined with adaptable synthesis strategies, make TMDs highly suitable for a range of sustainable energy technologies (Fig. 6(d)) (Sovizi et al., 2023).

However, it is critical to highlight the testing conditions under which these performance metrics are obtained. The electrolyte type used in the experiments plays a significant role in the reported performance. For instance, the energy density and capacitance may vary depending on whether aqueous electrolytes, such as KOH or Na_2SO_4, or non-aqueous electrolytes are used. Furthermore, electrode mass loading directly affects the energy density, with higher mass loadings generally resulting in lower capacitance per gram of material. It is essential to normalize current density across different studies to ensure fair comparisons, as varying current densities can significantly impact the reported efficiency and stability of TMD-based systems. Additionally, the configuration of devices, whether symmetric or asymmetric, or hybrid versus pure systems should be considered as it can have a substantial effect on the overall performance. Therefore, the testing conditions need to be clearly reported and standardized to enable meaningful comparisons of data across studies.

2.3.1. *Properties and applications of TMDs*

The unique energy-related functionality of TMDs stems from their tunable band structures, layer-dependent electronic transitions, and polymorphic phases. In monolayer form, TMDs such as MoS_2 and WS_2 exhibit a direct bandgap (approximately 1.6 to 2.0 eV), contrasting with the indirect bandgap (around 1.2 to 1.3 eV) observed in their bulk forms, significantly enhancing photoluminescence and optoelectronic behavior (Okuno et al., 2018; Tan et al., 2018). This thickness-dependent transition is experimentally validated by Cho et al. (2023), who fabricated Au–MoS_2–Au devices with both bulk and monolayer configurations and demonstrated that the monolayer device produced a markedly higher photocurrent response under red (650 nm), green (532 nm), and blue (450 nm) illumination. Similarly, Poornimadevi et al. (2022) observed similar transitions for WS_2 and $MoSe_2$, with bandgap values of ~1.6-1.8 eV for WS_2 and ~1.5-1.6 eV for $MoSe_2$. Complementing this, Dominguez Godinez et al. (2024) employed density functional theory (DFT) to show that oxidation of MoS_2 and $MoSe_2$ monolayers induces a direct-to-indirect bandgap transition, reducing their bandgap energies from 1.62 to 1.12 eV for MoSO and from 1.45 to 0.83 eV for MoSeO as oxygen content increases. Their study also found that Janus-type oxidized phases are particularly stable in oxygen-rich environments. Das et al. (2021) highlighted that the 2H phase of TMDs, such as MoS_2 and WS_2, is semiconducting and suitable for FETs and optoelectronics, while the 1T phase, as seen in 1T-MoS_2, is metallic and offers higher conductivity, beneficial for applications in catalysis and energy storage. Furthermore, Khare and Dwivedi (2021) observed that the transition to a monolayer form improves charge carrier mobility due to reduced scattering and enhanced quantum confinement effects, underscoring the tunability of TMDs for various energy-related applications. These insights are visualized in Fig. 7(a)–(d), which capture the oxidation-induced bandgap variation, formation energy profiles, and structural stability, further emphasizing the versatility of TMDs.

However, it is important to consider the testing conditions that influence these reported performance metrics. The choice of electrolyte has a direct effect on the electrochemical performance of TMDs. For instance, the capacitance and energy density may vary significantly between aqueous electrolytes. Electrolyte ionic conductivity and chemical compatibility with TMDs should be standardized and reported in studies for accurate comparison. Moreover, it is crucial that future studies clearly report and standardize key testing parameters such as electrolyte type, electrode mass loading, exfoliation techniques, and device configurations to ensure meaningful and accurate comparisons across studies.

Different exfoliation techniques significantly influence the surface properties, defect density, and charge transport characteristics of TMDs, which in turn affect their performance across various applications. LPE, known for its scalability, produces materials with large surface areas but often introduces defects and contamination due to the use of surfactants, which can reduce charge carrier mobility and complicate material properties (Bai et al., 2025; Jeong and Samorì, 2024). In contrast, mechanical exfoliation, especially when assisted by metals like gold, helps preserve the intrinsic properties of TMDs, resulting in high-quality monolayers with minimal defects and improved charge carrier mobility (Velický et al., 2018). CVD synthesizes high-quality defect-free crystalline TMDs, but it is generally substrate and growth condition limited, constraining surface area (Jernigan et al., 2020). The exfoliation

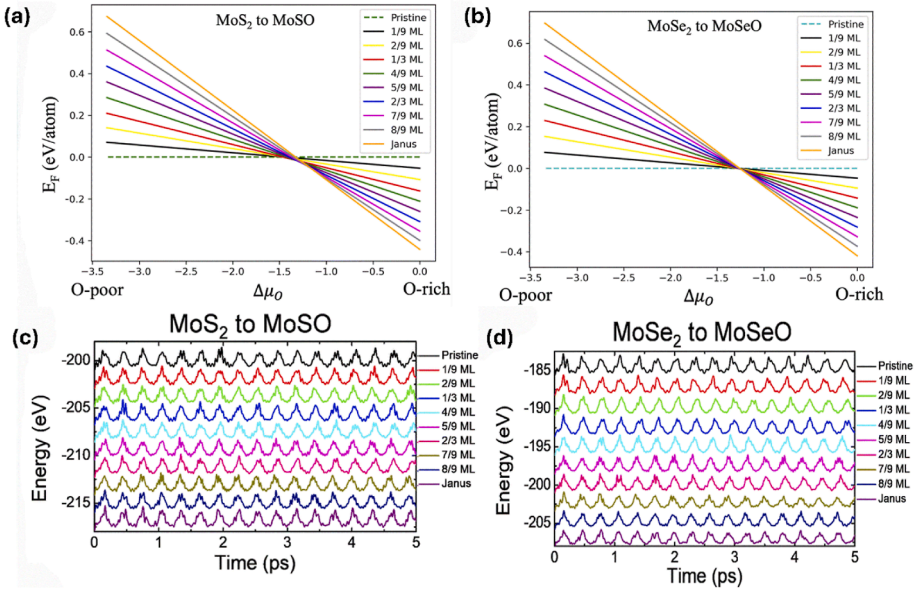


Fig. 7. (a) Bandgap variation in MoS_2 and $MoSe_2$ monolayers under oxidation, with direct-to-indirect transition and reduced energies (MoSO: 1.62–1.12 eV; MoSeO: 1.45–0.83 eV); (b) Formation energy under different oxygen potentials showing stable Janus phases; (c) Structural evolution and stability of oxidized monolayers; (d) Band alignment shifts in oxidized structures (Adapted from Ref. (Dominguez Godinez et al., 2024)).

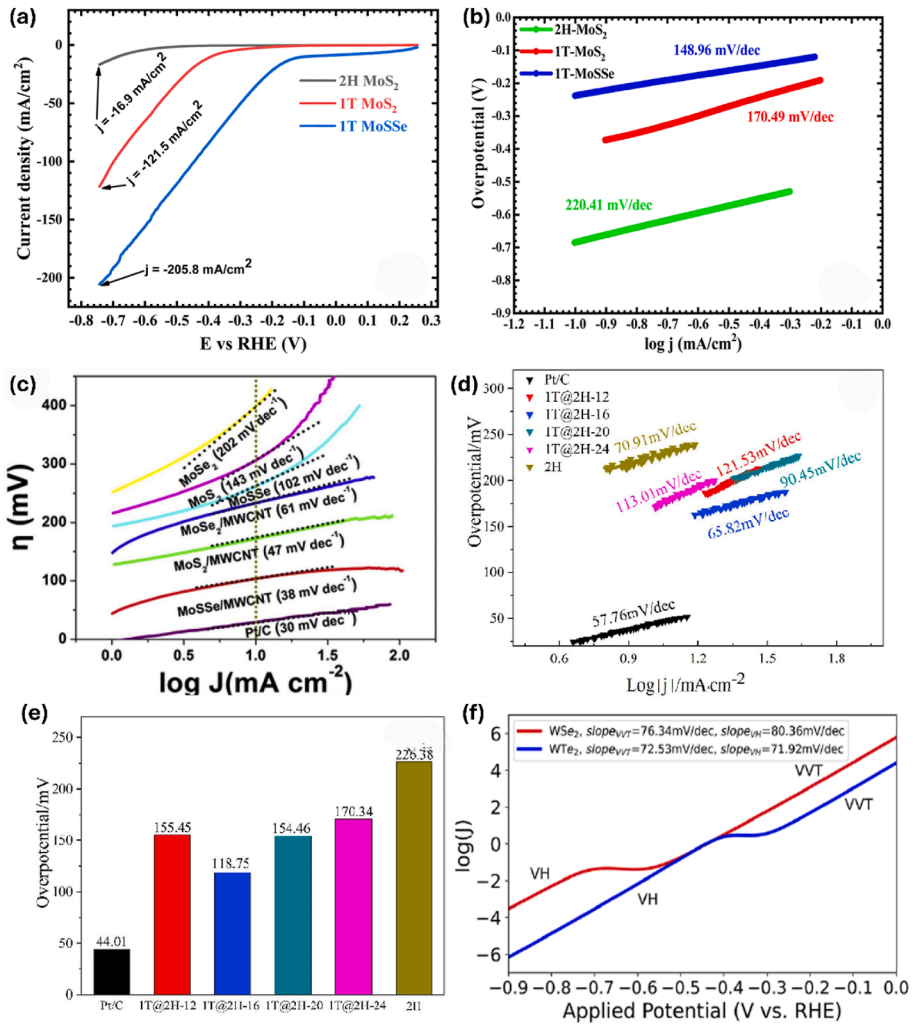


Fig. 8. (a) Current density vs. potential for TMDs showing superior catalytic performance of Ni-doped 1T-MoS_2 over 2H-MoS_2; (b) Tafel plots highlighting lower slope and overpotential of 1T-MoS_2 for HER (Adapted from Ref. (Mazumder et al., 2025)); (c) Comparison of 1T-WS_2 and 2H-WS_2 showing 38 mV/dec Tafel slope and 102 mV overpotential for 1T-WS_2 (Adapted from Ref. (Qiao et al., 2019)); (d) 1T@2H-$MoSe_2$ with 65.8 mV/dec slope and 118 mV overpotential indicating strong HER activity; (e) Bar graph comparing overpotentials of TMD composites, showing superior performance of 1T@2H-MoS_2 (Adapted from Ref. (Liu et al., 2022)); (f) WSe_2 and WTe_2 plots with 1T′-WSe_2 exhibiting −0.53 V onset potential and 70 mV/dec slope, further improved by electrochemical activation (Adapted from Ref. (Song et al., 2021)).

method also plays a critical role in performance, particularly for energy storage and harvesting applications. LPE-exfoliated TMDs are often better suited for supercapacitors and batteries, while mechanical exfoliation and CVD are preferred for applications requiring defect-free, high-quality monolayers, such as optoelectronics and catalysis. Furthermore, electrode mass loading should be carefully controlled across studies, as higher mass loadings typically lead to lower capacitance per gram, affecting overall energy density. Normalizing current density is essential to ensure fair comparisons of performance metrics across studies.

Energy application-based LPE and mechanical exfoliation increase the efficiency of HER by raising the surface area and accessible sites, while TMDs grown by CVD are less utilized in HER application (Mazánek et al., 2018). Also, LPE-prepared exfoliated TMDs can be utilized in supercapacitors and enhance electrochemical characteristics, provided that defects are kept in check and do not lower the characteristics (Jeong and Samorì, 2024). Hence, it is application-dependent as to which exfoliation technique is chosen, and mechanical exfoliation and CVD are usually favored exfoliation techniques in creating defect-free, high-quality TMDs in application areas involving electronic and optoelectronic equipment, while in producing large quantities of TMDs needed in application fields requiring particular surface area, LPE is a more effective choice, especially in creating TMDs in energy application fields. In addition, configurations of the devices, such as symmetric versus asymmetric setups, can impact the energy storage or conversion performance significantly. This should be reported and standardized across studies to allow for an accurate comparison of performance across different TMD-based systems.

The catalytic activity of TMDs in the HER is strongly dependent on their phase, defects, and morphology. Mazumder et al. (2025) demonstrated that Ni-doped 1T-MoS_2 tunes the S-H bond strength in a way that it results in a Tafel slope of 148 mV/dec and an overpotential of 87.8 mV at 10 mA/cm^2. Fig. 8(a) demonstrates the enhancement, with 1T-MoS_2 presenting a better response compared to 2H-MoS_2. Fig. 8(b) verifies the same, with a lower Tafel slope and overpotential in 1T-MoS_2, underscoring its improved catalytic activity in hydrogen evolving reactions. Qiao et al. (2019) observed in a similar vein that WS_2 in the 1T phase delivers a Tafel slope as low as 38 mV/dec and an overpotential as low as 102 mV at 10 mA/cm^2, underscoring improved catalytic activity compared to the 2H phase, as depicted in Fig. 8(c), wherein the 1T-WS_2 curve demonstrates a Tafel slope and overpotential of 38 mV/dec and 102 mV, respectively, stressing the improved 1T-WS_2 response in the HER. Liu et al. (2022) showed that 1T@2H composite phase of $MoSe_2$ presents a low overpotential of 118 mV and a low Tafel slope of 65.8 mV/dec. Fig. 8(d) depicts it clearly, wherein 1T@2H $MoSe_2$ curve demonstrates the Tafel slope, 65.8 mV/dec. Moreover, Fig. 8(e) demonstrates the corresponding overpotential, 118 mV, in 1T@2H $MoSe_2$, stressing improved catalytic activity in the HER. Song et al. (2021) observed that WSe_2 in its 1T′ stage presents an onset potential as low as −0.53 V and a Tafel slope as low as 70 mV/dec as depicted in Fig. 8(f), with electrochemical activation yet enhancing its activity. The catalytic activity of TMDs is also enhanced by edge sites and defects, such as chalcogen vacancies, which provide additional active sites for HER.

Furthermore, Prabhu et al. (2020) showed that heterostructures like MoS_2/WS_2 and $MoSe_2/WSe_2$ exhibit improved HER performance due to enhanced electron transfer and increased active sites. MoS_2 and its doped or phase-engineered variants, particularly the Ni-doped 1T-MoS_2 and Janus 1T-MoSSe, show the best HER performance with low overpotentials and favorable Tafel slopes (Hao et al., 2019; Mazumder et al., 2025). However, TMDs with high edge site density, well-engineered defects, and optimal heterostructures, such as MoS_2 and WS_2, exhibit the lowest overpotentials and highest HER efficiency among the various TMDs.

Hybrid systems and doped structures of TMDs have demonstrated significantly improved performance in energy harvesting applications, surpassing pristine TMDs in various aspects such as energy density, cycle life, and HER kinetics. For instance, Imran et al. (2024) built a MoS_2@VZnS//AC hybrid supercapacitor delivering 1025 c/g, 39.5 Wh/kg at 2462 Wh/kg, and 91.32% retention after 5000 cycles, outperforming pristine MoS_2. Zhuang et al. (2019) showed edge-rich 1T′-$ReSe_2$ on CNTs with $\eta_{10} = 23$ mV and Tafel = 37 mV/dec, and bifunctionality for Na-ion storage. Ogunkunle et al. (2024) found Cu/Ni/Co-doped defective 1T′-MoS_2 boosts alkaline HER via optimized OH* desorption at active sites, beating undoped analogs. Pawar et al. (2019) reported a polymorphic 1T″-Mo_6Te_6/2H-$MoTe_2$ electrode with 1542 mF/cm^2 areal capacitance and 96% stability, surpassing single-phase $MoTe_2$. Manyepedza et al. (2024, 2025) demonstrated WS_2/MoS_2, $MoSe_2/MoS_2$, and ternary $MoS_2/MoSe_2/WS_2$ heterostructures with lower onset overpotentials and higher rate constants than single TMDs to interfacial charge transfer and added edge sites. Chen et al. (2016) achieved $\eta_{10} = 183$ mV, Tafel = 55.5 mV/dec, and durability over 2000 cycles with vertical $MoS_{2(1-x)}Se_{2x}$ nanosheets. Gong et al. (2016) showed $MO_xW_{1-x}(S_\gamma Se_{1-\gamma})_2$ alloy nanoflakes with small onset η/Tafel and robust stability via composition–activity tuning. These hybrid systems consistently outperform pristine TMDs in real-world energy devices, with higher energy/capacitance, longer cycle life, and faster HER kinetics. However, the performance of these hybrid systems is also strongly dependent on the testing conditions, such as the electrolyte type, electrode mass loading, and current density. It is crucial that future studies clearly report these conditions to ensure accurate comparisons across different TMD-based systems.

2.3.2. TMDs in energy harvesting

TMDs have demonstrated significant potential in enhancing the performance of energy harvesting devices, particularly in piezoelectric generators (PENGs) and triboelectric nanogenerators (TENGs). TMDs such as MoS, SnS_2, and VS_2 are being integrated into these devices to enhance power output, efficiency, and energy conversion. For instance, SnS_2/SnS heterostructures have demonstrated an output voltage of 60 mV and a current density of 11.4 nA/cm^2 at 0.6% tensile strain, showing a 40% improvement in piezoelectric response compared to SnS_2 thin films alone (Cao et al., 2021). Similarly, MoS_2 nanosheets have been shown to generate 400.4 mV and a current of 40.7 nA under 0.57% bending strain, demonstrating their potential in centimeter-scale PENGs, harvesting energy from human motions (Jung et al., 2022). Additionally, VS_2/PVDF nanocomposites have been reported to produce an output voltage of ~83 V, current of ~52 μA, and power of 2115.25 μW, with a power density of 114.4 μW/cm^2 under a biomechanical force of 7-8 N, showing excellent energy harvesting potential for wearable and flexible devices (Verma et al., 2024). For TENGs, the $Mo_{0.5}W_{0.5}S_2$ ternary alloy has shown an increase in voltage by 62% and current by 253% under visible light illumination, with photoresponsivity reaching ~45.5 V/mW under ultralow illumination, demonstrating its potential for energy harvesting in low-light conditions (Bhattacharya et al., 2023). Surface-crumpled MoS_2 has also been shown to enhance performance with an output voltage of ~25 V, current of ~1.2 μA, and ~40% more power than flat MoS_2 due to increased surface roughness and work function changes (Park et al., 2020). These results highlight the significant improvements in energy density and efficiency achieved by TMD-based materials in energy harvesting applications.

However, it is important to consider the testing conditions that influence these reported performance metrics. For example, the tensile strain applied to TMDs in PENGs, such as the 0.6% strain for SnS_2/SnS heterostructures, directly affects the piezoelectric response, and similar testing conditions should be reported across studies for accurate comparisons. Additionally, the light conditions under which TENGs are tested, such as the enhancement observed in $Mo_{0.5}W_{0.5}S_2$ under visible light illumination, are critical to performance metrics such as photoresponsivity and output voltage. Reporting the exact light intensity and wavelength for TENGs is necessary to ensure a fair comparison across studies. Furthermore, the biomechanical force applied in the case of VS_2/PVDF nanocomposites is another important variable, influencing the output voltage and current. Standardizing the force applied across different studies will allow for meaningful comparisons of energy density and efficiency. To facilitate accurate comparison of energy density and efficiency values across different TMD-based energy harvesting systems, future studies should carefully report and standardize these testing conditions, ensuring that key factors such as strain, light conditions, and mechanical forces are consistent across configurations.

While these TMD-based materials have demonstrated significant performance improvements in individual components (such as PENGs and TENGs), it is important to note that fully integrated devices, such as packaged supercapacitors, PENGs, or TENGs, utilizing these hybrid materials are still in the early stages of development. Future studies should focus on the integration of these hybrid systems into fully functional devices and compare their performance metrics, including power output, energy density, and efficiency, with commercial benchmarks to assess their practical applicability and scalability in real-world applications.

The thickness or number of layers in TMDs decides significantly their performability in energy harvesting devices. Direct bandgaps are achieved by monolayers in MoS_2, which are needed in optoelectronic devices, while multilayered TMDs lead to a shift in bandgaps towards indirect ones, affecting their performances in devices like solar cells (Thomas et al., 2021). Enhanced photovoltaic efficiency has been achieved in monolayer MoS_2 doped with materials such as graphene, and 11.1% conversion efficiency was achieved (Tsuboi et al., 2015). Nevertheless, multilayered TMDs such as MoS_2 and $MoSe_2$ achieve 25% power conversion efficiencies (PCEs) or higher if duly well-tailored in thickness (Nazif et al., 2023). The electrical conductivity is also improved by the layer number as well, as has been observed in the case in WSe_2 doped in PEDOT:SS which enhances hole transport and suppresses charge recombination loss, thus providing improved PCE in organic solar cells (Koo et al., 2018). These findings reflect how layer number and thickness are crucial determining parameters that govern the energy conversion efficiency, electrical properties, and functionality of TMDs in energy harvesting devices.

TMDs have shown immense ability in energy harvesting devices, namely in PENGs and TENGs, and the layer number and thickness of the TMDs significantly govern their functionality. For example, multilayer TMDs, such as MoS_2, support direct bandgaps, perfect for optoelectronic devices like solar cells and photodetectors, while thick TMDs transform into indirect bandgaps, affecting efficiency in solar cells. The electronic conductivity in TMDs enhances with layer number as there are fewer charge trapping sites and fewer impurities in multilayer designs, thus boosting functionality in energy harvesting applications (Yu et al., 2017). Furthermore, multilayer TMDs, namely MoS_2, $MoSe_2$, and WS_2, have reached record high PCE up to 25% as they are optimized in material quality and thickness (Nazif et al., 2023). Structural alterations such as crumpling on the surface and formation of a heterostructure transform triboelectric functionality in TMDs, offering enhanced active sites as well as improved energy conversion efficacy (Park et al., 2020). Such developments emphasize the functionality of TMDs in creating efficient energy harvesting devices, and continuous material and

architectural enhancements are opening up paths towards sustainability.

2.4. Key differences between 2D-MOFs and TMDs

The characteristic structural differences between 2D-MOFs and TMDs significantly impact their charge storage and transfer properties. 2D-MOFs are composed of metal ions coordinated by organic ligands, forming a porous material with adjustable pore sizes and extensive porosity, which promotes charge delocalization and mobility. In contrast, TMDs feature layered structures stabilized by van der Waals forces, facilitating exfoliation into monolayers and offering impressive charge carrier mobility, particularly in the monolayer form. These structural differences contribute to their respective strengths in energy storage, catalysis, and electronics. Charge carrier mobility in 2D-MOFs is driven by the π-conjugation in the extended layers, while in TMDs, it relies on individual metal and chalcogen elements, as well as defects. Both materials exhibit improved charge transfer rates, with 2D-MOFs benefiting from abundant active sites and TMDs offering efficient electron transport in the layers, although this can be compromised by defects. In energy storage, 2D-MOFs excel with adjustable pores and high porosity, while TMDs, with their layered structure, allow ion intercalation, though energy capacity depends on interlayer spacing and material composition. The complementary nature of 2D-MOFs and TMDs establishes the foundation for synergistic hybridization. While 2D-MOFs provide high porosity, structural tunability, and abundant catalytic sites, TMDs contribute superior electronic conductivity, efficient charge transport, and robust mechanical stability. The limitations of each material class, low conductivity in MOFs and stability challenges in TMDs, can be effectively addressed through strategic hybridization. This synergistic integration enables the development of multifunctional hybrid systems with emergent properties that surpass the capabilities of individual components in energy harvesting applications. A detailed comparison of their properties is summarized in Table 3.

Table 3
Properties comparison of 2D-MOFs and TMDs.

Property	2D-MOFs	TMDs
Structure	Atomically thin materials combining organic molecules with crystalline inorganic solids (Grisan Qiu et al., 2025).	Layered materials with strong in-plane covalent bonds and weak van der Waals forces between layers (Kasbe et al., 2021).
Electronic Properties	Exhibits hybrid electronic bands and distinct magnetic properties due to interactions between transition metal centers and organic ligands (Mearini et al., 2024).	Excellent electronic properties, including high conductivity and tunable band gaps (Luo et al., 2024).
Magnetic Properties	Magnetic properties can be tuned by selecting different transition metals (Grisan Qiu et al., 2025).	Magnetic properties influenced by defects and interfaces (Luo et al., 2024)
Thermal Properties	Good thermal stability due to π-electron conjugation and effective interaction between metal and organic ligands (Li et al., 2022).	Thermal conductivity varies with composition and structure, influenced by phonon dispersion and lifetimes (Farris et al., 2024).
Mechanical Properties	High mechanical stiffness and structural stability (Ghosh et al., 2023).	High mechanical stiffness, but properties can be affected by defects (Li et al., 2023).
Catalytic Properties	Effective for HER and OER catalysis, with active sites on O and TM atoms (Li et al., 2022).	Efficient charge transfer and catalytic properties, especially in HER applications (Ashraf et al., 2026).
Gas Sensing	Enhanced gas sensing capabilities when combined with TMDs (Wang et al., 2022).	High surface-to-volume ratio makes them suitable for gas sensing, but responsivity can be low without optimization (Wang et al., 2022).
Energy Storage	High porosity and surface area make them suitable for energy storage applications (Ashraf et al., 2026).	Promising electrode materials for energy storage due to conductivity and catalytic properties (Mohamed et al., 2020).

3. Synergy between 2D-MOFs and TMDs

The true potential of 2D-MOF/TMD systems is unlocked not by the simple addition of their individual properties, but through the profound synergy that emerges at their interface. This synergy, arising from the complementary integration of MOFs' tunable porosity and abundant active sites with TMDs' superior conductivity, catalytic edge states, and strong light absorption, creates a new class of materials with capabilities exceeding the sum of their parts. The synergy between 2D-MOFs and TMDs arises from the complementary integration of MOFs' tunable porosity and abundant active sites with TMDs' superior conductivity, catalytic edge states, and strong light absorption. Recent studies show that hybrid structures overcome the limitations of each material when used alone: for example, MoS_2@MOF composites exhibit improved photochemical stability and charge separation efficiency, enhancing photocatalytic activity (Hosseini and Safarifard, 2024), while a MOF-5/WSe_2@g-C_3N_4 hybrid demonstrates superior hydrogen evolution and electrochemical stability due to efficient charge transfer and structural robustness (Ashraf et al., 2026). In addition to improved conductivity and stability, hybridization also adjusts electronic and optical properties, enabling broader light absorption for solar applications (Idisi and Mwakikunga, 2023), while incorporating TMD nanoparticles into MOF frameworks exposes more active sites and increases catalytic efficiency in electrochemical reactions (Zhang et al., 2024). These findings confirm that 2D-MOF/TMD hybrids achieve notable improvements in energy harvesting through interactions that neither material can achieve alone. The following subsections explore these interactions in detail through hybridization strategies, underlying mechanisms, and interface engineering.

3.1. Hybridization of 2D-MOFs and TMDs

Hybridizing 2D-MOFs with TMDs is a versatile strategy for designing multifunctional materials with properties that neither material could achieve alone. The crystalline coordination networks in MOFs provide tunable metal–ligand interactions and ordered porosities, while TMDs contribute layered structures with in-plane conductivity and catalytic edge states. This combination results in hybrids with enhanced structural stability and complementary physicochemical properties. Beyond TMDs, hybridizing 2D metal–organic frameworks (MOFs) with other 2D layered materials such as graphene, hexagonal boron nitride (hBN), MoS_2, WSe_2, and fluorographene broadens the material's functionality. In these systems, the MOF lattice offers tunable porosity and abundant active sites, while the 2D layers provide superior conductivity, chemical stability, and diverse catalytic or electronic properties. The integration of these materials, illustrated in Fig. 9, leads to notable improvements in charge transport, electronic band modulation, and catalytic activity, reinforcing their structural and functional complementarity.

One of the most notable outcomes of this hybridization is the modulation of electronic structure. In MOFs, charge transport is often restricted by their organic linkers, whereas TMDs, such as MoS_2 and WSe_2, provide efficient pathways for electron and ion mobility. Intimate MOF–TMD interfaces promote rapid charge transfer, suppress recombination, and generate new electronic states that enable enhanced photocatalytic and electrochemical responses (Kan et al., 2024). This cooperative effect also allows the hybrids to operate effectively across wider potential windows and under broader light absorption ranges compared with their pristine counterparts. Catalytically, the dense unsaturated coordination sites of MOFs create abundant centers for adsorption and activation (Xue et al., 2021), while the edge-rich TMD surfaces accelerate electron donation and reaction kinetics (Hosseini

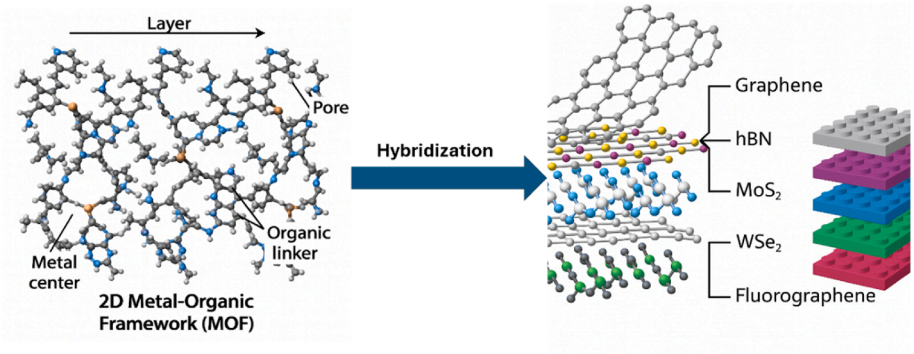


Fig. 9. Schematic of 2D-MOF hybridization with layered materials (graphene, hBN, MoS_2, WSe_2, fluorographene).

and Safarifard, 2024). The porous MOF framework ensures access to these active centers, while the conductive TMD layers prevent charge accumulation and structural collapse under cycling conditions.

Recent studies provide strong experimental validation of these hybridization strategies, demonstrating clear performance advantages over pristine counterparts. In energy storage, Sun et al. (2023) reported that amorphous Cu_3BHT grown on 1T(H)-MoS_2 achieved a specific capacitance of 329.9 F/g, more than double that of pure MoS_2, while MOF–MXene hybrids delivered further improvements through the combination of ion-accessible porosity and high conductivity (Gaba et al., 2024). Ashraf et al. (2026) advanced this concept with MOF-5/WSe_2@g-C_3N_4 composites, which attained exceptional energy and power densities in supercapatteries. Catalytic applications show similar benefits, Zhou et al. (2025) reviewed progress on MOF-based materials and highlighted that integrating Ni-MOF nanosheets with Pt nanostructures can markedly enhance hydrogen evolution activity, and Ma et al. (2019) synthesized $Cu_{0.9}Co_{2.1}S_4$@MoS_2 composites from bimetallic MOFs that achieved hydrogen production rates exceeding 40000 μmol/h/g under visible light, significantly surpassing undoped analogs. Hybridization has also been used to extend sensing and electronic functionality, as was evidenced by Koo et al. (2018) in WS_2 encapsulated in Co,N-doped hollow carbon nanocages, which showed superior NO_2 sensing, and by Zou et al. (2017) as Au nanoparticle/MoS_2 heterostructures, which improved electrochemical biomolecule detection. Also, hybridizing TMDs with GaN substrate materials was shown by Zhang et al. (2018) as enhancing vertical transport, enabling tunneling and a diode-like nature absent in isolated TMD layers. Collectively, these communications indicate how tailored MOF–TMD interfaces lead to emergent properties such as expanded capacitance, enhanced catalytic turnover, and expanded sensitivity well in excess of additive contributions by the pristine individual materials.

3.2. *Mechanisms of synergy in energy harvesting*

The superior efficiency of 2D-MOF/TMD hybrids in energy harvesting stems from interfacial charge-transfer processes and favorable band alignment that jointly suppress carrier recombination and extend light absorption as illustrated in Fig. 10. At the MOF–TMD interface, ultrafast electron migration circumvents momentum mismatch, a phenomenon observed in TMD heterostructures where excess electronic energy and defect-mediated states enable efficient charge separation even without lattice matching (Zhu et al., 2017). This rapid transfer reduces exciton binding energy and prevents electron–hole recombination, particularly when guided by type-II band alignment that spatially separates carriers across layers (Hu et al., 2024). Additionally, bandgap tuning of TMDs, such as the shift from indirect to direct transitions in monolayer MoS_2 broadens light absorption and facilitates stronger coupling with MOF-based excitonic states, enhancing photon-to-charge conversion efficiency (Al-Ghiffari et al., 2022). Computational investigations confirm that lateral heterostructures, with stronger orbital hybridization, exhibit faster electron transfer dynamics than vertical stacking, highlighting the role of interfacial geometry in dictating synergy (Zheng et al., 2019).

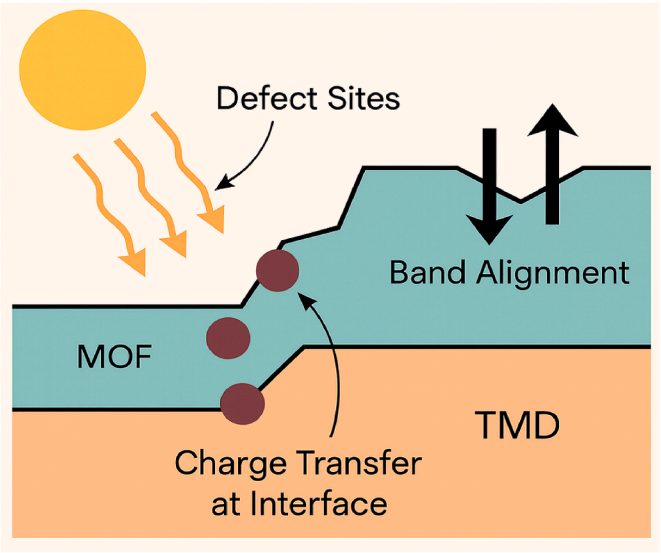


Fig. 10. Schematic illustration of mechanisms in 2D-MOF/TMD hybrids for energy harvesting.

The superior efficiency of 2D-MOF/TMD hybrids arises from three quantifiable synergistic mechanisms operating at the heterojunction interface: (1) type-II bands alignment-driven charge separation, (2) interfacial orbital hybridization and charge transfer kinetics, and (3) defect-mediated catalytic site generation.

Electronic band alignment and carrier separation: Type-II band alignment at 2D-MOF/TMD interfaces ensures spatial separation of photogenerated electrons and holes across layers, suppressing recombination. Specifically, when MOF valence band maximum (VBM) energy is lower than TMD VBM, and MOF conduction band minimum (CBM) is higher than TMD CBM, electrons preferentially accumulate in the TMD layer while holes localize in the MOF layer. This energy cascade creates an ‘energy downhill' pathway (as quantified through DFT calculations with GW corrections) that reduces the effective barrier for carrier transfer. Recent computational studies reveal that this band offset typically ranges from 0.3 to 0.8 eV depending on MOF/TMD composition, with optimal offsets maximizing carrier lifetime while maintaining transfer efficiency (Guan and Han, 2019; Ma et al., 2023; Tong et al., 2025). Interface quality directly impacts band alignment: atomic-scale defects, disorder, or residual adsorbates shift band edges by 50–200 meV, thereby modulating charge extraction by 10%–40%.

Charge transfer kinetics at heterojunctions: Electron transfer at 2D-MOF/TMD interfaces proceeds via coherent and incoherent pathways. Time-resolved pump-probe spectroscopy reveals that coherent transfer occurs within 10–100 fs at pristine, well-ordered interfaces, driven by orbital overlap of MOF ligand π-states with TMD metal d-orbitals. This ultrafast timescale circumvents momentum mismatch limitations observed in direct band-to-band transitions. Quantitatively, charge transfer efficiency (defined as the fraction of photogenerated carriers transferred before recombination) improves from ~60% in isolated TMDs to >90% in optimized hybrids. Interfacial resistance (measured by electrochemical impedance spectroscopy (EIS)) decreases from 100 to 500 Ω cm^2 for pristine MOFs to 5–50 Ω cm^2 for MOF/TMD composites, directly proportional to improved photocurrent. The Marcus theory framework predicts that transfer rates scale with reorganization energy (λ) and electronic coupling ($|V|^2$); optimal design minimizes λ while maximizing interfacial coupling through defect engineering and composition tuning (Hu et al., 2024; Zhang et al., 2025).

Interfacial chemical bonding and defect-assisted catalysis: At the molecular scale, heterojunction interfaces form through van der Waals interactions or, in some designs, covalent bonding between MOF metal nodes (e.g., Zn^{2+}, Co^{2+}) and TMD chalcogen vacancies. These interactions create new electronic states at the Fermi level, quantified by density of states (DOS) calculations. Importantly, oxygen vacancies in MOF linkers and sulfur vacancies in TMDs act as catalytically active sites, not detrimental defects but rather functional elements. Defect concentrations can be tuned (typically 0.1%–5% of lattice sites) to optimize the balance between enhanced catalytic activity and acceptable electronic quality. X-ray absorption fine structure (XAFS) spectroscopy and X-ray photoelectron spectroscopy (XPS) reveal that defects create localized electronic states 0.2–0.5 eV above the Fermi level, which serve as nucleation sites for adsorbates (e.g., *OH, *OOH in OER). Synergistic catalytic ensembles emerge when metal nodes in MOFs cooperate spatially with TMD edge sites, reducing activation barriers for multi-step reactions by 30–60 kJ/mol compared to single materials (Chakraborty et al., 2021; Gao et al., 2025; Lu et al., 2023; Singh and Sivaramakrishna, 2024).

Experimental and computational studies have quantified these interfacial processes. For instance, charge transfer dynamics at 2D-MOF/TMD junctions have been investigated using EIS, which quantifies interfacial resistance, and time-resolved spectroscopy to measure the rate of electron transfer at the junctions (Raikwar and Panda, 2025). Additionally, DFT studies have been used to predict the band alignment at 2D-MOF/TMD interfaces, revealing the role of type-II band alignment in facilitating efficient charge separation (Oh et al., 2024). These computational and experimental approaches provide a detailed understanding of how charge transfer, band alignment, and interfacial resistance contribute to the performance of 2D-MOF/TMD hybrids in energy harvesting.

Decoupling the contribution of intrinsic defects from true interfacial synergy is challenging but essential for understanding how they each contribute to the enhanced electrochemical or catalytic performance of 2D-MOF/TMD hybrids (Ramachandran et al., 2026). While intrinsic defects, such as vacancies and dopants, play an important role in modulating electronic properties and introducing active sites for reactions, their contribution to performance must be carefully distinguished from the effects of interfacial synergy. Experimental and computational approaches, such as controlled defect engineering and interface characterization techniques, can help decouple these contributions.

To optimize the performance of hybrid 2D-MOF/TMD systems, the following design principles are proposed. First, pore size should be adjusted to suit the TMD phase, with smaller pores being ideal for monolayer TMDs to enhance charge transfer, while larger pores are more appropriate for multilayer TMDs to boost catalytic activity. Second, metal node selection in 2D-MOFs should be based on compatibility with the TMD phases, particularly concerning band alignment. For example, transition metals like Ni or Co in MOFs should be paired with TMDs like MoS_2 to promote type-II band alignment for efficient charge separation. Lastly, defect engineering should be employed by introducing defects, such as vacancies or dopants, in both MOFs and TMDs, creating active sites for catalysis without compromising material stability. These design rules can be experimentally tested using DFT simulations, electrochemical techniques, and material characterization methods.

While these 2D-MOF/TMD materials show significant improvements in individual components (such as charge transfer and band alignment), the integration of these systems into fully packaged devices such as supercapacitors, PENGs, and TENGs is still an area of ongoing development. Future studies should focus on integrating these hybrid systems into fully functional energy-harvesting devices and comparing their performance metrics, including energy density, efficiency, and power output, with commercial benchmarks to assess their scalability and practical applicability in real-world applications.

Beyond electronic alignment, structural defects, catalytic ensembles, and excitonic effects contribute significantly to the cooperative activity of these hybrids. Defect engineering introduces cationic vacancies in both MOFs and TMDs, which not only enrich surface electron density but also act as catalytically active centers for reactions such as hydrogen evolution and CO_2 reduction (Ding et al., 2023). These defect sites modulate phonon modes, slowing down nonradiative recombination pathways in favorable cases (Li and Carter, 2019). Furthermore, catalytic ensembles, where metal nodes in MOFs cooperate with sulfur or selenium edge sites in TMDs, create complementary reactivity that exceeds the sum of their standalone activities (Wun et al., 2024). Excitonic effects further enhance cooperation: the formation of long-lived interlayer excitons in TMD domains coupled with MOF porosity ensures prolonged lifetimes for charge carriers, sustaining photocatalytic and electrocatalytic cycles (Fang and Ju, 2018). Collectively, these mechanisms, including interfacial charge transfer, bandgap alignment, defect-assisted catalysis, and excitonic stabilization, create a collaborative platform in which MOFs and TMDs reinforce each other's strengths, enabling highly efficient and durable energy-harvesting systems.

3.3. Role of interface engineering

Engineering the interface between 2D-MOFs and TMDs plays a crucial role in optimizing charge dynamics, stability, and multifunctional performance in energy-harvesting devices. Interface modification, such as introducing organic molecules or polymers onto TMD surfaces, can passivate surface defects, enhance charge separation, and improve the interfacial properties. This leads to efficient charge transfer, which is critical for applications such as photovoltaics and photoelectrochemical cells (Cho et al., 2019). Additionally, quantum coherence at the $MoS_2/MoSe_2$ interface has been shown to facilitate rapid charge transfer, with electron and hole carriers moving in sub-picosecond timescales, which is essential for efficient light-to-electricity conversion (Long and Prezhdo, 2016).

In terms of stability, composite structures made from TMDs and materials like biochar or covalent organic frameworks (COFs) enhance both the structural integrity and performance of the devices. For instance, the $C@WS_2–MoS_2$ heterostructures anchored on biochar exhibit high cycling stability in lithium-ion batteries, while COF-supported Cu_2WS_4 nanoparticles show improved performance in mercury removal (Wang et al., 2022; Xie et al., 2025). Strain engineering and phase transitions in TMDs, like MoS_2, have also been demonstrated to improve their stability by tuning band structures, making them more robust under operational conditions (Ouyang et al., 2016).

To further enhance multifunctional performance, lateral heterojunctions with sharp interfaces can promote high separation efficiency of photogenerated carriers, leading to superior photoelectric properties. $MoS_2–WS_2$ lateral heterojunctions, for instance, exhibit high external quantum efficiency (EQE), improving performance for optoelectronic

applications (Li et al., 2022). Additionally, surface functionalization with thiolated ligands has been shown to improve triboelectric nanogenerator (TENG) performance by increasing output voltage and power density, thanks to defect engineering and p-type doping effects (Kim et al., 2021).

However, interface engineering in 2D-MOF/TMD hybrids leverages functionalization, nano-structuring, and advanced design strategies like Z-schemes and hetero-phase TMDs to significantly enhance charge dynamics, redox activity, and long-term stability. These strategies contribute to the development of highly efficient and durable energy-harvesting devices.

Quantitative descriptors such as band offsets and charge-transfer resistance play key roles in this optimization. Band alignment, which refers to the relative positioning of the conduction and valence bands of the two materials, is crucial for enhancing charge transfer at the interface. For instance, larger energy level offsets result in lower charge transfer efficiency but longer charge-separated state lifetimes, as reported in a study on monolayer MoS_2 combined with organic semiconductors (Raoufi et al., 2023).

In addition to charge transfer, interfacial binding energies, which can be assessed through XPS or DFT, provide insight into the strength of interactions between the 2D-MOF and TMD layers. Stronger binding energies generally lead to more stable hybrids, reducing material degradation during device cycling. Studies show that strong coupling between excitons in TMD monolayers and optical nanocavities, facilitated by various optical resonances, results in large binding energies in these heterostructures (Li et al., 2025). Spectroscopic techniques, such as fluorescence spectroscopy, fluorescence lifetime tests, and photocurrent response measurements, provide further evidence for enhanced charge transfer in hybrid materials like $Cu_{0.9}Co_{2.1}S_4$@MoS_2 composites, which exhibit improved photocatalytic hydrogen evolution performance (Ma et al., 2019).

Additionally, charge-transfer resistance can be quantitatively analyzed using EIS. Integrating MoS_2 nanosheets into a covalent organic framework (COF) has been shown to significantly reduce charge transfer resistance, enhancing charge separation and stability during photocatalytic reactions (Kumar et al., 2025). Similarly, hybridization of $Cu_{0.9}Co_{2.1}S_4$@MoS_2 composites results in low resistance electron transfer, which improves the photocatalytic performance (Ma et al., 2019).

To further enhance performance, introducing quantum coherence at the MoS_2/$MoSe_2$ interface has been shown to facilitate rapid charge transfer in sub-picosecond timescales, essential for efficient light-to-electricity conversion (Bai et al., 2025). This quantum coherence can be quantified by measuring the electron-hole recombination time, a metric that directly impacts device efficiency in photovoltaic and photoelectrochemical applications.

Interface engineering in 2D-MOF/TMD hybrids leverages a combination of functionalization, nano-structuring, and advanced design strategies such as Z-schemes and hetero-phase TMDs. These strategies not only enhance charge dynamics but also significantly improve redox activity and long-term stability. For instance, hybridizing TMDs with materials like biochar or COFs can improve structural integrity and cycling stability, while also enhancing electrocatalytic activity for energy conversion processes (Ashraf et al., 2026).

Table 4
Translating 2D-MOF/TMD materials and interface descriptors into device-level figures of merit (FoM) and operational lifetime endpoints for energy-harvesting applications.

Descriptor (materials/ interface metric)	Device-level mechanism	Device FoM(s) impacted (units/ conditions)	Realistic stressor/ failure mode	Mitigation and recommended stability endpoint	Ref.
Band alignment and interface quality (e.g., high work-function interlayers)	Improves extraction; suppresses interfacial recombination	PV: PCE 28.96%, short-circuit current density (J_{sc}) 31.4 mA/cm^2, FF 80.8%, V_{oc} = 632 mV	Moisture/thermal instability; interfacial degradation; performance drift	Interface/band alignment optimization; PCE/V_{oc}/J_{sc}/ FF retention after light soaking/bias	Chen et al. (2024); Hu et al. (2024a)
MOF stability as encapsulant	Enhances moisture/ thermal robustness in-device	PV: stability expected to improve via MOF encapsulation	Moisture-driven degradation; photo/ thermal instability	Encapsulation and interface engineering; efficiency retention vs time under realistic exposure	Satnami et al. (2024)
High surface area and pore structure (BET)	More active sites; improved ion transport	SC: 1668.7 F/g @ 2 A/g; 90.3% @ 5000 cycles (5 A/g); device 57.29 Wh/kg @ 160 W/kg	Cycling-induced fade	Pore/surface optimization; retention and energy/power density at stated rates	Zhang et al. (2018)
Pore hierarchy/pore-size tuning	Boosts rate capability; enables ultra-long cycling	78.8% retention (1 → 100 A/g); 2.2% loss @ 200000 cycles (50 A/g); plus device energy/power	High-rate limits; long-term electrode aging	Pore engineering; high-rate retention and very-long cycle stability	Miao et al. (2022)
Hybrid device assembly (Ni//Cu MOF and AC)	Practical device output under cycling/current load	Hybrid capacitor: 57 Wh/kg @ 1500 W/kg; Pmax 48000 W/kg; 9 Wh/kg @ 32 A/g; 94.3% @ 7000 cycles	Cycling/current stress degradation	Ragone-relevant performance; energy–power points plus retention after thousands of cycles	Deng et al. (2020)
Thermoelectric descriptors (S, σ, κ, mobility; interface phonon scattering)	Sets power factor/ZT; interfaces lower κ while preserving transport	$ZT = S^2\sigma T/\kappa$; $MoTe_2$ (1T'): μ 1434 cm^2/V/s, S 750 μV/K	Thermal gradients/ cycling; contact/ interface degradation	Interface/dimensionality/ chemical modification; power factor or ZT stability vs T or ΔT cycling.	Ge et al. (2020); Hippalgaonkar et al. (2017); Talin et al. (2016)
Piezoelectric descriptors (symmetry breaking; Janus coefficients; MOF ferroelectricity)	Higher polarization → higher output	MoS_2: 30 → 100 pA, 10 → 20 mV; MoSSe: 0.058 C/m^2, heterojunction 0.081 C/m^2; MOF composite: 12.20 V, 14.85 μW/cm^2	Mechanical fatigue; environmental exposure	Mechanical/structural design; output retention after repeated loading cycles (aligned with durability stressors)	Cui et al. (2018); Mula (2024); Prajesh et al. (2025); Rana et al. (2022)
Triboelectric descriptors (surface morphology; polymer matrix pairing)	Higher surface charge density; stronger contact electrification	MoS_2 TENG: 7.48 V, 0.82 μA; polymer matrices enhance charge density/morphology	Humidity/wear → charge decay	Protective coatings/ packaging; output vs RH% and retention after wear cycles	Prajesh et al. (2025); Priyadarshini et al. (2025); Rana et al. (2022)
Environmental durability (humidity/UV/ temperature; mechanical stress)	Defines operational lifetime; differentiates MOF vs TMD failure pathways	Degradation under moisture, UV, temperature fluctuations; MOF collapse/transformations (high humidity); TMD delamination/ fracture (extreme conditions)	Structural collapse (MOF); delamination/ fracture (TMD)	Protective coatings and self-healing matrices; FoM retention after humidity/UV/ thermal cycling	He et al. (2025); Kim et al. (2023)

While the preceding sections discuss key materials descriptors such as band alignment, defect chemistry, conductivity, porosity, and interfacial coupling, their implications for device-level performance should be made explicit. Accordingly, Table 4 maps commonly reported 2D-MOF/TMD material and interface metrics to the device figures of merit that govern practical energy-harvesting performance (efficiency, power density, and thermoelectric *ZT*) and to operational lifetime endpoints under realistic stressors (humidity, thermal cycling, UV/illumination, electrical bias, and mechanical fatigue). This translation framework is used to guide the application-focused discussion in Section 4.

4. Energy harvesting applications

The synergistic mechanisms detailed in the previous section, including enhanced charge separation, optimized band alignment, and superior structural stability, translate directly into tangible performance gains across a spectrum of energy harvesting applications. This section explores how 2D-MOF/TMD hybrids are being leveraged in photovoltaics, thermoelectrics, and mechanical energy harvesting, consistently demonstrating how their cooperative effects lead to efficiencies and functionalities unattainable by the parent materials alone.

4.1. Photovoltaic applications

4.1.1. Solar energy conversion

The synergy between 2D-MOFs and TMDs represents a paradigm shift in photovoltaic device architecture, offering unprecedented opportunities for enhanced solar energy conversion efficiency. This integrated approach leverages the unique properties of both material classes to overcome individual limitations while amplifying collective strengths (Ahmad et al., 2021; Hu et al., 2024). The integration of 2D-MOFs with TMDs creates multifunctional heterostructures that facilitate superior light harvesting, charge separation, increased porosity, and transport properties, all of which are essential for high-performance photovoltaic devices. TMDs such as $MoSe_2$, WSe_2, and MoS_2 exhibit exceptional optical and electronic properties that make them attractive for photovoltaic applications. Recent studies demonstrate that $MoSe_2$-based tandem photovoltaic architectures can achieve remarkable PCEs of 28.96% when optimally configured with silicon bottom cells (Hu et al., 2024). The key advantage lies in $MoSe_2$'s suitable bandgap of approximately 1.5 eV, which enables efficient light absorption in the visible spectrum while minimizing thermalization losses as shown in Fig. 11. The material's relatively lower bandgap compared to other TMDs like WS_2 and WSe_2 results in higher proportional light absorption, making it particularly effective for tandem cell configurations.

The integration of 2D-MOFs into TMD-based photovoltaic systems provides multiple benefits, including enhanced light-harvesting efficiency (LHE), improved charge transport properties, and superior interfacial engineering capabilities. MOF-derived transition metal oxides, synthesized through controlled thermal decomposition of parent MOF structures, offer tunable electronic properties and morphological characteristics that complement TMD absorption layers (Nizamudeen et al., 2023). For instance, Mn, Fe, and Ni-doped TiO_2 nanocrystals derived from MIL-125 MOF precursors demonstrate significant improvements in dye-sensitized solar cell performance, with PCEs reaching up to 20% (Hu et al., 2024; Nizamudeen et al., 2023). The porous structure of 2D-MOFs enables effective dye molecule adsorption, thereby improving LHE in hybrid photovoltaic devices (Nizamudeen et al., 2023). This increased porosity, combined with the inherent properties of MOF materials, provides numerous active sites for photon absorption and subsequent charge generation. Furthermore, the tunable nature of MOF chemistry allows for precise control over electronic band positions, enabling optimal energy level alignment with TMD components for efficient charge transfer processes. Hybrid organic-inorganic perovskite solar cells incorporating 2D-MOFs and TMDs have shown particular promise, with recent developments achieving PCEs exceeding 25.2% (Hu et al., 2024). The 2D layered materials counter certain challenges associated with perovskite systems, which are, namely, moisture stability, halide segregation, and hysteresis effects. The materials, TMD, MoS_2 and WSe_2, are well-suited as a hole transport layer, and

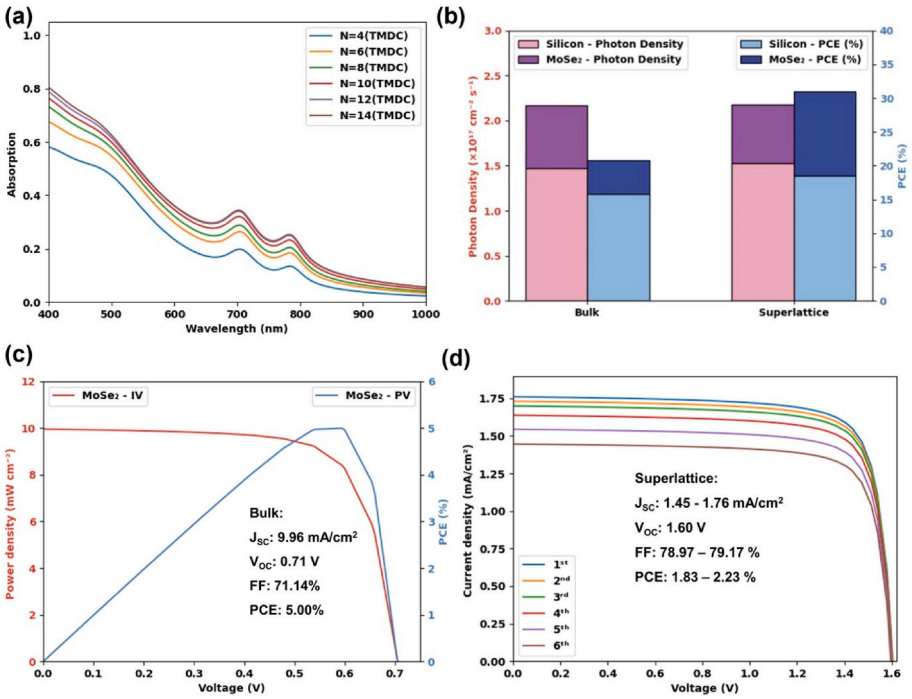


Fig. 11. Optimization of the superlattice top cell: (a) spectral absorption as a function of the number of TMDC layers; (b) comparison of photon absorption and efficiency between the superlattice design and a bulk-heterojunction cell; (c) I–V curve of the bulk cell; (d) I–V curves of individual superlattice layers (Hu et al., 2024).

2D-MOFs exhibit structural stability and efficient charge carrier dynamics.

4.1.2. Performance metrics

The energy conversion efficiency in 2D-MOF and TMD devices is characterized by a variety of performance indices, namely, PCE, EQE, and open-circuit voltage (V_{oc}). As recent findings have evidenced, photovoltaic devices based on TMDs have been capable of reaching upmarket EQE and PCE levels. Some impressive developments in heterojunction devices based on TMDs have been documented in other research works. A specific example is a monolayer MoS_2/p-Si heterojunction silicon photovoltaic solar cell demonstrating a 5.23% PCE value (Marwaha, 2025). Ongoing research on direct 2D-MOF/TMD hybrids remains new, yet 2D-material-based systems in perovskite solar cells (PSCs) give a sense of the potential. The integration of TMDs as hole or electron transport layers in PSCs has pushed efficiencies significantly (Satnami et al., 2024). By improving charge extraction and reducing recombination, these 2D layers contribute to higher J_{sc} and V_{oc}. It is projected that by optimizing the band alignment and interface quality in 2D-MOF/TMD heterostructures, PCE values well into the double digits are achievable. For example, some advanced tandem solar cell designs incorporating 2D materials are projected to reach efficiencies over 28% (Bankura and Biswas, 2025). The stability of these devices, another critical metric, is also expected to improve, with the MOF acting as a robust encapsulant (Satnami et al., 2024).

The performance evaluation of 2D-MOF/TMD hybrid photovoltaic devices reveals significant improvements across multiple metrics compared to individual component systems. Systematic analysis of tandem photovoltaic architectures incorporating six-layer $MoSe_2$ superlattices with optimized 40 nm SiO_2 antireflective coatings demonstrates PCEs of 28.96%, representing substantial improvement over single-junction c-Si solar cells (23.28%) (Hu et al., 2024). This enhancement results from the complementary absorption characteristics of the hybrid system, where TMDs capture high-energy photons while silicon efficiently harvests lower-energy portions of the solar spectrum. Current density improvements in hybrid systems are particularly noteworthy, with $MoSe_2$-based devices achieving J_{sc} of 31.4 mA/cm^2 when integrated with high-work-function interface layers such as MoO_3 (Chen et al., 2024). The enhanced current collection efficiency stems from improved built-in potential and reduced interface recombination losses.

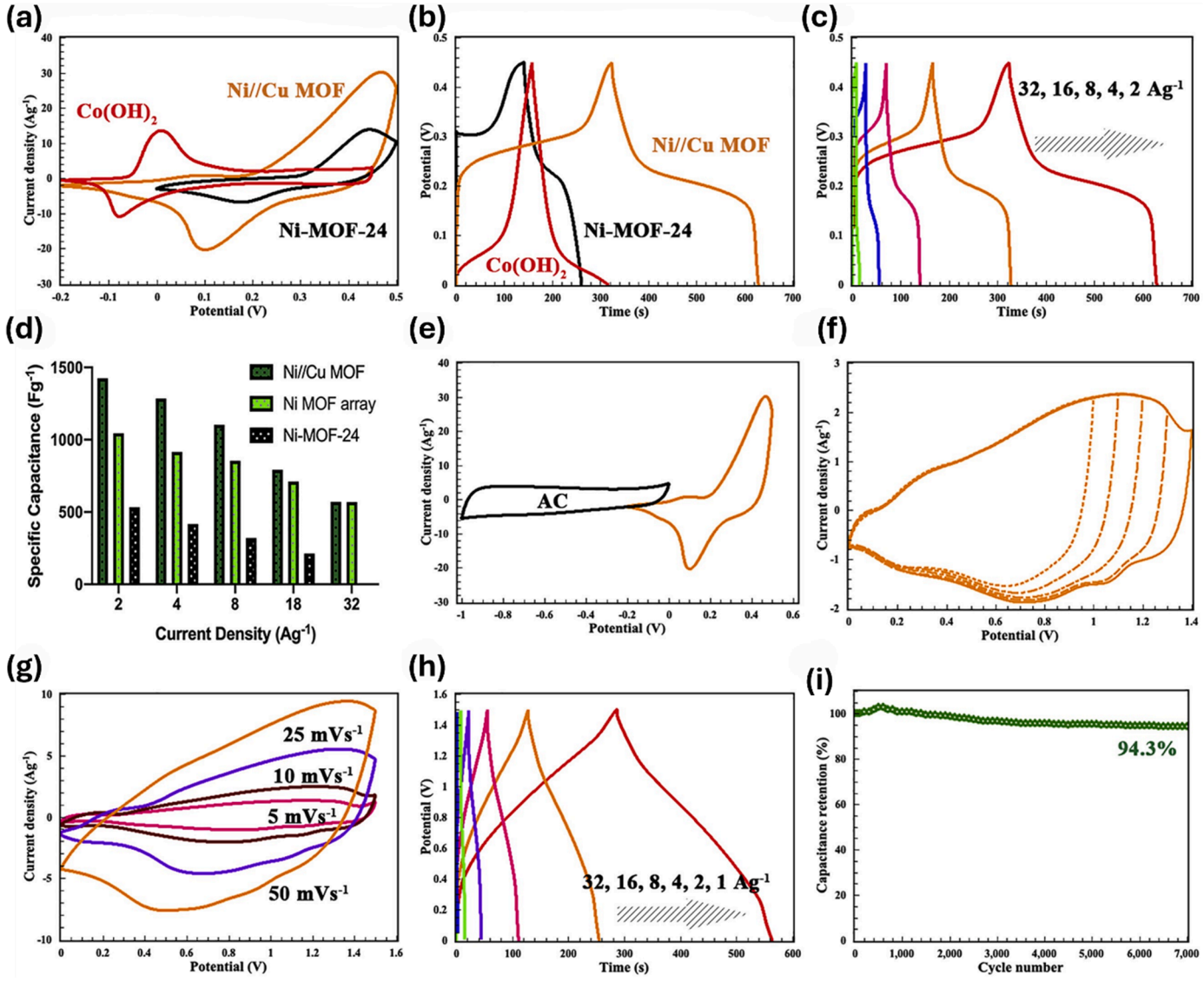


Fig. 12. Electrochemical performance of the Ni//Cu MOF electrode and hybrid supercapacitor. (a)–(d) Ni//Cu MOF shows high capacitance (1472 F/g) and excellent rate capability; (e)–(i) the assembled device with Ni//Cu MOF and AC electrodes delivers stable operation, good rate performance, and 94.3% retention after 7000 cycles (Deng et al., 2020).

Fill factors in optimized hybrid devices reach 80.8%, indicating excellent charge transport and collection properties. Voc enhancement represents another critical performance improvement, with hybrid PEDOT:PSS/Si solar cells incorporating MoO_3 interface layers achieving V_{oc} values of 632 mV (Chen et al., 2024). The electrochemical properties analysis of the Ni//Cu MOF electrode and the assembled hybrid supercapacitor is illustrated in Fig. 12. This hybrid capacitor can deliver a maximum energy density of 57 Wh/kg at a power density of 1500 W/kg at 1 A/g and a maximum power density of 48000 W/kg while the energy density remains 9 Wh/kg at 32 A/g (Deng et al., 2020).

This improvement results from enhanced charge separation at the heterojunction interface and reduced recombination losses. The high work function of integrated components creates favorable energy band alignment that facilitates efficient charge extraction while minimizing back-recombination processes. Spectral response analysis reveals that hybrid 2D-MOF/TMD systems exhibit superior performance across broader wavelength ranges compared to single-material devices. The complementary absorption characteristics of different TMD materials (WS_2, MoS_2, WSe_2, $MoSe_2$) enable tailored spectral response optimization (Romero et al., 2025; Shi et al., 2025). Despite similar total light absorption across various TMD materials, $MoSe_2$ demonstrates superior performance due to its optimal bandgap positioning and reduced excitonic binding energy effects. Stability metrics for hybrid photovoltaic devices show significant improvements over conventional organic photovoltaic systems. The integration of 2D-MOFs provides enhanced moisture resistance and thermal stability, while TMD components offer superior photostability under prolonged illumination. Long-term performance evaluation demonstrates maintained efficiency over extended operational periods, addressing critical commercialization requirements for photovoltaic technologies (Ding et al., 2025; Nam et al., 2024).

4.2. Thermoelectric applications

4.2.1. Energy conversion via heat gradients

TMDs have shown great potential for thermoelectric applications due to their unique electronic, thermal, and mechanical properties. The ability to independently modulate electrical and thermal conductivity in TMDs makes them ideal candidates for thermoelectric energy conversion (Ng et al., 2024; Zhou et al., 2022). For instance, the quantum size effect and layer-dependent properties of TMDs can be exploited to enhance their thermoelectric performance (Ng et al., 2024). The thermoelectric properties of hybrid 2D-MOF/TMD materials represent a frontier in waste heat recovery and energy conversion technologies. These materials combine the unique electronic structures of TMDs with the tunable porosity and chemical diversity of MOFs to create superior thermoelectric performance characteristics (Ge et al., 2020; Hippalgaonkar et al., 2017). The fundamental thermoelectric performance is governed by the dimensionless figure of merit $ZT = S^2\sigma T/\kappa$, where S represents the See-beck coefficient, σ denotes electrical conductivity, T is absolute temperature, and κ represents thermal conductivity. The $1T''$ phase of TMDs shows particularly promising thermoelectric characteristics, with theoretical calculations predicting ZT values exceeding unity at moderate temperatures. $MoTe_2$ in the $1T''$ phase demonstrates hole carrier mobility of 1434 $cm^2/V/s$ at room temperature, significantly higher than other TMD phases (Ge et al., 2020). This enhanced mobility, combined with favorable See-beck coefficients reaching 750 μV/K, results in exceptional thermoelectric power factors.

The integration of 2D-MOFs into TMD-based thermoelectric devices provides several advantages including reduced thermal conductivity through phonon scattering at interfaces and enhanced electrical conductivity through improved charge transport pathways (Hippalgaonkar et al., 2017; Talin et al., 2016). MOF-derived materials exhibit inherently low thermal conductivity due to their porous structure and organic-inorganic hybrid composition. Cu_3(2,3,6,7,10,11-hexahydroxytriphenylene)$_2$ (Cu_3(HHTP)$_2$) MOFs demonstrate power factors of 0.757 μW/m/K when optimized through molecular iodine incorporation (Gonzalez-Juarez et al., 2023). The guest molecule infiltration strategy in MOF systems significantly enhances thermoelectric performance by modifying electronic structure and transport properties. TCNQ@Cu_3(BTC)$_2$ systems show drastically improved electrical conductivity ($\sigma = 0.45$ S/m) compared to pristine MOF materials, although thermal conductivity also increases (Talin et al., 2016). The challenge lies in optimizing the trade-off between enhanced electrical conductivity and increased thermal conductivity to maximize overall ZT performance.

4.2.2. Recent advancements

Recent advancements in hybrid 2D-MOF/TMD thermoelectric systems focus on interface engineering, dimensionality control, and chemical modification strategies to optimize performance metrics (Muchuweni and Mombeshora, 2023; Pallecchi et al., 2020). Field-effect tunability in TMD-based thermoelectric devices enables reversible optimization of power factors through electrostatic gating, with single-layer MoS_2 and WSe_2 films demonstrating nearly order-of-magnitude power factor tuning through ambipolar field effect (Pallecchi et al., 2020). Nano-structuring approaches using LPE of TMDs combined with polymer composites have achieved significant performance improvements. TMD nanoflake assemblies with optimized morphology and concentration demonstrate power factors reaching 0.046-0.049 mW/m/K at 3 wt%-5 wt% MoS_2 concentration (Pallecchi et al., 2020). The extremely low thermal conductivity (0.27 W/m/K) in these composite systems enables ZT values of 0.04 at room temperature, representing a substantial improvement over individual component material (Ali et al., 2024; Bilc et al., 2021).

Advanced synthesis techniques, including CVD and layer-by-layer growth methods, enable precise control over hybrid material architecture and interface properties (Luo et al., 2024; Shekhah, 2010). Low-temperature CVD synthesis of TMDs allows for direct integration with temperature-sensitive MOF components while maintaining material quality and performance. Multi-step CVD approaches demonstrate successful growth of MOF thin films with controlled thickness and orientation, enabling optimized thermoelectric device architectures (Zhang et al., 2023). The development of flexible and wearable thermoelectric devices utilizing hybrid 2D-MOF/TMD materials represents a significant advancement toward practical applications. These systems combine mechanical flexibility with maintained thermoelectric performance, enabling integration into wearable electronics and IoT sensor networks. The low-dimensional nature of both MOF and TMD components provides inherent mechanical flexibility while preserving electronic transport properties essential for thermoelectric function.

4.3. Piezoelectric and triboelectric energy harvesting

The piezoelectric and triboelectric energy harvesting capabilities of hybrid 2D-MOF/TMD materials stem from their unique structural and electronic properties that enable efficient mechanical-to-electrical energy conversion (Pang et al., 2025; Yang and Lee, 2019). Piezoelectric effects in these materials arise from non-centrosymmetric crystal structures that generate electric polarization under mechanical stress, while triboelectric mechanisms involve contact electrification and electrostatic induction processes. TMDs exhibit remarkable piezoelectric properties due to their layered crystal structure and broken inversion symmetry in odd-numbered layers (Cui et al., 2018; Mula, 2024). MoS_2 demonstrates significant piezoelectric coefficients, with surface treatment enhancing current output from 30 to 100 pA and voltage increasing from 10 to 20 mV (Mula, 2024). The piezoelectric response can be further enhanced through defect engineering and chemical modification, with sulfur treatment of MoS_2 showing ten-fold enhancement in maximum power output (Cui et al., 2018).

Janus TMD structures, featuring asymmetric sandwich construction with different chalcogen atoms, exhibit exceptionally high out-of-plane piezoelectricity. MoSSe Janus structures demonstrate piezoelectric

coefficients of 0.058 C/m^2 for monolayers, with van der Waals heterojunctions of MoSSe-BlueP achieving even higher values of 0.081 C/m^2 (Rana et al., 2022). This enhanced piezoelectric response results from broken reflection symmetry and out-of-plane electric polarization in addition to conventional in-plane effects. 2D-MOFs contribute to piezoelectric energy harvesting through their ferroelectric properties and structural flexibility. Octahedral cage assemblies such as $Co_6(H_2O)_{12}(TPTA)_{812}{\cdot}50H_2O$ demonstrate pronounced ferroelectric

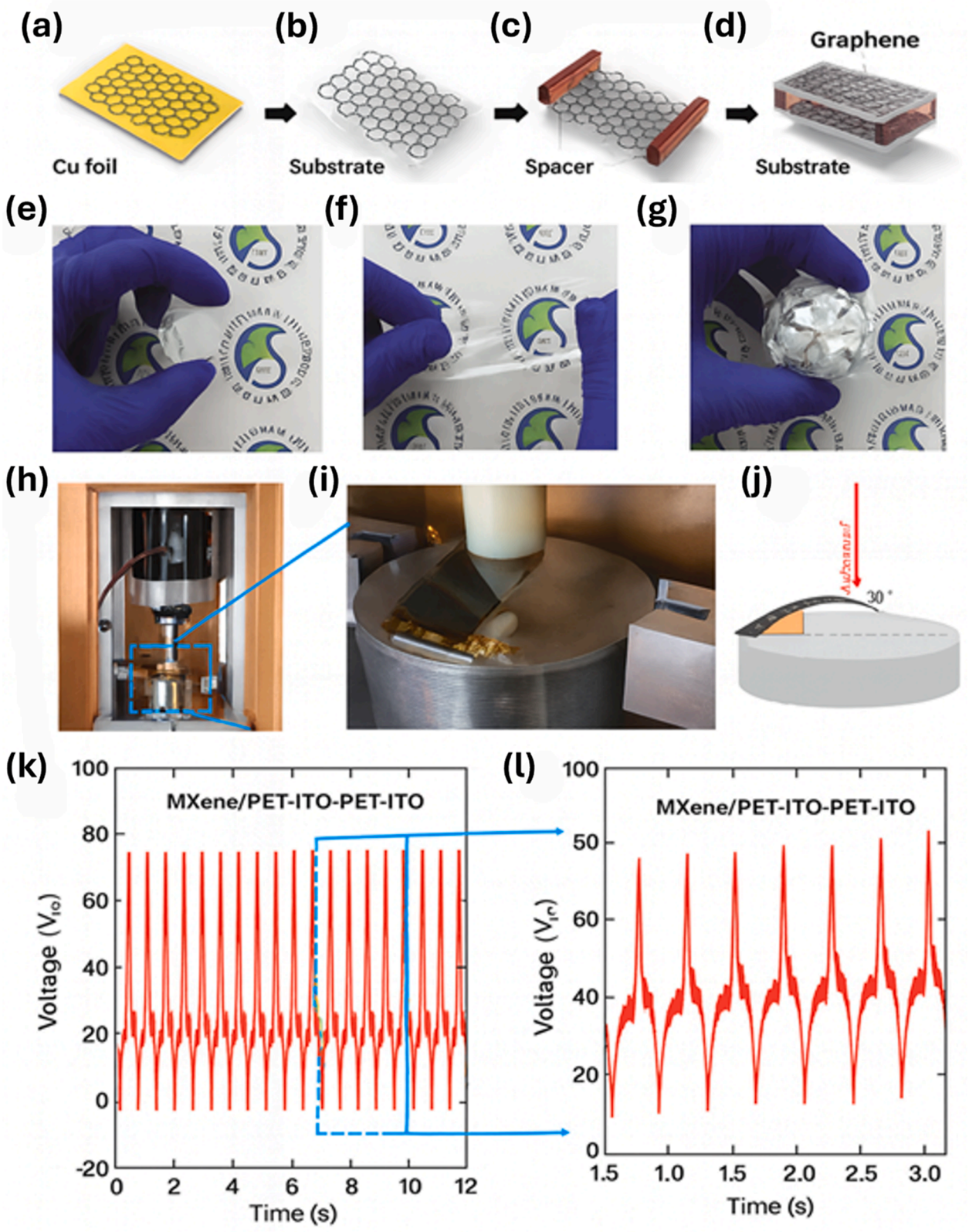


Fig. 13. Schematic diagrams of device fabrication and compatibility of graphene with an arbitrary substrate (a)–(g). The flexible MXene TENG was operated with a force of 1 N applied at 2 Hz by the mandrel (h)–(l) (Dong et al., 2018a; Kim et al., 2014).

behavior with remnant polarization of 6.84 μC/cm (Prajesh et al., 2025). These MOF-based systems exhibit characteristic amplitude-butterfly and phase-hysteresis loops confirming their piezoelectric nature, with composite devices achieving maximum peak output voltages of 12.20 V and power densities of 14.85 μW/cm (Prajesh et al., 2025).

Triboelectric mechanisms in hybrid systems involve contact electrification between different materials and subsequent electrostatic induction (Priyadarshini et al., 2025; Rana et al., 2022). Researchers have made several attempts to fabricate triboelectric devices using 2D materials to better understand and evaluate their triboelectric properties. For instance, Kim et al. (2014) pioneered the development of a flexible, transparent TENG device using graphene, which could power commercial LEDs without any external energy source. Similarly, Dong et al. (2018) demonstrated high-performance TENG devices using novel materials like fluorinated MXene, showcasing their potential in both rigid and flexible TENG applications. These MXene-based TENGs can be seamlessly integrated into various accessories, such as wrist bands and textiles as illustrated in Fig. 13. TMDs exhibit distinct positions in the triboelectric series, with MoS_2 and $MoSe_2$ showing negative polarity while other 2D materials demonstrate positive polarities (Rana et al., 2022). MoS_2-based TENGs achieve output voltages of 7.48 V and currents of 0.82 μA, representing the highest negative triboelectric charging characteristics among investigated 2D materials. The combination of TMDs with polymer matrices enables enhanced triboelectric performance through optimized surface morphology and charge density (Prajesh et al., 2025; Priyadarshini et al., 2025). Electrospinning techniques facilitate dipole alignment and β-phase formation in polymer components, while TMD nanofillers provide enhanced mechanical properties and electrical conductivity. These composite systems demonstrate superior performance metrics including output voltages up to 145 V and current densities of 350 $\mu A/cm^2$ (Kim et al., 2021; Rana et al., 2022).

To quantitatively underscore the performance advantages conferred by synergistic hybridization, Table 5 provides a comparative analysis of key performance metrics for hybrid 2D-MOF/TMD systems versus their individual components across different energy harvesting applications. The data clearly illustrate that the integration of these materials leads to substantial, quantifiable improvements in efficiency, energy/power density, and output, directly validating the impact of the synergistic effects discussed.

4.4. Computational design and interface engineering

Computational studies, including DFT and machine learning (ML), have provided critical insights into interface design, defect engineering, and phase selection in 2D-MOF/TMD hybrids, guiding experimental strategies and accelerating the development of energy-harvesting devices. These methods have been instrumental in predicting material properties, optimizing charge transfer, and improving device performance.

DFT plays a central role in predicting band alignments and energy offsets at the interfaces of 2D-MOF/TMD hybrids. For instance, DFT calculations combined with graph neural networks (GNNs) have been used to predict band offsets with high accuracy. These predictions help optimize charge transfer and reduce carrier recombination at heterojunctions, crucial for improving the performance of energy devices such as photovoltaics and photoelectrochemical cells (Choudhary and Garrity, 2024). The InterMat framework, which combines DFT and GNNs, has been instrumental in assessing work functions and electron affinities, achieving remarkable accuracy and guiding interface design for TMD/MOF hybrids. Additionally, the use of Zur's algorithm and unified GNN force-fields helps in predicting high-quality interfaces, addressing conformation challenges in interface design, and ensuring that hybrid systems exhibit optimal electronic properties (Choudhary and Garrity, 2024).

In the realm of defect engineering, DFT has enabled the design of active sites for catalytic reactions by introducing specific defects such as vacancies, dopants, or interfaces. These defects modulate the electronic structure, leading to enhanced catalytic activity. For example, studies on MoS_2 polymorphs have shown that defective monolayers exhibit significantly higher catalytic performance for HER compared to pristine materials (Zhang et al., 2025). X-ray absorption fine structure (XAFS) techniques are used to quantify defect concentrations and validate the effects of these defects on the catalytic properties, further demonstrating the effectiveness of DFT in optimizing catalytic systems. These findings, based on computational predictions, have been experimentally verified, highlighting the importance of defect engineering in improving material performance.

Furthermore, ML has become a valuable tool in material science, particularly for predicting phase stability and optimizing material properties. By analyzing large datasets of DFT-calculated energies, ML models such as K-nearest Neighbor (K-NN) and Support Vector Machines (SVM) are used to predict the thermodynamic stability of materials and screen potential candidates for energy applications. These ML models accelerate the discovery of new materials by efficiently navigating vast chemical spaces and predicting material properties. In the context of energy materials, ML has been applied to batteries, electrocatalysts, and solar cells, enabling rapid screening and optimization of materials for specific applications, such as increasing electrocatalytic activity and enhancing energy storage efficiency (Shetty et al., 2022). However, challenges remain in terms of data quality and model generalization. To address these, emerging solutions like equivariant architectures and

Table 5
Comparison of performance metrics for hybrid system and individual components.

Application	Material system	Key performance metric	Pristine value	Hybrid value	Performance gain (%)	Ref.
Supercapacitor	Cu_3BHT/MoS_2	Specific capacitance	~155 F/g (Pristine MoS_2)	329.9 F/g	112.8%	Sun et al. (2023)
Supercapacitor	Ni-MOF/Graphene	Cycling stability (10000 cycles)	~85% (Pristine Ni-MOF)	97.7%	14.9%	Gautam et al. (2024)
Battery-supercapacitor hybrid	MoS_2@VZnS//AC	Energy density	~25 Wh/kg (Pristine MoS_2)	39.5 Wh/kg	58.0%	Imran et al. (2024)
Photovoltaics	$MoSe_2$/Silicon	Power conversion efficiency (PCE)	23.28% (c-Si cell)	28.96% (Tandem cell)	24.4%	Hu et al. (2024)
Piezoelectric (PENG)	MoS_2 (Surface treated)	Output current	30 pA	100 pA	233.3%	Pang et al. (2025)
Piezoelectric (PENG)	SnS_2/SnS	Output voltage	~42 mV (Pristine SnS_2)	60 mV	42.8%	Khan (2024); Xia et al. (2025)
Triboelectric (TENG)	$Mo_{0.5}W_{0.5}S_2$ (with light)	Output current	~0.5 μA (Dark)	~1.76 μA (Light)	252.0%	Chen et al. (2026)
Hydrogen evolution (HER)	1T′-$ReSe_2$/CNTs	Overpotential (η_{10})	~95 mV (Pristine $ReSe_2$)	23 mV	−75.8% (Lower is better)	Ndala (2022)

physics-informed neural networks are improving the accuracy and predictive capabilities of ML models, enabling more robust material designs (Kim, 2026). These studies directly quantify the charge transfer dynamics, band alignment, and interfacial resistance at 2D-MOF/TMD junctions, offering both theoretical predictions and experimental validation that guide the design of high-performance hybrid materials for energy harvesting and catalytic applications.

However, the integration of DFT, defect engineering, and ML has greatly advanced the understanding of 2D-MOF/TMD hybrids. These computational insights not only provide a deeper understanding of the interface design and defect engineering processes but also accelerate the development of materials with enhanced electronic and catalytic properties. The combination of theoretical predictions and experimental validation continues to shape the design of high-performance materials for energy harvesting and catalytic applications, setting the stage for the next generation of 2D hybrid systems.

5. Fabrication and characterization techniques

5.1. Synthesis techniques for 2D-MOFs and TMDs

The successful fabrication of synergistic 2D-MOF/TMD hybrids is fundamentally dependent on synthesis techniques that can precisely control the interface where these cooperative effects originate. Similarly, advanced characterization methods are essential to probe and confirm the structural and electronic interactions that define this synergy. This section reviews the key fabrication and characterization techniques that enable the rational design and verification of high-performance hybrid materials, with a focus on methods that are crucial for engineering and understanding the MOF-TMD interface.

5.1.1. Solvothermal and hydrothermal methods for 2D-MOFs

Solvothermal and hydrothermal synthesis methods represent the most widely adopted approaches for 2D-MOF fabrication, offering precise control over crystal growth kinetics, morphology, and structural properties (Bai et al., 2021; Li et al., 2021). These techniques utilize elevated temperature and pressure conditions within sealed reaction vessels to promote controlled nucleation and growth processes essential for high-quality 2D-MOF formation. The hydrothermal method involves the reaction of metal salts with organic ligands in aqueous solutions at temperatures typically ranging from 80°C to 200°C under autogenous pressure. This approach has proven particularly effective for synthesizing 2D microporous Al-MOFs such as CYCU-7 and CAU-11, where systematic control of reaction conditions enables tunable defect concentrations and structural properties (Udourioh et al., 2023). Water-based hydrothermal synthesis generally produces MOFs with fewer linker-missing defects compared to ethanol-based solvothermal approaches, highlighting the critical role of solvent selection in determining final material quality (Udourioh et al., 2023). A typical synthesis method employed for the preparation of MoS_2/PVDF-HFP fiber membrane used in triboelectric nanogenerator application is illustrated in Fig. 14.

Solvothermal synthesis broadens the hydrothermal principle to non-aqueous solvents, providing access to MOF structures that are unstable or inaccessible in aqueous media (Lin et al., 2018). The technique generally utilizes organic solvents like methanol, DMF, or ethanol as reaction media. Recent work shows the potential to modulate Lewis/Brønsted catalytic activity in materials in the Hf-MOF-808 class through judicious choice of solvent during solvothermal synthesis, showing the dramatic influence of synthesis conditions on functional properties (Udourioh et al., 2023). Computer control over multi-step hydrothermal synthesis is a major improvement in 2D-MOF synthesis technology (Ghosh et al., 2023). The technique employs 3D-printed reactor systems equipped with chambered compartments that allow sequence and time control on reaction steps. Fabrication involves polypropylene reactor build-up with computer-programmed pauses in response to reagent addition, followed by hermetic sealing and thermal annealing control (Li et al., 2021). The technique allows access to kinetically controlled product and new phases of MOF hitherto unreachable via traditional single-step synthesis. Layer-by-layer growth techniques allow exquisite control over 2D-MOF thin-film thickness and orientation (Ghosh et al., 2023). The technique involves a sequence of substrate immersion in solutions containing metal nodes and organic ligands, facilitating controlled build-up of MOF structures with atomic-scale accuracy on a layer-by-layer basis (Bai et al., 2021). The LBL technique has been used successfully in preparing a range of

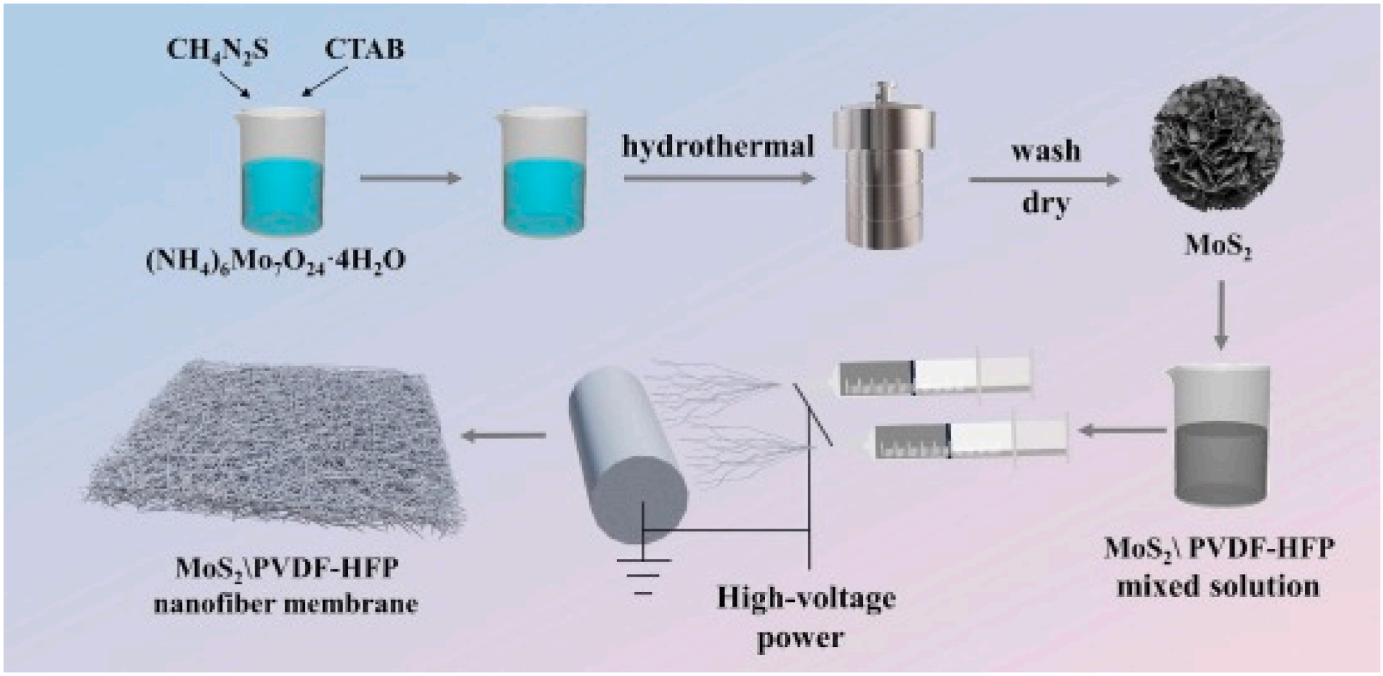


Fig. 14. Production process of MoS_2/PVDF-HFP composite nanofiber membrane (Zhao et al., 2025).

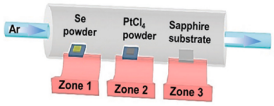
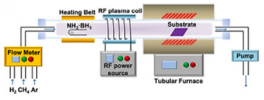
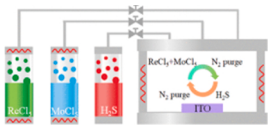
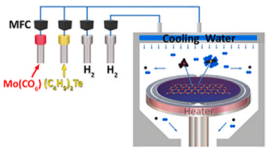
different MOF structures including $Cu_3(btc)_2$, Zn-based systems, and mixed ligand systems and incontrollable morphology and crystallography orientation (Lin et al., 2018). Special reactor designs with time-dependent mixing functionality are used in assessing kinetically controlled synthesis pathways (Zhao et al., 2010). Multicompartment reactors are capable of separate initial storage of initial reactants followed by mixing in a well-defined time-dependent sequence, leading to access to new phases and morphology in the field of MOF. This approach has successfully produced novel bimetallic Co-Cd MOF systems with unique trinuclear secondary building units and enhanced structural diversity (Li et al., 2021).

5.1.2. CVD and other methods for TMDs

CVD is considered the gold standard for producing high-quality TMDs, providing excellent control over the number of layers, crystal quality, and spatial uniformity. In a typical CVD process, solid precursors such as MoO_3 and sulfur powder are heated in a tube furnace. The vaporized precursors are carried by a gas (like Argon) to a downstream substrate, where they react and form a thin TMD film. Critical parameters such as temperature, pressure, gas flow rate, and precursor selection are precisely managed to adjust the film's thickness, domain size, and quality. Low-temperature CVD methods have gained importance for applications that require integration with temperature-sensitive substrates or conditions. The key to successful TMD growth is maintaining a consistent precursor flux and optimizing temperature profiles to produce uniform, layer-by-layer growth. Metal-organic chemical vapor deposition (MOCVD) uses organometallic precursors with high vapor pressure and low decomposition temperatures. This approach is especially effective for TMD growth because the organic groups help control precursor delivery and ensure uniform decomposition rates. The process involves pyrolysis-induced removal of organic groups followed by reactions of the resulting species to form epitaxial layers. Although growth rates are generally slow, MOCVD allows for wafer-scale uniformity, which is crucial for device applications. The comparison of different CVD techniques used for TMD synthesis, highlighting their advantages and limitations, were summarized in Table 6.

Self-condensation-assisted CVD represents a novel approach for MOF thin film growth that addresses fundamental challenges in atomic-level control (Zhang et al., 2023). This method leverages programmed temperature profiles and precursor delivery to achieve large monolayer domain formation. Unlike conventional CVD processes that rely on high-temperature atom diffusion, this approach utilizes controlled condensation and surface chemistry to achieve high-quality film growth at reduced temperatures (Zhang et al., 2023). Physical exfoliation methods provide alternative routes to 2D material synthesis, particularly for applications requiring minimal structural modification. Ultrasonic exfoliation techniques harness external ultrasonic forces to delicately separate layered bulk materials into monolayer or few-layer nanosheets. The process typically involves three sequential steps: solvent selection, ultrasonic parameter optimization, and centrifugal separation. Precise control over exfoliation conditions enables thickness control and minimizes structural damage. Soft physical exfoliation methods combine wet ball milling with ultrasonic treatment to address limitations of conventional mechanical exfoliation (Ghosh et al., 2023). This synergistic approach provides larger surface contact and uniform forces while minimizing coordination bond cleavage and structural disruption. The technique has successfully produced monolayer 2D $Zn_2(bim)_4$ nanosheets using volatile solvents such as methanol and propanol. The electrochemical and electromechanical processes of exfoliation allow greater control during 2D material preparation. The processes incorporate electric stress or potential in causing delamination of layers without harming the material structurally. The processes are most efficient in materials with close interlayer interactions, which resist normal exfoliation processes.

Table 6
Comparison of various CVD techniques (Lee et al., 2019; Liu et al., 2020; Xu et al., 2019).

CVD Technique	Benefits	Limitations
Thermal CVD 	✓ Economical ✓ Simple setup ✓ Adaptable for different uses	✓ Requires elevated temperatures ✓ Thickness and composition not easily controlled ✓ Inconsistent coating over wide surfaces
Plasma-Enhanced CVD (PECVD) 	✓ Operates at reduced temperatures ✓ Produces more uniform coatings ✓ Allows adjustment of film properties	✓ Growth rate is relatively low ✓ Thickness control remains limited ✓ Plasma interaction may harm the substrate
Atomic Layer Deposition (ALD) 	✓ Exceptional precision in thickness and composition ✓ Generates highly uniform films ✓ Suitable for complex, high–aspect ratio surfaces	✓ Deposition is slow ✓ Equipment is expensive ✓ Scaling up is difficult
Metal-Organic CVD (MOCVD) 	✓ Rapid film growth ✓ Compositional control of coatings ✓ Capable of depositing a wide material range	✓ High operating temperatures restrict substrate selection ✓ Cost of equipment is high ✓ Limited precision in film thickness control

5.2. Characterization techniques

5.2.1. X-ray diffraction (XRD)

XRD is a primary method of characterizing 2D material crystal structure. The technique gives details on the phase, degree of crystallinity, and lattice parameters of the resultant materials. The most important application of XRD is in confirming 2D MOF and 2D TMD successful synthesis through revealing their distinctive diffraction peaks (Ashraf et al., 2026; Ismael et al., 2025). The case in point is the application of XRD in determining the crystal structure and composition of the elementals in Co-W-S composites obtained through carbonization of zeolitic imidazolate frameworks (Mohamed et al., 2020). Verification of a structural model necessitates combining the results from XRD with computer work and supplementary characterization techniques (Dhingra et al., 2025). High-resolution transmission electron microscopy (HRTEM) imaging provides direct structural visualization, while N_2 sorption measurements distinguish porosity and structural differences. X-ray absorption spectroscopy (XAS) offers additional insight into local atomic environments and electronic structure (Hu et al., 2017). Grazing incidence X-ray diffraction (GIXRD) proves particularly valuable for thin film characterization, enabling assessment of film orientation and crystalline quality while minimizing substrate interference. This technique provides enhanced surface sensitivity essential for evaluating 2D material films and multilayer heterostructures. XRD analysis, shown in Fig. 15(a), was used to verify the crystal structures of the initial materials. The pattern for MOF-5 displayed its characteristic diffraction peaks, confirming a well-ordered structure consistent with its standard file (JCPDS No. 89-0511). Similarly, the peaks for WSe_2 corresponded to its known hexagonal phase (JCPDS No. 38-1388) (M. Wang et al., 2020). SEM analysis as shown in Fig. 15(b) revealed a well-integrated

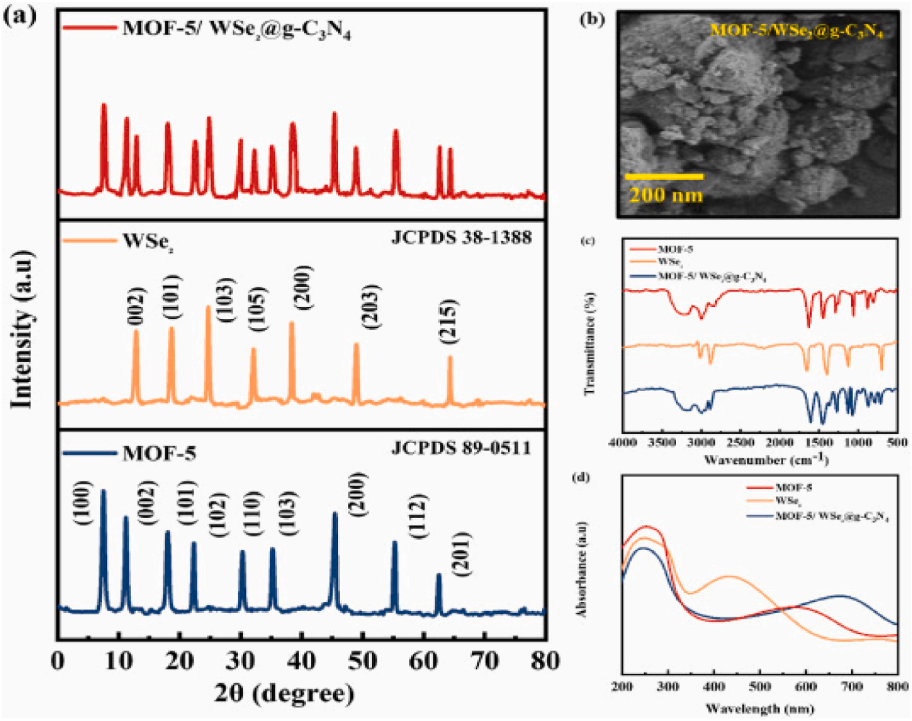


Fig. 15. (a) XRD, (b) SEM, (c) FTIR, and (d) UV-spectra of MOF-5, WSe_2, and MOF-5/WSe_2@g-C_3N_4 (Ashraf et al., 2026).

MOF-5/WSe_2@g-C_3N_4 composite with preserved MOF-5 porosity, which is crucial for ion transport. FTIR spectroscopy as illustrated in Fig. 15(c) confirmed the chemical integrity of the hybrid, as the signature peaks of both MOF-5 and WSe_2 were retained after synthesis. Finally, UV-vis spectroscopy as shown in Fig. 15(d) characterized the optical properties, determining MOF-5's band gap (~3.1 eV) and providing insight into the composite's charge transfer behavior.

5.2.2. *Scanning electron microscopy (SEM)*

SEM is utilized to study the 2D material surface morphology and microstructure. SEM produces high-resolution images exhibiting 2D MOF and TMD size, shape, and layer thickness details (Hu et al., 2017; Mohamed et al., 2020). SEM has been applied, for instance, in characterizing Co-W-S composite morphology and surface functional groups, revealing nanosheet composition and surface alterations (Mohamed et al., 2020). SEM is also amenable to correlative use with other analytical techniques, including energy-dispersive X-ray spectroscopy (EDS), in determining materials' elemental composition and distribution. High-resolution SEM imaging discerns crystal morphology, domain arrangement, and surface roughness properties essential in materials property and electronic device understanding. Field emission scanning electron microscopy (FESEM) provides higher resolution and lower charging effect conditions useful in characterizing insulating MOF material and layered TMD materials (Zhu et al., 2025). Cross-sectional SEM investigation reports on material film thickness, layer consistency, and interface quality in multilayer heterostructures. EDS, in conjunction with SEM, allows elemental composition mapping and synthesis success validation. Environmental scanning electron microscopy (ESEM) functionality allows in-situ material observation within controlled atmospheric conditions, reporting on stability and environmental response material properties. This method is especially useful in determining MOF stability in humidity exposure and TMD oxidation material properties.

5.2.3. *Raman spectroscopy*

Raman spectroscopy provides detailed insights into the chemical composition and structural properties of 2D materials. It is particularly useful for studying the interactions between different components in hybrid materials. It also provides detailed information about vibrational modes, structural quality, and layer-dependent properties in 2D-MOF and TMD materials (Foti et al., 2025; Li et al., 2025). For TMDs, Raman spectroscopy enables precise determination of layer number through characteristic frequency shifts and mode splitting patterns. The technique reveals fundamental vibrational modes, including in-plane E′ and E″ modes and out-of-plane A′1 and A1g modes. Layer-dependent Raman features in TMDs demonstrate systematic trends with increasing layer number, where E2g modes shift to lower frequencies and A1g modes shift to higher frequencies (O'Brien et al., 2016). New high-frequency first-order modes appear in few-layered systems, enabling precise identification of layer thickness. Mode splitting around A′1 and A1g positions provides additional structural information, with exterior and interior layers exhibiting different vibrational frequencies (Sarkar and Pal, 2017). These characterization techniques complement each other and help thoroughly investigate the properties of materials, providing a clearer understanding of the science behind their performance in any intended applications. An illustration of this is shown in the Multi-characterization technique adopted in explaining the properties of 2D MOF film in Fig. 16.

Two-dimensional infrared (2D-IR) spectroscopy represents an advanced characterization approach for probing ultrafast structural dynamics in MOF materials (O'Brien et al., 2016). This technique enables investigation of structural elasticity and fluctuation timescales essential for understanding functional properties. 2D-IR measurements on functionalized MOFs reveal structural fluctuation time constants of 7 and 670 ps, providing insights into framework flexibility and guest molecule interactions (O'Brien et al., 2016). Resonance Raman spectroscopy provides enhanced sensitivity for specific vibrational modes and enables selective characterization of different components in hybrid materials. This approach proves particularly valuable for distinguishing between MOF and TMD contributions in composite systems and assessing interfacial interactions.

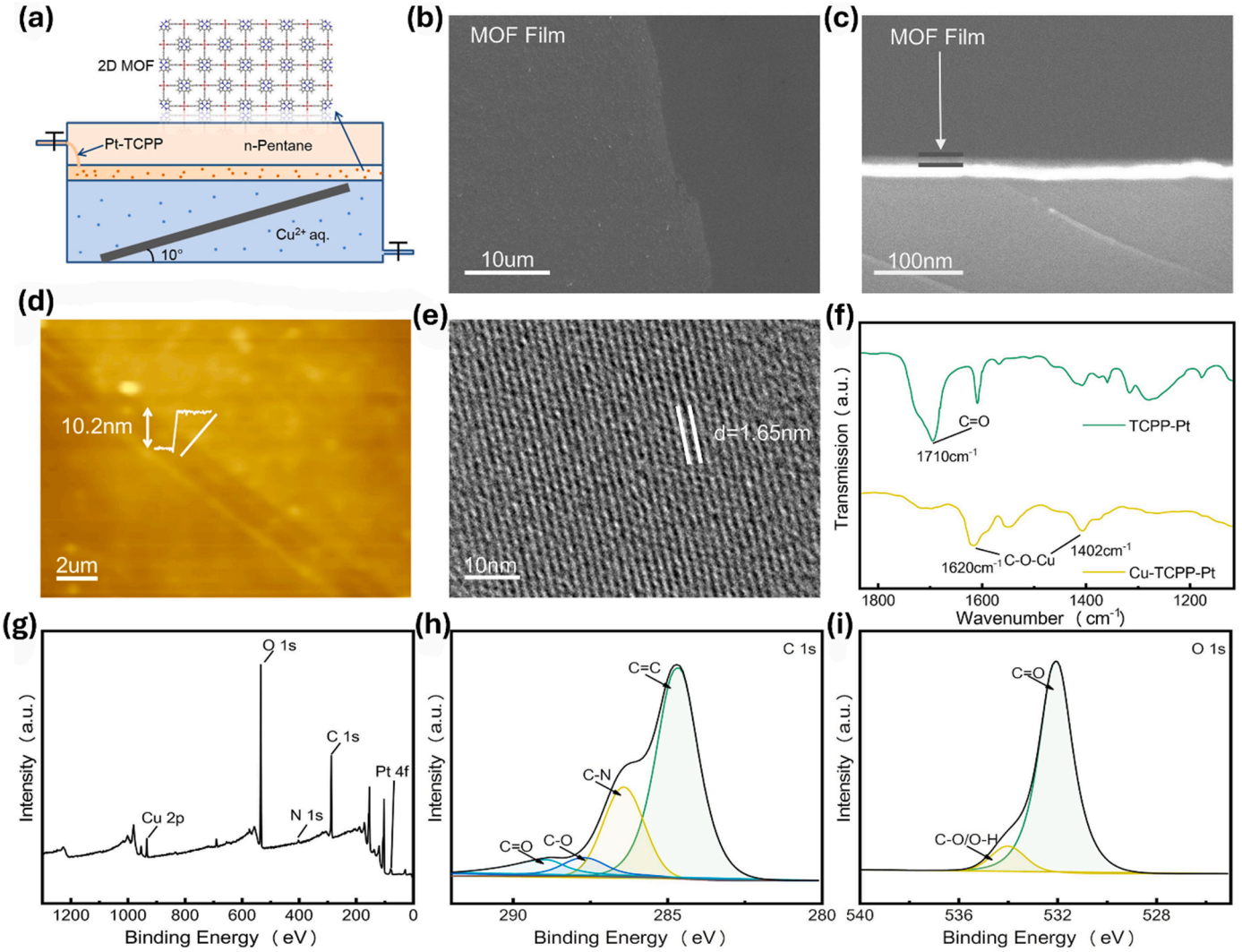


Fig. 16. Multi-technique analysis of 2D MOF film properties and structure: (a) Diagrammatic representation of the synthesis approach, (b) and (c) Surface and cross-sectional SEM imaging of films grown on Si wafers, (d) AFM surface topography measurements, (e) TEM morphological characterization, (f) Comparative FTIR analysis of TCPP-Pt starting material and synthesized 2D MOF films, (g)-(i) X-ray photoelectron spectroscopy investigation including survey spectrum and detailed C 1s and O 1s core-level analyses (Shi et al., 2025).

5.2.4. Other key methods

Transmission electron microscopy (TEM) and scanning transmission electron microscopy (STEM) provide atomic-resolution structural characterization essential for understanding interfacial properties and structural defects in hybrid 2D materials (Patil and Lee, 2018). These methods allow direct visualization of interface quality, grain boundaries, and crystal structure at the atomic level. The selected area electron diffraction (SAED) provides, in addition to imaging, crystallographic details about local orientation relationships and local structural quality. The structural development of MoS_2/NC@rGO composite materials is illustrated schematically in Fig. 17(a). Low-magnification TEM images revealing the morphological characteristics of MoS_2/NC@rGO structures are presented in Fig. 17(b), while Fig. 17(c) displays the corresponding high-magnification TEM analysis. HRTEM examination of the MoS_2/NC@rGO composite is depicted in Fig. 17(d). The crystallographic structure is further analyzed through SAED patterns, as demonstrated in Fig. 17(e). Finally, the elemental distribution within the MoS_2/NC@rGO composite is characterized using TEM-energy dispersive spectroscopy (TEM-EDS) mapping, with results illustrated in Fig. 17(f) (Jing et al., 2023).

XPS provides surface-sensitive chemical analysis, enabling assessment of elemental composition, oxidation states, and surface chemistry modifications. This technique proves essential for understanding interface chemistry in hybrid systems and verifying successful synthesis and modification procedures (Chen et al., 2018). Atomic force microscopy (AFM) enables topographical characterization and thickness determination with sub-nanometer precision. The nature of forces that MOFs are strongly bonded with are determined by AFM in addition to the surface profile as shown in Fig. 18. Piezoresponse force microscopy (PFM) broadens the capability of AFM to measure ferroelectric and piezoelectric properties directly, and it delivers critical information on energy harvesting applications. Single-point bias-dependent PFM spectroscopy demonstrates characteristic amplitude-butterfly and phase-hysteresis loops verifying the piezoelectricity (Nishida et al., 2014). Sorption analysis provides a quantitative measure of porosity, surface area, and pore size distribution in the pores of MOF materials. The nitrogen sorption isotherm can be used for calculation of the BET surface area and pore volume characteristics, which are critical in determining gas storage and catalytic ability. The mercury intrusion porosimetry gives a complementary picture about the macropore nature and connectivity. Photoluminescence measurement and UV-visible spectroscopy describe the optical properties in terms of band gap, absorption bands, and excitonic characteristics. These techniques deliver crucial information for photovoltaic applications and help evaluate electronic structure

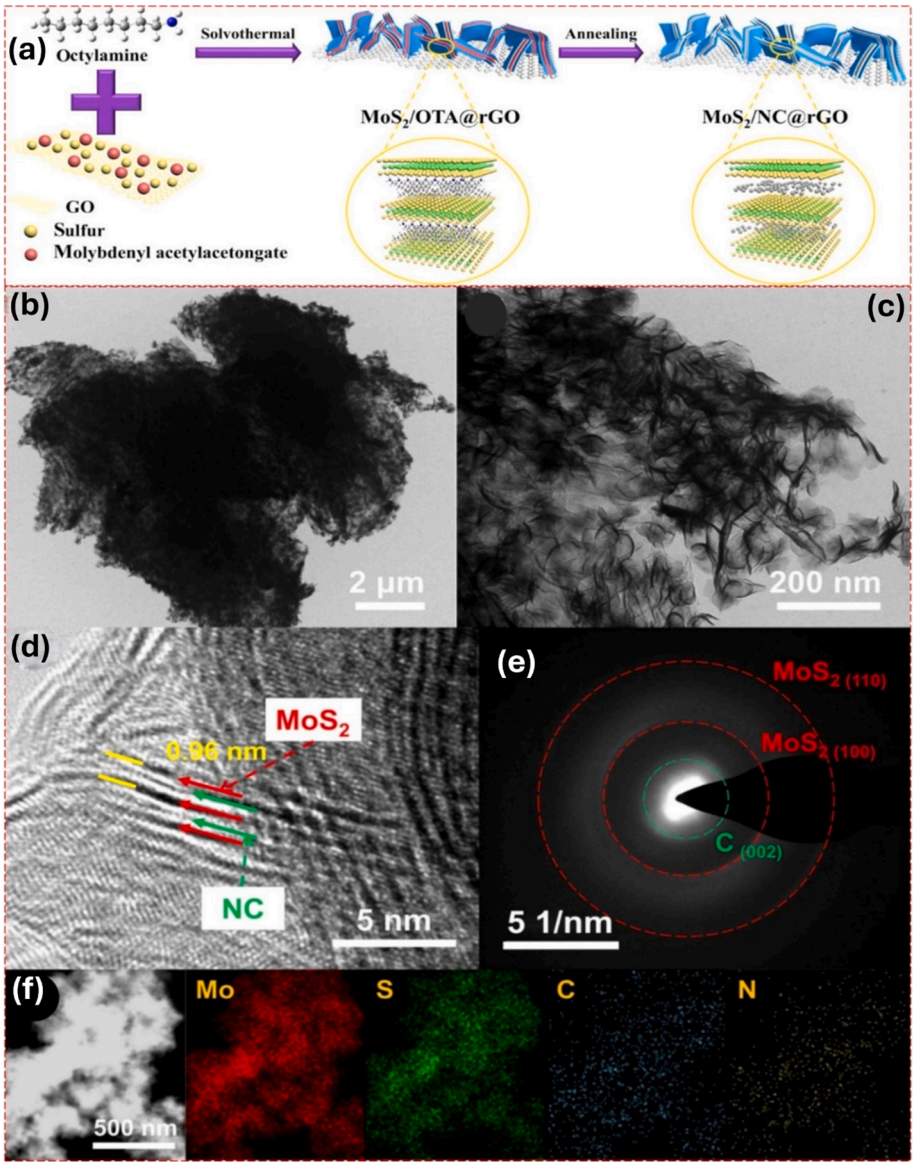


Fig. 17. Structural and compositional analysis of MoS_2/NC@rGO composites through multiple characterization techniques: (a) Schematic depiction of formation evolution; (b) and (c) TEM imaging at low and high magnifications respectively; (d) High-resolution TEM investigation; (e) SEAD patterns; and (f) Energy-dispersive X-ray spectroscopy elemental mapping (Jing et al., 2023).

modifications in hybrid systems. Time-resolved spectroscopy methods give further insights into charge carrier behavior and recombination processes, which are vital for energy conversion efficiency. The comprehensive characterization of 2D-MOF/TMD hybrid systems is essential for understanding and optimizing their synergistic effects. Interface quality, determined through TEM and STEM, directly influences charge transfer efficiency between MOF and TMD components. XPS analysis reveals chemical interactions at the heterojunction that enhance stability and catalytic activity. Raman spectroscopy provides insights into strain effects and electronic coupling that emerge from hybridization. By correlating these characterization results with device performance metrics, researchers can establish structure-property relationships that guide the rational design of synergistic hybrid systems with superior energy harvesting capabilities. The integration of advanced in-situ characterization techniques will further accelerate the optimization of these hybrid materials for next-generation energy applications.

6. Challenges and limitations

6.1. Scalability and commercialization challenges

Scaling up the synthesis of 2D-MOFs and TMDs for commercial applications presents challenges related to material yield, consistency in quality, and cost-efficiency. For 2D-MOFs, the use of templates and surfactants in complex synthesis methods often leads to lower yields due to aggregation and restacking, reducing accessibility and performance (Wang et al., 2025). Similarly, TMDs face issues in achieving high-quality nanosheet production at scale. Methods like CVD are still limited by scalability, despite promising results using microcrystalline NaCl templates (Huan et al., 2019). Variations in batch production and multistep synthesis processes in 2D-MOFs contribute to inconsistencies, while TMDs suffer from defects on surfaces and thickness non-uniformity, affecting their reliability (Zhang et al., 2024).

The key trade-offs between performance enhancement and scalability arise as we move from laboratory-scale synthesis to industrially viable processes. On one hand, laboratory-scale synthesis often leads to

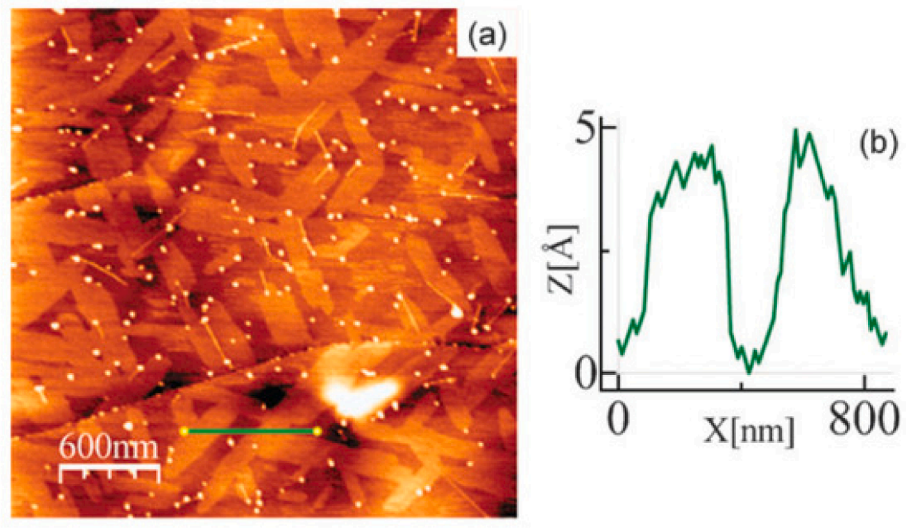


Fig. 18. One-atom-thick flakes of a copper-based MOP. (a) An atomic force microscope (AFM) obtained a micrograph showing topography; (b) Depth profile obtained along the green line (Amo-Ochoa et al., 2010).

high-quality materials with optimal properties, such as high surface area, minimal defects, and precise layer control. However, when scaling up these processes for commercial production, maintaining these performance characteristics becomes challenging due to issues like lower yields, surface defects, and batch-to-batch inconsistency. This often leads to compromised performance at larger scales, as the materials may lose some of their desired properties (e.g., charge transfer, stability) during the scaling process.

To address these challenges, synthesis yield and batch-to-batch reproducibility need further optimization to ensure more consistent material production at scale. Additionally, the cost of ligands and precursors remains a critical factor, requiring the development of cost-efficient alternatives for commercial viability. Ensuring compatibility with large-scale fabrication methods, such as roll-to-roll (R2R) or wafer-scale processes, is also essential for the practical application of these materials in commercial energy harvesting devices.

Green synthesis methods for 2D-MOFs offer a pathway to reduce costs by eliminating harmful modulators and simplifying the synthesis process (Wang et al., 2025). For TMDs, interface engineering and the introduction of organic molecules aim to passivate surface defects and improve material properties. The development of universal synthetic routes, such as those compatible with dissolution-filtration processes, holds promise for improving the cost-efficiency of TMD production. In addition to synthesis, ensuring long-term stability is critical for commercial viability. Hybrid 2D-MOF/TMD systems often degrade when exposed to environmental stressors like moisture, UV radiation, and temperature fluctuations. To enhance stability, researchers are investigating protective coatings and self-healing materials, such as carbon-based matrices or advanced polymer coatings, that could extend the lifespan of these materials in operational conditions.

Furthermore, the integration of these materials into commercial energy harvesting devices requires overcoming challenges related to uniformity, reproducibility, and device compatibility. For successful commercialization, hybrid systems need to be integrated into functional devices that can scale efficiently. Emerging designs such as flexible energy harvesting systems and self-powered devices for applications in wearable electronics and autonomous sensors are a promising starting point for bridging the gap between material performance and market deployment. As these innovations evolve, they could significantly improve the scalability and commercial viability of both 2D-MOFs and TMDs, as shown in Fig. 19.

To bridge the gap between laboratory synthesis and industrial production, researchers are actively exploring advanced, scalable manufacturing techniques. For flexible energy harvesting devices, R2R processing stands out as a particularly promising route. This method involves the continuous deposition of 2D-MOF/TMD inks onto a flexible substrate that moves between rollers, enabling high-throughput fabrication of devices like flexible solar cells and nanogenerators. While

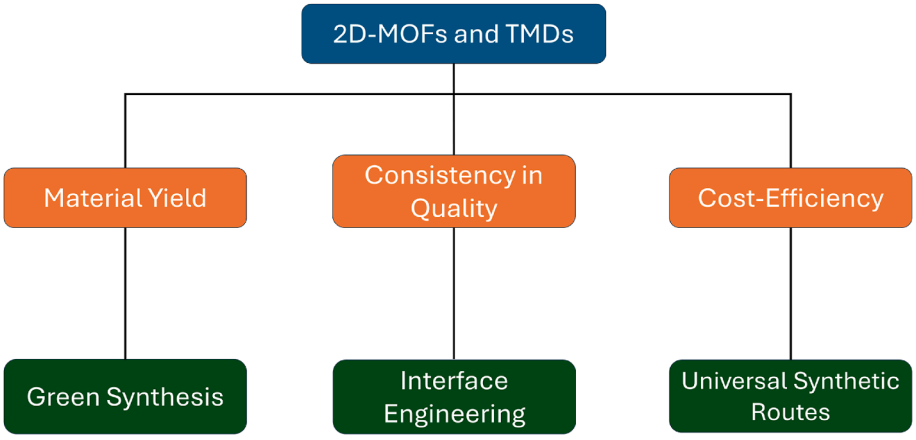


Fig. 19. Scalability challenges and strategies for synthesizing 2D-MOFs and TMDs.

challenges in ink formulation and maintaining film uniformity over large areas remain, successful demonstrations are emerging (Darr et al., 2017; Xin and Li, 2018). For the synthesis of the materials themselves, continuous flow synthesis offers a powerful alternative to traditional batch processes. In a flow reactor, precursors are continuously pumped and mixed under precisely controlled conditions, leading to higher yields, better batch-to-batch consistency, and improved safety. This approach is being adapted for both MOFs and the LPE of TMDs, showing potential for producing industrial quantities of high-quality nanosheets with reproducible properties (Bayliss et al., 2014; Rubio-Martinez et al., 2017). The successful implementation of these techniques will be critical for realizing the commercial potential of 2D-MOF/TMD technologies.

6.2. Stability and durability

The stability of 2D-MOFs and TMDs is a critical factor for their long-term performance in energy harvesting applications, particularly in wearable and outdoor energy harvesting devices. MOFs are particularly sensitive to environmental factors such as humidity, temperature, and mechanical stress, all of which can significantly affect their performance (Jasuja and Walton, 2013; Xiang et al., 2025). High humidity can cause MOFs to undergo structural collapse or transformation, negatively impacting their functionality in real-world environments. While technologies such as catenation and pillaring have been employed to improve their water stability, these strategies are not universally effective. Temperature fluctuations also pose a challenge, as many MOFs are poorly thermally stable (del Angel et al., 2021). Even a slight increase in temperature can cause them to morphologically transform, limiting their application in hot conditions. Additionally, MOFs with lower rigidity are susceptible to mechanical deformation under stress, which compromises their structural integrity.

In contrast, TMDs, including materials like MoS_2, exhibit a higher resistance to environmental stressors, particularly humidity and temperature. However, they are still vulnerable to moisture exposure and high temperatures, which can cause delamination or fracture in extreme conditions. Their layered structure provides some protection against mechanical stress, but when subjected to extreme conditions, TMDs can still experience degradation.

The stability issues associated with both 2D-MOFs and TMDs significantly affect their applicability in practical energy harvesting devices. For instance, instability in MOFs under varying environmental conditions can lower the efficiency and lifespan of energy storage and harvesting devices, such as batteries and supercapacitors (Ashraf et al., 2026; Hosseini and Safarifard, 2024). To address this, hybridization of MOFs with TMDs has been proposed as a promising strategy to enhance their stability, mechanical strength, and resistance to environmental stress (Ashraf et al., 2026; Xu et al., 2022). This hybridization helps offset the inherent sensitivity of MOFs and improves their long-term performance in energy harvesting systems.

While TMDs are known for their electrical conductivity and catalytic activity, their long-term stability under environmental stress remains a crucial factor for their continuous functionality in practical applications. Hybrid systems, combining the best properties of both MOFs and TMDs, have the potential to offer a balanced solution. By leveraging the stability of TMDs and the structural integrity provided by MOFs, hybrid materials can resist the environmental challenges that each material faces individually, leading to enhanced performance, mechanical strength, and resilience in heat, humidity, and mechanical stress.

As these hybrid materials evolve, they could offer a durable, reliable solution for long-term energy harvesting systems, enabling their widespread use in applications that require continuous operation over extended periods. These advancements could also contribute to commercialization by ensuring that energy devices powered by hybrid 2D-MOF/TMD systems have the stability required for real-world applications, especially in wearable and outdoor environments.

7. Future prospects and opportunities

7.1. Emerging trends in 2D-MOF and TMD research

7.1.1. Materials and synthesis trends enabling performance gains

Recent advances in two-dimensional 2D-MOF and TMD have accelerated the development of high-surface-area catalysts, conductive heterostructures, and mechanically compliant thin films for energy conversion, sensing, and environmental engineering. In 2D-MOFs, electrocatalysis remains a dominant growth area, particularly for transition-metal systems (e.g., Ni-, Co-, and Cu-based frameworks) where the ultrathin morphology increases the density of accessible active sites and supports efficient OER (Huang et al., 2020). Parallel improvements in synthesis, especially co-assembly strategies and template-assisted growth, are enabling better thickness control, improved defect regulation, and higher stability, which collectively improves reproducibility and strengthens the case for scalable fabrication.

In hybrid architectures, MOF/TMD composites (e.g., MoS_2@MOF) are increasingly designed to enhance photochemical stability and promote interfacial charge separation, which benefits photocatalysis and solar energy conversion. Beyond stability, combining MOFs with TMDs is frequently reported to improve electronic transport pathways, supporting performance improvements in solar cells and water splitting systems (Hosseini and Safarifard, 2024). In addition, heterometallic MOFs (HMOFs) that integrate lanthanides with transition metals are expanding the functional scope of 2D-MOF platforms toward sensing, optical response tuning, and emerging quantum-relevant device components (Zhang and Cheng, 2015).

For 2D-TMDs, progress in chemical exfoliation, CVD, and atomic layer deposition (ALD) continues to raise materials quality and property tunability, strengthening applications in electronics and optoelectronics (Song et al., 2022). MOF-derived routes are also gaining traction; for example, carbonization of zeolitic imidazolate frameworks yields porous carbon-based structures with improved electrochemical response, supporting energy storage applications (Mohamed et al., 2020). Finally, while MXenes are distinct from TMDs, their increasing integration into lamellar membrane platforms is shaping environmental engineering directions (e.g., water purification and desalination), largely because mechanically robust, high-flux architectures can be engineered alongside antibacterial effects. Collectively, these trends indicate that synthesis control, hybridization, and interface engineering are becoming the decisive levers that move 2D-MOF/TMD systems from laboratory demonstrations toward scalable devices for energy harvesting, storage, and environmental remediation.

7.1.2. Technological evolution pathways for 2D-MOF/TMD hybrids

Early hybrid systems primarily relied on physical mixing of pre-synthesized MOFs and TMDs, typically driven by van der Waals attraction and electrostatic interactions. Although these composites often reported proof-of-concept improvements (commonly ~20%–40%), they frequently exhibited weak interfacial adhesion, unstable charge-transfer behavior, and significant batch-to-batch variability. More recent studies increasingly emphasize interfacial chemical design, including metal–ligand coordination between MOF nodes and TMD vacancy sites, as well as π–π interactions between aromatic linkers and TMD basal planes. For example (Han et al., 2025), reports that covalently engineered MOF-5/WSe_2 interfaces deliver substantially larger performance gains (≈60%–90%) and stronger cycling stability (>95% retention after 10000 cycles) than electrostatically bound counterparts. Moving forward, the most impactful direction is expected to be programmable interfacial bonding, enabled by rational linker design (e.g., thiolated ligands targeting S-deficient sites) and deliberate tuning of interfacial energy barriers to control charge-transfer directionality and suppress recombination losses.

Early work largely optimized one dominant mechanism at a time (photovoltaics or thermoelectrics or piezoelectrics). Emerging hybrid platforms increasingly integrate multiple functions within a single architecture, such as thin-film systems that simultaneously support (i) photovoltaic energy conversion, (ii) thermal regulation, and (iii) mechanical strain sensing (Hanan et al., 2024; Jayaramulu et al., 2022; Kumar et al., 2021). This trend is significant because it shifts evaluation from "best-in-class single metrics" to "system-level utility," particularly for autonomous devices. Next-generation concepts point toward hierarchically integrated thin films that unify multiple harvesting routes with embedded storage and power conditioning, enabling self-powered sensors and Internet-of-Things (IoT) nodes driven by ambient light, heat gradients, and mechanical motion.

Traditional screening of MOF/TMD combinations relied heavily on DFT calculations or iterative experimental trial-and-error, both of which impose high time and compute costs (often 10–100 CPU-hours per candidate and slow synthesis cycles). Recent advances increasingly employ GNNs and other ML models to predict band alignment, charge-transfer barriers, and thermal properties at near-real-time speeds, enabling rapid narrowing of candidate spaces. The InterMat framework, trained on 44,850 calculated band offsets, reports predictive accuracy near 0.26 eV, which is positioned as an improvement over older semi-empirical uncertainty ranges (~0.5–1.0 eV) and shortens discovery cycles from years to weeks (AL-Maatoq et al., 2022; Lee and Wu, 2022; Mohd Nurazzi et al., 2021). Priority directions now include (a) extending training targets to environmental durability under humidity, thermal cycling, and mechanical fatigue, and (b) using active learning to prioritize experiments that maximize information gain while accelerating identification of high-impact hybrid pairs for validation.

7.1.3. Critical research gaps limiting translation and reliability

While static performance metrics are widely reported, the degradation kinetics under repeated mechanical loading (≈10000 to 1000000 cycles) are still under-characterized. Reports in triboelectric and flexible platforms indicate failure modes beyond simple performance decay, including interfacial delamination and MOF ligand rupture at high cycle counts (>100000) (Khandelwal et al., 2023; Wang et al., 2021). A clear priority is to quantify fatigue thresholds systematically and develop mechanically resilient interface strategies (e.g., self-healing interlayers or multilayer architectures that resist crack propagation and delamination).

Most studies still rely on static characterization (XRD, SEM, XPS), which provides limited insight into dynamic processes such as ion migration, charge redistribution, and strain evolution during operation. Operando and in situ methods, such as operando X-ray absorption spectroscopy and time-resolved spectroelectrochemistry, remain comparatively rare in MOF/TMD hybrids despite being central to mechanistic claims (Choudhary and Garrity, 2024). Targeted investment in advanced measurement access (e.g., synchrotron beamtime) would enable direct mapping of charge distribution, bonding evolution, and strain localization while devices operate.

Current protocols often evaluate stressors independently (humidity, temperature, UV), whereas outdoor and field systems experience simultaneous stress coupling. Accelerated protocols that combine high humidity (~85% RH), thermal cycling (−20 to +60°C over >1000 cycles), UV exposure (e.g., 340 nm for >1000 h), and electrical bias, with failure-mode attribution, are still not consistently adopted (Hörmann et al., 2025; Jardine et al., 2025). Without multi-stressor datasets, reported stability remains difficult to extrapolate to year-scale service lifetimes.

Defect introduction (vacancies, dopants) frequently improves catalytic activity by increasing active sites, but it can also degrade electronic quality, mechanical integrity, or long-term stability. The field lacks robust design rules for "optimal defect windows" across coupled metrics (charge transport, catalysis, and mechanical strength) (Chang et al., 2025; de Araujo and Farrusseng, 2025; Wu et al., 2024). High-value work would use combinatorial designs that systematically vary defect density (e.g., ~0.1%–5% lattice sites) and quantify multi-objective trade-offs, ideally using ML to infer structure–property correlations.

A substantial portion of the literature remains materials-centric, with comparatively few fully packaged devices demonstrated under realistic conditions. A key translational gap is the lack of complete system demonstrations (energy harvester, storage and power management) using MOF/TMD hybrids operating continuously for >1 year under field-relevant environments (Jardine et al., 2025; Wu et al., 2024). Closing this gap likely requires tighter collaboration between materials researchers and device engineers to align materials design with manufacturability, encapsulation, and circuit-level constraints.

7.2. Commercialization of energy harvesting devices

The commercialization of 2D-MOFs and TMDs for energy harvesting and storage applications shows significant promise, thanks to their unique properties and recent advancements. TMDs, such as MoS_2 and WSe_2, offer large surface areas, excellent electrical conductivity, and tunable properties, making them ideal for supercapacitors and batteries. Their scalability, aided by enhanced epitaxial growth methods, facilitates integration into current manufacturing processes (Chen et al., 2022; Hakami et al., 2023; Mohamed et al., 2020). However, challenges remain in terms of stability and defect control, requiring further development of composite materials and hybrid systems to improve their functionality and durability (Hakami et al., 2023; Sovizi et al., 2023).

On the other hand, MOFs, known for their high porosity and large surface areas, have demonstrated significant potential in charge storage and electrochemical applications (Lu et al., 2022). When combined with TMDs, MOFs address key issues of conductivity and stability, resulting in hybrid materials with improved functionality for energy storage and photocatalysis (Hosseini and Safarifard, 2024). Despite their success in the lab, scaling MOFs for large-scale production presents challenges, including maintaining quality and performance at industrial levels. The potential of these materials for supercapacitors, solar cells, and photocatalytic applications emphasizes their commercial potential in the energy sector.

To unlock the full commercial application of 2D-MOFs and TMDs, further work is needed to address scalability and stability challenges. Developing more efficient and cost-effective manufacturing processes and hybrid materials that combine the best properties of MOFs and TMDs will be crucial for their widespread adoption in energy storage and harvesting technologies.

7.3. Future applications in energy harvesting

The combination of 2D-MOFs and TMDs presents tremendous potential in advancing energy harvesting technologies. In photovoltaic energy harvesting, 2D-TMDs such as MoS_2 and WS_2 are ideal candidates due to their intense light absorption and high optical conductivity, enabling the development of ultrathin photovoltaics and energy-cascade-type devices. These innovations enhance light harvesting and energy conversion efficiency, making TMDs valuable for the next generation of solar cells (Peng et al., 2015).

The synergy between 2D-MOFs and TMDs in hybrid materials further enhances their photocatalytic stability, charge separation, and light absorption. These hybrid systems are particularly well-suited for sustainable energy production and offer promising solutions for increasing the efficiency of energy conversion processes (Hosseini and Safarifard, 2024; Takhar and Banerjee, 2025). As shown in Fig. 20, these materials are integral in solar energy harvesting, photocatalysis, and other energy applications, contributing to energy sustainability.

In addition to solar energy, the potential for energy harvesting in wearable devices and thermoelectric applications is significant. The flexibility, porosity, and efficient ion transport properties of 2D TMDs make them ideal for wearable electronics and energy storage devices.

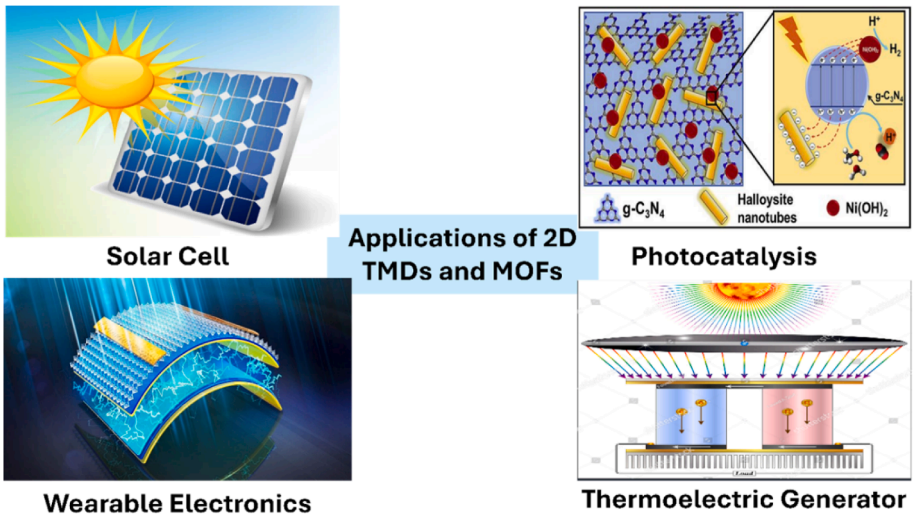


Fig. 20. Schematic representation of the future applications of 2D-MOFs and TMDs in solar energy harvesting, photocatalysis, wearable electronics, and thermoelectric energy harvesting.

Devices based on MoS_2 or TENGs can effectively harvest energy from mechanical actions, powering self-powered sensors and contributing to energy autonomy in wearables (Kumar et al., 2024; Park et al., 2020).

Moreover, TMDs like MoS_2 and WS_2, with their large see-beck coefficients and excellent electrical conductivity, are excellent candidates for thermoelectric energy harvesting. These materials can efficiently convert waste heat into electricity, providing a sustainable solution for heat recovery systems in industrial and wearable applications. Future research focusing on doping strategies to optimize their performance will be crucial for improving the functionality of these materials, making them more effective in waste heat recovery and thermoelectric devices (Awasthi and Islam, 2023; Moon et al., 2025).

These advancements demonstrate that hybrid 2D-MOF/TMD systems have the potential to revolutionize energy harvesting across various domains, from solar energy and wearable electronics to thermoelectric applications, supporting the transition to sustainable energy systems.

8. Conclusion

The growing global demand for sustainable energy, combined with the limitations of fossil fuels, underscores the urgency of developing innovative energy harvesting technologies. Hybrid 2D-MOF/TMD systems represent a paradigm shift in this effort, offering a platform that merges the high porosity, chemical tunability, and catalytic ensembles of MOFs with the conductivity, optical absorption, and layered structures of TMDs. This synergy has enabled significant progress in photovoltaics, thermoelectrics, piezoelectrics, and triboelectrics, where performance metrics consistently surpass those of conventional materials.

A central insight of this synthesis is that hybridization overcomes the intrinsic weaknesses of each material class when used independently. MOFs, though versatile, suffer from poor conductivity, while TMDs, despite their strong electronic and catalytic properties, face challenges in stability and scalability. Their integration generates cooperative effects such as enhanced charge separation, optimized band alignment, reduced recombination losses, and improved durability that cannot be achieved otherwise. These findings position hybrid 2D-MOF/TMD systems as leading candidates for multifunctional energy harvesting platforms.

Despite encouraging advances, several critical obstacles remain before these systems can achieve large-scale practical deployment. Scalability of synthesis remains one of the greatest hurdles, as many reported methods are energy-intensive, solvent-dependent, or difficult to reproduce at industrial scale. Similarly, long-term stability under real-world operating conditions including humidity, temperature fluctuations, and mechanical stress is insufficiently explored. Integration into commercial-scale devices requires not only robust material design but also cost-effective and reproducible fabrication strategies. Addressing these gaps will demand sustained collaboration across materials chemistry, device physics, and engineering design.

Looking ahead, several promising avenues warrant attention. Atomic-level interface engineering should be prioritized to fine-tune charge transfer and structural stability. Eco-friendly synthesis techniques, including mechanochemical and green-chemistry approaches, offer a sustainable pathway toward commercialization. Coupling experimental work with computational modeling and ML could accelerate the identification of optimized architectures and reduce trial-and-error in the lab. Finally, device-level integration of 2D-MOF/TMD hybrids into real-world photovoltaic modules, flexible thermoelectric generators, and wearable nanogenerators represents the most impactful step forward.

In summary, hybrid 2D-MOF/TMD systems are emerging as transformative materials for next-generation energy harvesting. Although challenges remain, the steady progress in synthesis, engineering, and theoretical modeling is rapidly advancing their journey from laboratory-scale innovations to commercially viable technologies. Their development holds the promise of revolutionizing sustainable energy systems and contributing meaningfully to a greener and more energy-secure future.

CRediT authorship contribution statement

Kehinde Temitope Alao: Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Data curation, Conceptualization. **Abdulhammed K. Hamzat:** Writing – review & editing, Writing – original draft, Investigation, Conceptualization. **Kamaruzzaman Sopian:** Writing – review & editing, Supervision, Investigation, Funding acquisition, Conceptualization. **Syed Ihtsham Ul Haq Gilani:** Writing – review & editing, Writing – original draft, Supervision, Methodology, Investigation, Conceptualization. **Taiwo Onaopemipo Alao:** Writing – review & editing, Data curation, Conceptualization. **Zeshan Aslam:** Writing – review & editing. **Hussein A. Kazem:** Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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