

### MoS<sub>2</sub>-based nanocomposites

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### REVIEW



# MoS<sub>2</sub>-based nanocomposites: synthesis, structure, and applications in water remediation and energy storage: a review

M. I. A. Abdel Maksoud<sup>1</sup> · Ahmed G. Bedir<sup>2</sup> · Mohamad Bekhit<sup>1</sup> · Marwa Mohamed Abouelela<sup>2,3</sup> · Ramy Amer Fahim<sup>1</sup> · A. S. Awed<sup>4</sup> · Sayed Y. Attia<sup>5</sup> · Said M. Kassem<sup>1</sup> · M. Abd Elkodous<sup>3,6</sup> · Gharieb S. El-Sayyad<sup>7</sup> · Saad G. Mohamed<sup>5</sup> · Ahmed I. Osman<sup>8</sup> · Ala'a H. Al-Muhtaseb<sup>9</sup> · David W. Rooney<sup>8</sup>

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### Abstract

The world is currently facing critical water and energy issues due to the growing population and industrialization, calling for methods to obtain potable water, e.g., by photocatalysis, and to convert solar energy into fuels such as chemical or electrical energy, then storing this energy. Energy storage has been recently improved by using electrochemical capacitors and ion batteries. Research is actually focusing on the synthesis of materials and hybrids displaying improved electronic, physiochemical, electrical, and optical properties. Here, we review molybdenum disulfide ( $MoS_2$ ) materials and hybrids with focus on synthesis, electronic structure and properties, calculations of state, bandgap and charge density profiles, and applications in energy storage and water remediation.

Keywords Water treatment  $\cdot$  MoS<sub>2</sub>  $\cdot$  MoS<sub>2</sub>-based hybrids  $\cdot$  Energy storage  $\cdot$  Supercapacitors  $\cdot$  Two-dimensional layered nanomaterials

### Abbreviations

- EDLCs Electrochemical double-layer capacitorsHOMO Highest occupied molecular orbitalLUMO Lowest unoccupied molecular orbitalMHCS Mesoporous hollow carbon spheresNDMA N-Nitrosodimethylamine
- DOS Projected density of states

M. I. A. Abdel Maksoud muhamadmqsod@gmail.com

- Ahmed I. Osman aosmanahmed01@qub.ac.uk
- <sup>1</sup> National Center for Radiation Research and Technology (NCRRT), Egyptian Atomic Energy Authority (EAEA), Nasr City, Cairo, Egypt
- <sup>2</sup> Egyptian Petroleum Research Institute (EPRI), Nasr City, Cairo 11727, Egypt
- <sup>3</sup> Department of Electrical and Electronic Information Engineering, Toyohashi University of Technology, 1-1 Hibarigaoka, Tempaku-cho, Toyohashi, Aichi 441-8580, Japan
- <sup>4</sup> Higher Institute for Engineering and Technology at Manzala, Manzala, Egypt

### Introduction

Two-dimensional layered nanomaterials have drawn much research consideration from their interesting physicochemical properties such as the extraordinary electrical, optical, and physical characteristics that arose from their ultra-thin construction and their quantum size impact. Among these two-dimensional layered materials, transition metal dichalcogenides are a set of substances with several attractive

- <sup>5</sup> Tabbin Institute for Metallurgical Studies (TIMS), Tabbin, Helwan 109, Cairo 11421, Egypt
- <sup>6</sup> Center for Nanotechnology (CNT), School of Engineering and Applied Sciences, Nile University, Sheikh Zayed, Giza 16453, Egypt
- <sup>7</sup> Drug Radiation Research Department, National Center for Radiation Research and Technology (NCRRT), Egyptian Atomic Energy Authority (EAEA), Nasr City, Cairo, Egypt
- <sup>8</sup> School of Chemistry and Chemical Engineering, Queen's University Belfast, Belfast BT9 5AG, Northern Ireland, UK
- <sup>9</sup> Department of Petroleum and Chemical Engineering, College of Engineering, Sultan Qaboos University, Muscat, Oman

characteristics for fundamental research and promising applicability. The transition metal dichalcogenides have the general formulation notated as MX<sub>2</sub>, in which M stands for the transition metal atom, and X represents the chalcogen. They consist of weakly joined sandwich-like layers (X-M-X). The neighboring layers are connected via van der Waals forces. In each layer, M is bonded to X atoms by covalent bonds. Exfoliation of the bulk substances into a few layers mostly conserves their characteristics and also leads to additional features due to restriction impacts. These materials have sparked numerous interest due to their unique physical characteristics and special applications (Jayabal et al. 2017; Chhowalla et al. 2013; Arshad et al. 2019). In opposition to graphene possessing a zero bandgap, transition metal dichalcogenides have a bandgap comparable to Si or GaAs and offer an interesting ability for reducing the size of the technology and semiconductor to the nanoscale. Additionally, many years ago, transition metal dichalcogenides affirmed their applications in many fields like solid-state lubricants, rechargeable batteries and photovoltaic devices (Gourmelon et al. 1997; Fortin and Sears 1982; Gupta et al. 2020; Abdel Maksoud et al. 2021).

Among the family of transition metal dichalcogenides, molybdenum disulfide ( $MoS_2$ ) has recently been broadly studied in many research fields such as: lubrication, supercapacitors, lithium-ion batteries and drug delivery, because of its extraordinary activity and its perfect two-dimensional structure.  $MoS_2$  has also exhibited excellent performance in environmental remediation applications such as electroor photocatalysis, adsorption of heavy metals, ammonium nitrogen removal, and membrane-based separation (Kalin et al. 2012; Lin et al. 2015; Chang et al. 2016; Wang and Mi 2017; Zhang et al. 2017a; Fan et al. 2019; Liu et al. 2018a; Xing et al. 2018; Sheng et al. 2019; Zhou et al. 2020).

Herein, we reported the recent advances in  $MoS_2$  material and its hybrid forms for energy applications in detail. Firstly, the controllable synthesis of  $MoS_2$ , divided into topdown and bottom-up approaches, was reviewed. Then, its unique electronic structure and its associated characteristics were analyzed. After that, the density-functional theory calculations were utilized to identify  $MoS_2$  density of state, bandgap, charge density profiles, and work function. Later,  $MoS_2$ -based hybrids for water remediation were presented. Then,  $MoS_2$ -based hybrids for energy storage applications were presented, which started with supercapacitors and were then followed by three types of ion batteries.

### Structure and controllable synthesis of MoS<sub>2</sub>

 $MoS_2$  structure is a trigonal prismatic of S–Mo–S arrangement having two atomic planes of S surrounding an atomic plane of Mo in a sandwich-like structure. The length of

the Mo–S bond is 1.54 Å, while the S–S bond is 3.08 Å in length. Accordingly, the MoS<sub>2</sub> single-layer thickness is about 0.62 nm (Late et al. 2012). The MoS<sub>2</sub> semiconductor has an indirect bandgap of 1.2 eV, while the direct bandgap of a single-layered MoS<sub>2</sub> semiconductor is 1.8 eV (Arshad et al. 2019). In addition, although multilayer MoS<sub>2</sub> is not photoluminescent, exfoliation-induced changes in its electronic structure lead to photoluminescent behavior in exfoliated monolayers (Splendiani et al. 2010).

 $MoS_2$  has three main phases (Ding et al. 2016; Ali et al. 2018): 1 T MoS<sub>2</sub>, 2H MoS<sub>2</sub> and 3R MoS<sub>2</sub> (Fig. 1). In the 1 T MoS<sub>2</sub> unit cell, the sulfur atoms coordinate the molybdenum atoms octahedrally; 2H MoS<sub>2</sub> has the molybdenum atom coordinated by two S-Mo-S units in a trigonal prismatic geometry for each elemental cell; and with the same geometry as the 2H MoS<sub>2</sub>, coming to the third phase the 3R MoS<sub>2</sub> but three units of S-Mo-S are directed along the c-axis instead of two. The 1 T phase has metallic properties, while the 2H and the 3R phases are semiconductors (Acerce et al. 2015a; Toh et al. 2017; Wang et al. 2017a). Natural  $MoS_2$  exists as the thermodynamically favored 2H phase, while the 1 T phase does not occur naturally and is usually obtained from lithium-intercalated 2H-MoS<sub>2</sub> interlayers by chemical exfoliation (Lukowski et al. 2013; Eda et al. 2011; Wang et al. 2012; Fan et al. 2015). Furthermore, the monolayered 1 T-MoS<sub>2</sub> is metastable from the thermodynamic perspective, which tends to restructure to form the more stable phase, 2H-MoS<sub>2</sub>. Consequently, the 1 T phase commonly happens in a multiphase form along with the 2H phase (Chhowalla et al. 2013; Chua et al. 2016; Chou et al. 2015; Song et al. 2015).

2H-MoS<sub>2</sub> and their composites were extensively studied for energy-related applications, especially supercapacitors, due to their fascinating electronic, optical, catalytic characteristics, and considered the most common form in nature. (Ding et al. 2016; Xiao et al. 2017a; Liu et al. 2016; Shi et al. 2016). However, 2H-MoS<sub>2</sub> is less competitive to graphenebased materials in energy storage applications due to their semiconductivity and bandgap ( $\approx 1.3-1.9 \text{ eV}$ ) (Yang et al., 2013; Chen and McDonald 2016). From another point of view, 1 T-MoS<sub>2</sub> is metallic and superior to 2H-MoS<sub>2</sub> in electronic conductivity (nearly higher 107 times) that making 1 T-MoS<sub>2</sub> deliver an excellent platform or stage for electron transfer; this is the first point. Secondly, the abundance of in-plane active sites (in contrast to that in 2H phase, which assembled on the edges) affords an improved reactivity. Thirdly, the improved interlayer spacing ( $\approx 1$  nm) offers fast and wide ion-diffusion channels. Owing to the previous qualities, enhanced energy materials can be fabricated and designed by amendable structures of MoS<sub>2</sub> (1 T phase) via doping, stress, defection, intercalation, or heterojunction (Acerce et al. 2015b; Wang et al. 2017b; Ambrosi et al. 2015).

Where in the 1 T  $MoS_2$  unit cell, the sulfur atoms coordinate the molybdenum atoms octahedrally, in 2H  $MoS_2$ , the molybdenum atom is coordinated by two S–Mo–S units in a trigonal prismatic geometry for each elemental cell; with the same geometry as the 2H  $MoS_2$ , coming to the third phase the 3R  $MoS_2$  but three units of S–Mo–S are directed along the c-axis instead of two.

Many approaches have been established to synthesize  $MoS_2$  nanostructures. Generally, the methods for synthesizing  $MoS_2$  nanoparticles can usually involve either a "top-down" approach or a "bottom-up" approach.

### **Top-down**

The "top-down" strategy is an exfoliation process of bulk layered materials which widely includes mechanical, liquid, and electrochemical exfoliation.

### **Mechanical exfoliation**

Mechanical exfoliation or simply "micromechanical cleavage" was first used as an approach to prepare two-dimensional nanosheets from bulk layered materials by mechanical fragmentation as was applied to graphene (Late et al. 2012; Novoselov et al. 2004; Novoselov et al. 2005). Mechanical exfoliation, also known as the Scotch-tape method, means "detaching" or "peeling" of bulk crystals with adhesive tape or bulk crystals rubbing against a solid surface(Novoselov 2011; Li et al. 2014). The cleaning of the substrate before sticking the tape onto it gives better results (Huang et al., 2015a). Often, using a film of gold as an intermediary substrate enhances mechanical exfoliation because gold has a good tolerance for chalcogens, which effectively overcomes the van der Waals force among the top layer and the residue of the crystal (Magda et al. 2015; Desai et al. 2016).

Mechanical exfoliation, which does not require costly or specialized machinery, is the most effective way to create the cleanest, most crystalline, and atomically thin nanosheets of layered materials. (Kolobov and Tominaga 2016). Nevertheless, since this technique cannot be used for large-scale processing, it can only be used to prepare samples for research purposes.

Nanomechanical exfoliation, an expansion of mechanical exfoliation, has recently been documented to generate highquality  $MoS_2$  nanosheets having a definite layer. A particularly acute tungsten probe of a tip diameter of about 10 nm is used in nanomechanical exfoliation to peel nanosheets of a thick flake of  $MoS_2$  stacked on the substrate with an edge-on alignment. Piezoelectric actuators power the tungsten probe, and the entire process is observed in real-time using a highresolution transmission electron microscope (Tang et al. 2014). Miyake and Wang used an atomic force microscope

#### Liquid exfoliation

There are two types of liquid exfoliation: sonication and shear force-assisted.

Sonication-assisted liquid exfoliation Sonication has also been shown to aid in the exfoliation of layered substances in liquid suspensions that may assist in intercalating the barrier of activation (Nicolosi et al. 2013). Based on high sonication power and constituents (ions, polymers, surfactants) that reinforce the adhesion on the stratified  $MoS_2$  surface and facilitate their exfoliation, the process yields an excellent yield of the level of dispersion of few-layered  $MoS_2$ .

A wide variety of organic solvents identified the top 20 solvents for sonication-assisted  $MoS_2$  exfoliation was investigated. In ultraviolet–visible spectra, the absorbance values for solvents are at 672 nm (which is excitonic peak characteristic for a few layered  $MoS_2$ ) divided by the length of the cell. The  $A/l = \varepsilon C$  relationship, also identified as Beer–Lambert law, shows that the absorbance value is directly linear with concentration, where  $\varepsilon$  is the extinction coefficient (Coleman et al. 2011). On the other hand, transition metal dichalcogenides nanosheets prefer to accumulate unless a surfactant or polymer is used since they are still hydrophobic even after being exfoliated in H<sub>2</sub>O (i.e., through a long sonication period)(Samadi et al. 2018).

With the assistance of polyvinylpyrrolidone, (Liu et al. 2012) published a simple method to exfoliate and disperse  $MoS_2$ . Polyvinylpyrrolidone-coated  $MoS_2$  nanosheets that result are distributed in the ethanol, making preparation and system fabrication of thin film using the technique of solution processing much more straightforward.

To exfoliate  $MoS_2$ , (Xuan et al. 2017) used sodium alginate as a natural polysaccharide. The sonicating process lasted for 5.5 h, and during this period, a stirring was occurred for 1 min every 20 min to make the suspensions homogeneous.

To synthesize  $MoS_2$  nanosheets, (Liu et al. 2018b) demonstrated a simple exfoliation process with salt in the liquid phase. They used isopropyl alcohol as a medium for exfoliation and salts like sodium tartrate, potassium sodium tartrate, and potassium ferrocyanide as assistants. These salts have an effective impact on the exfoliation of  $MoS_2$ in isopropyl alcohol. In the isopropyl alcohol-K4Fe(CN)6 method, it was discovered that (K4Fe(CN)6) could increase the efficiency of exfoliation by about 73 times, accompanied by obtaining  $MoS_2$  nanosheets dispersion with concentrations of 0.240 mg mL<sup>-1</sup>.

Yuwen et al. (2016) claimed that via normal butyllithium as a lithiation mediator, ultrasonically enhanced Li intercalation could generate  $MoS_2$  nanosheets of matching morphology and features like conventional methods of lithium intercalation, which was produced by the work of (Joensen et al. 1986). Furthermore, ultrasonication-enhanced lithium intercalation will significantly reduce reaction time and yield high-yielding materials (Yuwen et al. 2016).

Nevertheless, the exfoliation method based on normal butyllithium intercalation has many drawbacks, including a long lithiation time, little yield, and the size of the flake is in the submicron range. Using lithium, potassium, and sodium naphthalenide, (Zheng et al. 2014) established a better methodology to exfoliate MoS<sub>2</sub> monolayered. The hydrazine (N<sub>2</sub>H<sub>4</sub>) along with sodium naphthalenide was used as double intercalants in this study to widen the gaps between interlayers of bulk MoS<sub>2</sub>, which is then exfoliated in water. A redox rearrangement model may describe the expansion process, in which part of the N<sub>2</sub>H<sub>4</sub> is oxidized to N<sub>2</sub>H<sub>5</sub><sup>+</sup> during intercalation. The intercalated  $N_2H_5^+$  is thermally unstable and will decompose into N<sub>2</sub>, NH<sub>3</sub>, and H<sub>2</sub> when the intercalated  $MoS_2$  films are heated to high temperatures. As intercalated N<sub>2</sub>H<sub>4</sub> molecules decompose and gasify, the sheets of MoS<sub>2</sub> extend by 100 times more than their initial length. The expanded crystal of MoS<sub>2</sub> is then undergoing intercalation with naphthalenide alkaline solution in a second step. Finally, to prevent sheet fragmentation, the intercalated MoS<sub>2</sub> is exfoliated by submerging it in low-power ultrasonic water. Sodium ions have a much greater ionic radius than lithium ions, allowing for a more significant expansion of interlayer space.

Furthermore, compared to Lix  $MoS_2$ , Nax  $MoS_2$  reacts more aggressively with water, resulting in extra  $H_2$  emitted in a shorter period, promoting exfoliation. This method achieved high-efficiency exfoliation, with lateral widths of around 10 µm in 80 percent of single-layer  $MoS_2$  sheets, approximately ten times greater than flakes identified using standard butyl lithium procedures. Some sodium-containing surfactants, such as sodium dodecyl benzene sulfonate, can be used as intercalation agents for  $MoS_2$  exfoliation besides sodium naphthalenide (Guan et al. 2018).

Guan et al. (2015) published a method for exfoliating  $MoS_2$  in an aqueous solution with high yields using a particular protein, bovine serum albumin. They discovered that bovine serum albumin could serve as an efficient exfoliating agent as well as a stabilizer, preventing monolayer nanosheets from reaggregating (Guan et al. 2015). The yield of  $MoS_2$  nanosheets (1.36 mg/mL) was significantly higher than 0.3 mg/mL of N-methylpyrrolidone agent (Coleman et al. 2011) and 0.5 mg/mL in case of use of surfactants (Smith et al. 2011).

Owing to the long period of induced scission and the creation of non-homogeneous  $MoS_2$  layers, the resulting  $MoS_2$ nanosheets have a relatively small dimension, which is a disadvantage in sonication-assisted exfoliation. Recently, a blend of bath and probe sonication results in a significantly faster exfoliation than bath sonication alone recorded by (Kaushik et al. 2020).

It is important to mention another method based on the sonication process and water expansion upon freezing called the water freezing-thawing approach. This approach is focused on the freezing behavior of water (Matsumoto et al. 2002), whereby when water freezes, it exerts a powerful extrusion force, causing pressures of about 2500 bar in a closed structure (Yoo et al. 2009), which can resolve the van der Waals interaction among neighboring layers in two-dimensional materials. The expansion of layered materials structure occurs as they thaw, ascribing to liquid water absorption. Exfoliation of two-dimensional nanosheets would be enhanced by repeated freezing and thawing cycles. H<sub>2</sub>O can soak into the interlayers of graphite, according to (Algara-Siller et al. 2015). A moderate H<sub>2</sub>O freeze-thaw method and polyvinylpyrrolidone as a stabilizer were used to prepare a few and monolayer two-dimensional nanosheets with no creation of scrolls or flaws. The results show that this method is efficient for exfoliating MoS<sub>2</sub> and MoO<sub>3</sub> nanosheets with fewer than 5 atomic layers, yielding around 32, 42, and 25 percent, respectively, upon 30 cycles of freeze-thaw. While time wasting, this method is economical and requires simple instrumentation, and it has much potential for two-dimensional exfoliating materials on a large scale (Zhu et al. 2019).

Shear force-assisted liquid exfoliation In this method, bulk  $MoS_2$  is exfoliated in suitable surfactant solutions or organic solvents using mechanical mixers with a high speed, like shearing laboratory mixers, ball milling, and even kitchen blenders produce local shear rate in a mixing vessel (usually with 1 L or higher capacity). A mixture of ball milling with low-energy besides sonication was used to report a simple, effective, and scalable method for  $MoS_2$  exfoliation. Ball milling produces compression and shear forces on layered materials, causing their exfoliation to form two-dimensional nanosheets from the edge outer surfaces. The  $MoS_2$  suspension as-fabricated was 0.8 mg/mL. The nanosheets of  $MoS_2$  with sizes in the range of 50—700 nm and thicknesses range of 1.2—8 nm were imaged using atomic force microscopy (Yao et al. 2012).

Sun et al. (2018) successfully fabricated MoS<sub>2</sub>/graphene nanosheets using hydrate salts of potassium sodium tartrate to ball mill both bulk MoS<sub>2</sub> and graphite. Intercalating agent potassium sodium tartrate dissociates into K<sup>+</sup>, Na<sup>+</sup>, and tartrate linker, which could then be intercalated into graphite and bulky MoS<sub>2</sub>, facilitating exfoliation (Sun et al. 2018). It is illustrated the exfoliated MoS<sub>2</sub> nanosheets with a size  $\approx$  of 100 nm and thickness of about 2–5 layers.

A kitchen blender was used to demonstrate exfoliation shear of  $MoS_2$  nanosheets on a large scale in a surfactant.

They achieved 0.4 mg/mL concentrations and 1.3 mg/min output rates by optimizing mixing factors (time of mixing, rotor speed,  $MoS_2$  concentration, and solution volume). Both length and thickness could be regulated from 40–220 nm in length and about 2–12 layers in thickness by changing the surfactant concentration (Varrla et al. 2015).

### **Electrochemical exfoliation**

The electrochemical exfoliation method is a promising process, usually carried out in mild conditions, simple, repeatable, and appropriate for large-scale production (Ji et al. 2019). An electrochemical method of lithium intercalation was used to exfoliate bulk layered MoS<sub>2</sub> (cathodic exfoliation of  $MoS_2$ ). Metal foils of lithium and  $MoS_2$  were used for cathodic and anodic poles, respectively, in this process. Lithium ions are intercalated within the bulk layered MoS<sub>2</sub> when discharging at constant current, weakening the van der Waals force among layers. After being washed with acetone, the intercalated compounds are ultrasonicated in H<sub>2</sub>O or C<sub>2</sub>H<sub>5</sub>OH to exfoliate and extract the two-dimensional nanosheets (Zeng et al. 2011). While this procedure can exfoliate multi-layered compounds into monolayers (for example, single-layer MoS<sub>2</sub>), it is hard to extract the residual lithium doping effect, which causes the MoS<sub>2</sub> nanosheets to lose their semiconducting properties. (Eda et al. 2011; Py and Haering 1983). Liu et al. have used electrochemical anodic exfoliation of bulk MoS2 to obtain thin nanosheets of MoS<sub>2</sub> with high quality(Liu et al. 2014a). The anode, counter electrode, and electrolyte were made up of a bulk layered MoS<sub>2</sub> crystal, a Pt thread, and a 0.5 M aqueous Na<sub>2</sub>SO<sub>4</sub> solution, respectively. Exfoliated monolayer and few-layer MoS<sub>2</sub> nanosheets with lateral sizes up to 50 m have excellent consistency and intrinsic structure.

### **Bottom-up methods**

Among these bottom-up methods, the hydro/solvothermal, microwave, and chemical vapor deposition synthesis routes are widely applied in  $MoS_2$  nanosheets synthesis.

### Hydro/solvothermal synthesis

This method is a traditional wet-chemical synthesis technique that operates at a high temperature of vapor pressure in a sealed autoclave to produce high yield, controllable size, and homogeneous layer thickness of nanomaterial. The only difference between hydrothermal and solvothermal synthesis is that the former uses an aqueous precursor (Gupta et al. 2015; Tan et al. 2017). The hydro/solvothermal synthesis method can be preceded with the assistant of ionic liquids. (Ma et al. 2008) used a hydrothermal process with 1-butyl-3-methylimidazolium tetrafluoroborate to make micro-spheres of  $MoS_2$  with 2.1 mm in diameter. (Du et al. 2015) prepared  $MoS_2$  nanospheres via a solvothermal method with the assistance of an ionic liquid. In dimethyl formamide/water mixed solvents, they used a template of 1-ethyl-3-methylimidazolium bromide. The ratio of dimethyl formamide to H<sub>2</sub>O has an important influence on the morphology and size of  $MoS_2$  produced. (Pirarath et al. 2021) used a surfactant-assisted hydrothermal system to make few-layered  $MoS_2$  nanosheets. The results indicated that the synthesized  $MoS_2$  nanosheets had a petal-like morphology.

### **Microwave synthesis**

The microwave synthesis technique for synthesizing MoS<sub>2</sub> is simple, secure, and time and energy-efficient (Lee et al. 2019; Baghbanzadeh et al. 2011). Nanotubes and fullerene-like MoS<sub>2</sub> nanoparticles were created using a method of microwave-assisted processing path. The amorphous powders of MoS<sub>2</sub> were calcined for 2 h at 600 <sup>0</sup>C in an argon atmosphere. Structural analysis shows that after 200 s of microwave irradiation, the synthesized MoS<sub>2</sub> is like fullerene in its structure with orientated at random, strongly doubled up layers of MoS<sub>2</sub> ordered in short range, whereas a longer time (600 s) of irradiation provided nanostructures similar to nanotube and fullerene in their morphology (Panigrahi and Pathak 2011). A microwave-assisted hydrothermal route was used to build MoS<sub>2</sub>/poly (ethylene glycol) nanoflowers. For 10 min, the precursors of MoS<sub>2</sub> were subjected to microwave irradiation at 220 °C. The nanoflowers form of MoS<sub>2</sub>/poly(ethylene glycol) comprises multi-layers of MoS<sub>2</sub> nanosheets (Sun et al. 2019).

A direct  $MoS_2$  growth on graphene substrate was reported by employing a safe, simple, scalable ultrafast, and efficient microwave-initiated method that did not involve inert gas (Sarwar et al. 2020). The dried blend of  $(NH_4)_2MoS_4$ -graphene-CS<sub>2</sub> was microwave irradiated for 60 s in a microwave oven for home use (2.45 GHz, 1250 W). Graphene was used as a substrate, absorbing microwave energy and converting it to heat, which caused the reduction of  $(NH_4)_2MoS_4$  to  $MoO_2$ , which was then transformed to  $MoS_2$  dispersed on the graphene substrate (Sarwar et al. 2020).

 $MoS_2$  nanosheets use conventional hydrothermal and microwave methods and compares their electrocatalytic performance for hydrogen evolution. The obtained  $MoS_2$ from both ways has similar crystal structural characteristics despite the 24-h hydrothermal synthesis process; microwaveassisted synthesis takes just 30 min. Both techniques give thin and combined nanosheets, but the microwave-formed  $MoS_2$  nanosheets have a smoother edge and less crumpled shape. Both  $MoS_2$  nanosheets were in nearly similar electrocatalytic performance (Solomon et al. 2020).

#### Chemical vapor deposition methods

On substrates such as SiO<sub>2</sub>/Si (Kang et al. 2015), sapphire(Yu et al. 2017), and glass (Yang et al. 2018; Yang et al. 2019), the chemical vapor deposition method is a promising bottom-up synthesizing of controllable size and thickness of MoS<sub>2</sub> with high quality. The correct precursors, MoO<sub>3</sub> and S, are first evaporated at a certain temperature in the chemical vapor deposition technique. The S vapor then gains access to the MoO<sub>3</sub> by passing through an inert gas such as argon (Lee et al. 2017). MoO<sub>3</sub> film is sulfurized in this case, and MoS<sub>2</sub> is formed on a SiO<sub>2</sub> substrate. It should be noted that the chemical vapor deposition condition can be used to monitor the thickness and size of the as-synthesized MoS<sub>2</sub> film. MoS<sub>2</sub> films made by chemical vapor deposition have a high degree of crystalline structure (Lee et al. 2017).

However, the small surface area of traditional chemical vapor deposition growth strategies makes mass development of monolayer or few layers  $MoS_2$  impossible. The  $MoS_2$  nanosheets have been synthesized by using microsized cubic NaCl crystal powders as a template. They chose NaCl as a substrate because it is inexpensive and scalable, with high chemical stability, allowing batch production of highly crystalline  $MoS_2$  powders. With raising the temperature from 500 to 650 °C, the average nanosheets thickness of  $MoS_2$  increases from 1.93 to 2.62 nm, and the suitable growth range was set as 550–650 °C (Zhu et al. 2020).

## Density-functional theory calculations of $MoS_2$

The electronic characteristics of MoS<sub>2</sub>, such as the bandgap, density of state, highest occupied molecular orbital HOMO and lowest unoccupied molecular orbital LUMO, charge density diagram, and work function, were studied via density-functional theory. The density-functional theory estimate of square nanotubes of MoS<sub>2</sub> was investigated by (Zhang et al. 2021). They discovered two groups of 4 bands near the Fermi level having identical energies. States at the square's 4 corners are defined by the conduction band minimum and valence band limit of nanotubes (see Fig. 2). The direct bandgap of the square nanotube is 0.23 eV in armchair structure and having an indirect bandgap of 0.28 eV in zigzag structure as a semiconductor. As the diameter grows, the bandgap grows as well. These values are much smaller than those of cylinder-shaped nanotubes: 0.4 eV, and monolayers MoS<sub>2</sub>: 1.738 eV (Seifert et al. 2000) due to the electronic states close to the 5-coordinated molybdenum atoms and the 2-coordinated sulfur atoms at the corners. In the top view and side view of a two-dimensional deformation charge density map of both cylinder and square nanotubes, thick and thin circles reflect Mo and S atoms, respectively.

In the top view and side view of a two-dimensional deformation charge density map of both cylinder and square nanotubes, thick and thin circles reflect Mo and S atoms, respectively. States at the square's 4 corners are defined by the conduction band minimum and valence band limit of nanotubes.

By the Brillouin zone's high symmetry K point, the direct bandgap of stacked vertically few-layer  $MoS_2$  drastically alters with thicknesses, according to (Majee et al. 2020). The valence band of 0.171 eV splits at the K level, according to a hypothetical band schematic for six layers of  $MoS_2$ , yielding two distinct excitons (A and B). The A and B were determined to have values of 1.73 and 1.90 eV, respectively. The existence of indirect transfers between the valence band maxima at high points of symmetry and the conduction band minima among the K points, based on the literature, is also suggested by the band structure estimation.

The optical band gap of MoS<sub>2</sub>/ZrO<sub>2</sub> was studied (Eid and Al-Hossainy 2021) in the high absorption area for indirect and direct, allowing transition. The  $E_{\sigma}$  can be computed by plotting  $(\alpha h\nu)^2$  versus  $(h\nu)$  and then extrapolation of the linear curve parts to zero absorption (Al-Hossainy et al. 2018). The Eg of [propylene glycol-MoS<sub>2</sub>/ZrO<sub>2</sub>]<sup>C</sup> and [propylene glycol -MoS<sub>2</sub>]<sup>C</sup> hybrid nanofluid films was 2.355 eV and 2.562 eV, respectively. This decrease in Eg resulted from the formation of new energy levels in Eg, attributed to increased defects that required electrons to be transferred from the valence to the conduction band, lowering bandgap as the loading was 0.50% wt. [ZrO<sub>2</sub>]. In universal reactivity descriptors, by using quantum predictions, HOMO and LUMO are essentially standard. The stability of a molecule is determined by the difference in energy between frontier molecular orbits. This plays a crucial part in the conductivity measurement of e-s, aiding in understanding electricity transport. The energy of HOMO and LUMO values is often negative, indicating that isolated compounds have stabilized. Aromatic compounds are predicted to target electrophilic locations based on the observed frontier molecular orbits. These orbitals must be combined in a variety of responses.

The density of states of  $MoS_2$  pristine phases and their intercalated Cs ion equivalents were investigated by (Ali et al. 2021). It is worth noting that the Mo atom's d orbital contributes the most to the density of state total, whereas Cs atom contributes a little. The influence of a Cs atom, on the other hand, was visible in the reorganization of the density of state for the 3 phases. The total density of state for the three phases increased as a result of the Cs intercalation. Furthermore, the intercalation with Cs caused a phase change thermodynamically in the 3R and 2H phases by means of moving fermi level near the valence band, converting the phase from semiconductor to metallic (Vatamanu et al. 2015; Azmi et al. 2016). Quantum capacitance of the  $MoS_2$  intercalated with Cs would be calculated using the density of state because it represents the quantum existence of materials. Estimation of quantum capacitance is critical when scheming electrodes for supercapacitor because it provides data about the electronic reaction of material when exposed to voltage and influences the electrode's electrical double-layer action. The useful potential for MoS<sub>2</sub> ranges from -0.5-0.5 V in this sample of aq. neutral electrolytes, which is the agreed potential window experimentally (Azmi et al. 2016). The Fermi level is the potential at zero charge, where the supercapacitor is unable to accept any extra charges in quantum capacitance calculations. The computed potential at zero charge shows the capacitance at no applied voltage since rich occupied states will accommodate charges, as shown by their quantum capacitance. The quantum capacitance of the three phases is raised by Cs intercalation to 2530, 3180, and 3257 F/g, respectively, for the 1 T, 2H, and 3R phases. The massive rise in quantum capacitance is due to the change in state density for 3R and 2H phases toward metallic existence.

Furthermore, the quantum capacitance improvement was only observed in the positive potential window, implying that 2H-MoS<sub>2</sub> could be used in asymmetric supercapacitor systems as a positive electrode. Cs–MoS<sub>2</sub> has a quantum capacitance that is 200% greater than doped graphene. In comparison with pristine MoS<sub>2</sub>, the difference in charge density was calculated. Charge transfer adsorption between Cs atoms and MoS<sub>2</sub> is signaled by the charges in the bonds between the Cs and S atoms. Bader charge analysis was used to investigate the charge transfer quantitatively (Tang et al. 2009). The Cs ion passes a charge to the MoS<sub>2</sub> system in the 1 T, 3R, and 2H stages, respectively, of 0.85, 0.86, and 0.86 lel, indicating the creation of ionic bonding.

Subramanian et al. (2020) predicted that the Schottky barrier at the epitaxial graphene/molybdenum disulfide interface would be lesser than that of the metal. To predict the Schottky barrier from first principles, estimates of work functions of the individual components pristine Ti, MoS<sub>2</sub>, graphene, and relaxed heterointerfaces (epitaxial graphene/ MoS<sub>2</sub> and Ti/MoS<sub>2</sub>) are needed. According to previous firstprinciples calculations, the work functions of undoped Ti, MoS<sub>2</sub>, and graphene are 4.38, 4.05, and 4.23 eV, respectively (Singh-Miller and Marzari 2009). The absolute value is significantly lowered by 0.3 eV here due to various parameterizations of the exchange–correlation functional and van der Waals interactions in other works since the choice of parameterizations affects the work function's absolute values.

Also, the density-functional theory was used to investigate the electrical and optical characteristics of N, Co, and Co–N co-doped  $MoS_2$  monolayers for visible light photocatalytic activity by (Cheriyan et al. 2018).

The electrical characteristics of  $MoS_2$  pristine and  $MoS_2$  doped with TM were investigated by (Deng et al. 2019). The energy of formation among S-vacancy of  $MoS_2$  and the

TM is given by  $[E_f = E_{vac} + E_{TM} - E_{(TM-MoS2)}]$ , where  $E_{vac}$ ,  $E_{TM}$ , and  $E_{TM-MoS2}$  stand for combined energies of MoS<sub>2</sub> monolayered with S vacant position, a free atom of transition metal, and the MoS<sub>2</sub> doped with the transition metal (Ma et al. 2016). Because of its high forming energy, Ti-doped MoS<sub>2</sub> has the highest binding power as well as the most stable structure (Deng et al. 2019). Since the Fermi level is in the energy gap region, all structures considered have semiconducting properties. The band distance of pristine MoS<sub>2</sub> is 1.70 eV, close to the experimental value of 1.69 eV (Kuc et al. 2011) and the theoretical result of 1.8 eV (Kam and Parkinson 1982). Pt-doped MoS<sub>2</sub> is a semiconductor with the indirect band gap type, while Ti-, Ni-, and Pd-doped MoS<sub>2</sub> are semiconductors with a direct band gap.

### MoS<sub>2</sub>-based nanocomposites for water remediation application

With the current global economic evolution, tackling prominent pollutants has become a global priority (Abdel Maksoud et al. 2020; Makvandi et al. 2021; Mamba et al. 2007; Singh et al. 2021). Hence, a variance of approaches has been undertaken to promote techniques for removing or decomposing pollutants, such as adsorption (Xiao et al. 2020), membrane separation (Luciano et al. 2020), biological (Oliveira et al. 2020), coagulation (Sillanpää et al. 2018), photo-oxidation (Onga et al. 2020), and photocatalysis technologies (Chenab et al. 2020).

In recent years,  $MoS_2$  has confirmed exceptional utilization potential in the water remediation field. Overall,  $MoS_2$ and its composites possess the capability to degrade and/or remove distinctive pollutants, which affords the potential for water remedy.  $MoS_2$  has been recognized as a proper photocatalyst and/or absorbent in water remediation, ascribing to its extraordinary specific uptake, cost-effective, exceptional specific surface area, and small bandgap. Notwithstanding, the display of absorbent or photocatalyst composed or based on  $MoS_2$  material is still far away from contentment, as it has a low surface area and an intrinsically lower electric conduction (Fageria et al. 2017). To defeat all the above obstacles,  $MoS_2$  incorporated with different proper photocatalysts such as carbonaceous material, metal oxides, and metal sulfides(Shanker et al. 2017).

### MoS<sub>2</sub>-carbon materials

One efficient strategy incorporates the  $MoS_2$  with carbonaceous materials with extraordinary electric conductivities and unique surface areas (Chen et al. 2017). Amongst them, the reduced graphene oxide possesses attracted great interest to synthesize reduced graphene oxide-based photocatalysts ascribing to its remarkable theoretical specific area and unique electric and thermo-mechanical features (Wang et al. 2016a; Shen et al. 2017; Jilani et al. 2018; Hebbar et al. 2017; Maddinedi et al. 2017; Patel et al. 2020), which can be availed as an electron collector for gaining and donating electrons (Lv et al. 2017). The MoS<sub>2</sub>/reduced graphene oxide composites have recently synthesized to degrade the ranitidine under visible light (Zou et al. 2020). The detected diffraction peaks confirmed the successful preparation of MoS<sub>2</sub>/reduced graphene oxide. The high resolution-transmission electron microscope image of the MoS<sub>2</sub>/reduced graphene oxide composite presents distinctive layer-like structures besides a marked lattice fringe and having a 7.2 Å as an interlayer distance. The photocatalytic potential is to degrade ranitidine via MoS<sub>2</sub>/reduced graphene oxide composites under visible radiation. The removal efficiencies of ranitidine via MoS<sub>2</sub> and reduced graphene oxide were reached about 33% and 35%, respectively. At the same time, the MoS<sub>2</sub>/reduced graphene oxide composites possess a photodegradation performance that reached 74% after 1 h of visible light exposure.

Further, the photodegradation efficiency toward ranitidine enhances with rising the reduced graphene oxide content. This behavior can be attributed to the incorporation of reduced graphene oxide outstandingly enhanced the separation performance for the generated pairs of photoelectrons in the MoS<sub>2</sub>/reduced graphene oxide composites, and it enhances the specific surface area of the composite. Besides, the attraction within the electrons of p-orbital for ranitidine and the reduced graphene oxide conjugated system  $(\pi - \pi)$  enhances polluters' adsorption via the utilizing of the MoS<sub>2</sub>/reduced graphene oxide composite photocatalyst. Exaggerated coating of reduced graphene oxide on the MoS<sub>2</sub> surface prevents the MoS<sub>2</sub> capacity from absorbing visible radiation. Hence, the MoS<sub>2</sub>/reduced graphene oxide composite exhibited a photocatalytic performance lower in contrast to that of pristine MoS<sub>2</sub>. The formation potential of N-Nitrosodimethylamine (NDMA) of the ranitidine solution after 60 min under visible-radiation exposure was illustrated. With the rising reduced graphene oxide ratio, the formation potential of NDMA for ranitidine has reduced (6.76%) and then enhanced (45.27%), which complies with the photodegradation behavior and the mineralization degree.

Recently, heavy metals permanently menace human health and global sustainable evolution. The hexavalent chromium Cr (VI) is a very serious mineral pollutant with non-bioreduction and carcinogenic features. Currently, the reduction of Cr(VI) via photodegradation strategies is considered an essential way of efficient approaches to mitigating Cr (VI) contamination (Fang et al. 2018).

Bai et al. (2018) have synthesized Red phosphorus coating on  $MoS_2$ /reduced graphene oxide hybrid for removal of Cr (VI) and Rhodamine B. Figure 3a-f demonstrates the comparative surface morphology of the hybrid  $MoS_2@$ 

reduced graphene oxide and Red phosphorus coating MoS<sub>2</sub>/ reduced graphene oxide, in addition to their partial magnification, showing the curly layers where the graphene oxide works as a scaffold resulting in an anchoring and stabilizing for the nanostructured sheets of MoS<sub>2</sub> and Red phosphorus. Figure 3g affirms a consistent distribution of carbon, oxygen, phosphorus, molybdenum, and sulfur for the Red phosphorus coating MoS<sub>2</sub>/reduced graphene oxide hybrid. The results also revealed that the MoS<sub>2</sub> and graphene oxide layers are owning an unstacked arrangement. In addition, the graphene oxide reduction and the coating of  $MoS_2$  on the surface of reduced graphene oxide layers have been occurred concurrently, ending in a regular and controllable distribution of the nanostructured sheets of MoS<sub>2</sub> on the surface of reduced graphene oxide layers. Further, the results unveiled that the Red phosphorus coating MoS<sub>2</sub>/reduced graphene oxide displays a hexagonal crystal arrangement in the nanoscale nature. Finally, the Red phosphorus coating MoS<sub>2</sub>/reduced graphene oxide composite was used to remove about 98.0% of Cr (VI) and about 99.3% from the rhodamine B over half-hour only.

The photodegradation performance of Red phosphorus coating  $MoS_2$ /reduced graphene oxide hybrid is notably correlated with the e<sup>-</sup> and h<sup>+</sup> amount and their activity. Besides, the graphene oxide demonstrated an essential function in collecting, shuttling the generated electrons, and distinguished adsorption. Most remarkably, Cr (VI) and rhodamine B working as a scavenger to each other may absorb e<sup>-</sup> and h<sup>+</sup> together, ending to occurring a synergy impact between the Cr (VI) removal and the rhodamine B oxidation as presented in the graphical photodegradation mechanism.

Also, the carbon nanotubes are one-dimensional material, showing excellent merits such as unique electric conduction, exceptional thermal conduction, and remarkable stability in the structure (Kim et al. 2005; Bindumadhavan et al. 2013). So, combining the unique properties of carbon nanotubes and MoS<sub>2</sub>, we can get a unique construction of the MoS<sub>2</sub>/ carbon nanotubes composite that can be utilized as a proper photocatalyst composite for environmental applications. In photocatalytic application, the electrons in carbon nanotubes can be immediately excited to MoS<sub>2</sub> under ultraviolet or visible irradiation, resulting in the robust separation of charge carriers of photoexcitation. Hence, carbon nanotubes with a large diameter are an excellent selection to gain huge photocatalysis if carbon nanotubes are utilized as decorated on the surface of MoS<sub>2</sub> (Zhang et al. 2017b).

The extraordinary adsorption potential for lead (0.9  $\mu$ g/g) and cadmium (~0.7  $\mu$ g/g) from manufacturing mine water via a photocatalyst nanocomposite based on MoS<sub>2</sub>/multi-wall-carbon nanotubes has been reported by (Gusain et al. 2019). The adsorption of lead/cadmium ions on the surface of photocatalyst nanocomposite ascribing to creating a complex (metal/sulfur) between the lead/cadmium ion

and the sulfur group is on the  $MoS_2$  over the exchange process via H<sup>+</sup> ions. Also, the negative charges being in the  $MoS_2$ /multiwall-carbon nanotubes surface tend to the electrostatic interaction that was occurring among the positive charges for lead/cadmium ions and the negative charges of the adsorbent.

Between the carbonaceous materials, carbon nanofibers have been examined as candidate materials used in many fields, such as catalyst carriers and flexible electrodes (Almeida et al. 2019). These merits are ascribed to its extraordinary electrical conduction, excellent mechanical characteristics, and a broad range of products simply. (Liang et al. 2020) have reported the preparation of composites of MoS<sub>2</sub>/carbon nanofibers, which seems as foxtail via the electrospinning technique. The outcomes reveal that the surface morphology of MoS<sub>2</sub> was verified by varying the precursor concentration, as exhibited in Fig. 4. Compared to pure MoS<sub>2</sub>, the MoS<sub>2</sub> carbon nanofibers composites showed remarkable photocatalytic potential toward dye degradation. It is ascribed to the synergistic influence between carbon nanofibers and MoS<sub>2</sub> which may be resulting from the heterogeneous interfaces and the excellent conduction properties of carbon nanofibers. Further, the exceptional adsorptive capacity of MoS<sub>2</sub>/carbon nanofibers composites can improve the apparent concentration of reactants. Besides, the hierarchical structure morphology can supply additional reactive sites.

It is ascribed to the synergistic influence between carbon nanofibers and  $MoS_{2}$ , which may be resulting from the heterogeneous interfaces. The hierarchical structure morphology can supply additional reactive sites.

Graphitic carbon nitride besides has a two-dimensional layered construction, and it is a layered material like graphite. Recently, graphitic carbon nitride has been shown to advantage exceptionally attractive, ascribed to its proper bandgap and extraordinary stability in tough chemical conditions (Pramoda et al. 2017). Nevertheless, pure graphitic carbon nitride possesses low photocatalytic performance resulting from that the hole-electrons, that photogenerated, suffer from the fast recombination. But, MoS<sub>2</sub> has a demanding structure, including unsaturated atoms of both atoms (Mo and S) at the edges, which give a promising edge activity over the photodegradation process. Combining MoS<sub>2</sub> and graphitic carbon nitride to create heterostructure catalysts has been confirmed to improve the catalytic performance resulting from the effective charge separation (Li et al. 2017; Li et al., 2018a; Lu et al. 2019; Yang and Wang 2021). Recently, (Liu et al. 2020a) have reported enhancing the charge separation in the Z-scheme MoS<sub>2</sub>/graphitic carbon nitride composite for improved photodegradation potential toward bisphenol-A. Compared with the graphitic carbon nitride sample, the MoS<sub>2</sub>/graphitic carbon nitride composite exhibited exceptionally improved photocatalytic potential.

Also, a significant repression toward bisphenol A degradation was seen ascribed to the scavenging impact.

Also, the MoS<sub>2</sub>/graphitic carbon nitride composite exhibited a notable performance toward heavy metals removal. The synthesis of the heterostructure MoS<sub>2</sub>/graphitic carbon nitride as a promising catalyst for removing U(VI) has been reported by (Zhang et al. 2020a). The heterostructure advanced the charge transference and improving the separation potential of photogenerated electron-hole pairs. Further, the heterostructure MoS<sub>2</sub>/graphitic carbon nitride sample showed extraordinary photoreduction performance toward U(VI), which was notably higher than that obtained of pure graphitic carbon nitride. Besides, the heterostructure MoS<sub>2</sub>/ graphitic carbon nitride sample exhibited noteworthy stability under visible radiation. The electrons (e<sup>-</sup>) are transported between the conduction bands, whereas the holes  $(h^+)$ were transported between valence bands for both (graphitic carbon nitride and  $MoS_2$ ). Besides, e<sup>-</sup> lessen dissolved  $O_2$ while decreasing U(VI), and the declining output interacts synergistically with e<sup>-</sup> to reduce U(VI).

Furthermore, compared with the earlier published bulk phase of the heterogeneous  $MoS_2@$  graphitic carbon nitride, the heterogeneous  $MoS_2$ /graphitic carbon nitride phase lessens the transport time and interval photoinduced carriers and therefore lowers the recombination feasibility of the carriers through transfer (Shi et al. 2018).

### MoS<sub>2</sub>-metals oxides materials

In recent decades, to address the problem of dangerous environmental contamination, photocatalysis based on semiconductor materials has been broadly examined for the photocatalysis of contaminations (Lee and Jang 2014).

Titania or titanium (IV) oxide TiO2-based photocatalysts have numerous merits, which are ascribed to outstanding benefits such as cost-effectiveness, excellent chemical stability, and friendliness to the environment. Nevertheless, the TiO<sub>2</sub> catalysts display excellent photocatalytic activity in the near UV attributable to its broad bandgap energy (3.2 eV) that is incapable of being used in the visible light region (Xiao et al. 2014). On the other hand,  $MoS_2/TiO_2$  nanocomposites have been published to display enhanced photocatalytic characteristics. A rising number of researchers are currently attempting to advance manufacturing techniques to achieve the heterostructure of MoS<sub>2</sub>/TiO<sub>2</sub> possessing uniform distribution, influential interaction, and singular structures for numerous utilizations. These strategies to synthesize the MoS<sub>2</sub>/TiO<sub>2</sub> heterostructure can be classified into two sections: ex situ synthetic approaches and in situ synthetic approaches (Chen et al. 2018).

Development of the N and  $Ti^{3+}$  co-substituted  $TiO_2$  incorporating with  $MoS_2$  has been reported by (Liu et al. 2017). Moreover, after conjugation with  $MoS_2$ , the photocatalytic

activity of the sample is notably improved, ascribed to the production of the heterogeneous structure, that not only efficiently prevents recombination of electron-hole pairs but also affords rich catalytic sites for contaminants removal.

Also, (Zhang et al. 2016) have successfully prepared the heterostructure of  $MoS_2/TiO_2$  via the hydrothermal approach. Remarkably, the heterostructure of  $MoS_2/TiO_2$ presents a more excellent adsorption capacity to degrade the organic dyes in contrast to pure TiO<sub>2</sub>. Also, the enrichment in the adsorption capacity for the heterostructure of  $MoS_2/$ TiO<sub>2</sub> photocatalysts can be notably ascribable to the exceptional specific surface area of the heterostructure of  $MoS_2/$ TiO<sub>2</sub>, which contributes to growing the active adsorption sites to degrade the organic dyes and promote the photocatalytic potential. All heterostructures of  $MoS_2/TiO_2$  display remarkably better photocatalytic potential than both pure TiO<sub>2</sub> and  $MoS_2$  after exposure to ultraviolet-light radiation.

Zinc oxide ZnO also has a broad bandgap and is active only under ultraviolet radiation. Besides, it is one n-type semiconductor, which is a desirable photocatalytic candidate ascribing to its direct bandgap (3.37 eV), extraordinary photostability, exceptional sensitivity, cost-effective, nontoxic characteristics, and unique exciting binding energy (60 meV). ZnO is further limited only to ultraviolet radiation, and besides, the fast recombination for the carriers restricts its possible utilizations. Diverse strategies have been established to address ZnO serving in the visible light zone and promote ZnO absorption under the energies with low value by performing electronic levels inside its bandgap (Ebrahimi et al. 2017; Colombo et al. 2017). Many investigations have examined the MoS<sub>2</sub> potential candidate as co-photocatalysts to promote the photocatalytic potential of ZnO in water purification utilization. MoS<sub>2</sub> is a p-type semiconductor material with a narrow bandgap, which presents exceptional absorption toward the visible area of the solar radiation and possesses the stable layered metal dichalcogenides, which are infirmly linked via van der Waals interactions, presenting the feasibility for the bulk phase  $MoS_2$ which exfoliated to thin nanolayers for an additional examination of the activity of  $MoS_2$  (Benavente et al. 2018).

Also, (Rahimi et al. 2019) have reported the enrichment of the photocatalytic potential of ZnO under sunlight via incorporating it with thin layers of MoS<sub>2</sub>. In the case of uses sunlight radiation, MoS<sub>2</sub> increments the photocatalytic potential of ZnO by 75%. Nevertheless, in the case of use of ultraviolet-blocked radiation, MoS<sub>2</sub> lessens the photocatalytic potential of ZnO to 67% of its original value. If the photon energy  $h\nu \ge 3.1eV$ , i.e.,  $\lambda < 400nm$ , both ZnO and MoS<sub>2</sub> would be excited, and MoS<sub>2</sub> promotes the separation/division of electrons and holes. If the photon energy ranged between 2.45 and 3.1 eV, i.e., the wavelength ranged between 400 and 507 nm, this energy is sufficient to excited electrons MoS<sub>2</sub> to its conduction

band. Also, this energy demanded the electrons of ZnO to be excited to its defect-energy level.

Consequently, the excited electrons in the conduction band of  $MoS_2$  possess energy used to flow at the ZnO defect-energy level. Also, ascribing to the broad bandgap of ZnO and when the ultraviolet region of the light is missing, ZnO is just partially excited, and  $MoS_2$  performs the chief photodegradation capacity, and ZnO works essentially in an electron-hole division/separation for the photoinduced electrons and holes. Finally, if the photon possesses energy equivalent to the bandgap of  $MoS_2$ , i.e., the wavelength range between 507 and 751 nm, the  $MoS_2$ would be excited, and the level of defect energy for ZnO supports their separation.

Since pure  $MoS_2$  is unmanageable to perform free radicals for degrading the organic pollutants, ascribing to its valence band edge capability is not oxidative sufficient. Additionally, pure  $MoS_2$  is not simple to be cyclic employed.

Spinel ferrites with superior magnetic features and small band gaps are a profitable procedure to defeat these shortcomings of  $MoS_2$ , where spinel ferrites can stimulate the existence of photoinduced charge carriers and improve the photodegradation sensitivity to visible light (Abdel Maksoud et al. 2020; Lu et al. 2020; Marcelo et al. 2021).

Recently, (Atacan et al. 2021) have reported synthesizing a magnetic photocatalyst nanocomposite based on  $CuFe_2O_4/$  $MoS_2$  via the hydrothermal method. The outcomes show that the CuFe<sub>2</sub>O<sub>4</sub>/MoS<sub>2</sub> displays the greatest photodecomposition in Rhodamine B degradation than those for pure MoS<sub>2</sub> and Cu-ferrite. The charge transference procedure formed through the p-n (CuFe<sub>2</sub>O<sub>4</sub>/MoS<sub>2</sub>) heterojunction positively influences the separation of photoinduced carriers. Also, the  $CuFe_2O_4/MoS_2$  photocatalyst showed ferromagnetically performance, and hence, it will enable fast rescue from the Rhodamine B solution by utilizing an external magnetic field. After the 5<sup>th</sup> cycle, an insignificant reduction in the photocatalytic capability of CuFe<sub>2</sub>O<sub>4</sub>/MoS<sub>2</sub> photocatalyst was marked. The photodegradation for CuFe<sub>2</sub>O<sub>4</sub>/MoS<sub>2</sub> photocatalyst was reduced by 3.5% than those obtained in the 1<sup>st</sup> cycle. The outcomes present extraordinary photocatalytic performance for the CuFe<sub>2</sub>O<sub>4</sub>/MoS<sub>2</sub> photocatalyst.

Also, (Jia et al. 2019) have enhanced the Au-decorated  $CoFe_2O_4/MoS_2$  photocatalyst against methyl orange with feasibility for magnetic recovery. Indeed, the presence of Au as decorating for the surface of cobalt ferrite can efficiently improve the interface conduction and stimulate the recombination process for the conduction band electrons for cobalt ferrite with the holes in the  $MoS_2$  valence band. They found a negligible reduction in the photocatalytic capability until the 4th recycle, showing that the Au-CoFe<sub>2</sub>O<sub>4</sub>/MoS<sub>2</sub> composite is durable for possible applications. The composites can be available to recover by utilizing a magnet.

Perovskite oxides also give a unique functional material character with a novel crystal structure. Also, these materials possessed extraordinary photocatalysis potential. Besides, they have an excellent performance in energy and environmental areas (Hu et al. 2020; Grabowska 2016; Kumar et al. 2019).

Recently, (Jiang et al. 2020) have reported the synthesis of  $MoS_2/CaTiO_3$  heterogeneous for degrading tetracycline in water. The  $MoS_2/CaTiO_3$  shows a higher photocatalytic achievement toward tetracycline than to pure  $MoS_2$  and  $CaTiO_3$ . The photodegradation enhancement is attributable to the electron transportation for the Z-scheme of the heterogeneous and the stimulating interaction between the  $MoS_2$  and the  $CaTiO_3$  perovskite. Moreover, the Z-scheme  $MoS_2/CaTiO_3$  heterogeneous possessed more suitable induced carrier separation, more active charge transportation, and a greater photoinduced carrier lifetime and considerably improved photodegradation activities.

### MoS<sub>2</sub>-metal sulfide composites

MoS<sub>2</sub>/CdS heterostructures have been extensively investigated for organic dyes degradation, for instance, methylene blue, methylene orange, and rhodamine B, due to their unique properties and narrow band gap (Wang et al., 2018a; Lian et al. 2018; Li et al. 2019a). The heterojunction between CdS and MoS<sub>2</sub> could facilitate photogenerated charge migration and separation, thereby boosting photocatalytic performance(Kumar et al. 2016; Jia et al. 2014). A singlestep hydrothermal process was used to prepare CdS/MoS<sub>2</sub> nanocomposite and tested it for methylene blue degradation under ultraviolet illumination. The percentage of methylene blue photodegradation using CdS/MoS<sub>2</sub> was higher by 48% compared to CdS and MoS<sub>2</sub> (Darsara et al. 2018). Montmorillonite/MoS<sub>2</sub>/CdS demonstrated a potential photocatalytic activity for rhodamine B degradation and achieved 98.8% when exposed to visible light for 45 min (Peng et al. 2019). The large surface area, high visible light-harvesting capacity, and low electron-hole pairs recombination rate were credited to the high performance. They proposed the mechanism of rhodamine B degradation. Under the visible light illumination, the electrons in  $MoS_2$  and CdS are excited to the conduction band, leaving positive holes  $(h^+)$  in the valence band. The photogenerated e<sup>-</sup> and h<sup>+</sup> transferred from CdS to the conduction band and valence band of MoS<sub>2</sub>, respectively, because the MoS<sub>2</sub> has a lower conduction band and higher valence band than CdS. The charge reunion rate was less in MoS<sub>2</sub> with an indirect band gap which prolonged their lifetime. The photogenerated electrons reacted with  $O_2$  to form  $O_2^{-}$ . The OH groups present in the montmorillonite surface worked as a hole trapper to generate OH<sup>-</sup> inhibiting the recombination of the electron-hole pairs. The  $h^+$ ,  $O_2^-$ ,

and OH<sup>•</sup> acted as a strong oxidizing agent for rhodamine B dye removal (Peng et al. 2019).

Also,  $MoS_2/CdS$  nanodots-on-nanorods structure demonstrated high photodegradation efficiency of rhodamine B with 99.11% within 45 min. The well-defined structure, which inhibited charge recombination and allowed many charge carriers to participate in the rhodamine B degradation, was credited with this high performance. They explained the detailed photocatalytic activity mechanism of  $MoS_2/CdS$ . The electrons leaped conduction band under light irradiation, producing positive h<sup>+</sup> in the valence band, and then, the electrons react with O<sub>2</sub> to form O<sub>2</sub> combined with h<sup>+</sup> to degrade rhodamine B (Li et al. 2019a).

The MoS<sub>2</sub>/CdS nanocomposite was prepared using a two-stage solvothermal process at different temperatures and investigated for its photocatalytic activity for methylene orange removal under visible light illumination (Alomar et al. 2019). The thinner MoS<sub>2</sub>/CdS sheet, which was prepared at 220 °C, exhibited the highest performance for methylene orange degradation with high stability under visible light. Compared to pristine MoS<sub>2</sub> and CdS, this nanocomposite's narrow bandgap, excellent separation, and low recombination of  $e^-$  and  $h^+$  were credited with the high performance.

 $Bi_2S_3/MoS_2/TiO_2$  showed the highest photocatalytic efficiency of methylene blue degradation under sunlight up to 99% after 4 min compared to bare TiO<sub>2</sub>, MoS<sub>2</sub>, and Bi<sub>2</sub>S<sub>3</sub>. This developed performance was ascribed to the large surface area and the construction of double Z-scheme heterojunction, which increased the active sites and charge separation efficiency (Drmosh et al. 2020).

Besides, (Zhang et al. 2018a) evenly distributed the  $MoS_2$ nanosheets with different  $Cu_2S$  snowflake to form  $MoS_2$ nanosheets/ $Cu_2S$  snowflake nanocomposites and examined their photocatalytic activity for methylene orange degradation under visible light illumination. The nanocomposite with 50 wt% of  $MoS_2$  demonstrated the highest performance for methylene orange photodegradation and reached to 90% after 60 min when exposed to visible light. This excellent efficiency was owed to the high specific surface area of the  $Cu_2S$  snowflake structure, which improved the light-trapping ability and enhanced charge separation in the composite heterojunction.

The  $MoS_2/Ag_2S/Ag$  ternary nanocomposite (flower-like structure) has been designed and examined it for the photodegradation of Congo red. This nanocomposite achieved 97.01% of Congo red degradation after 120 min when exposed to visible light. This outstanding performance was ascribed to the  $MoS_2$  flower-like structure, which supplied many active sites; the electron transporter function of Ag and Z-scheme constructed in the  $MoS_2/Ag_2S/Ag$  interface

boosted charge separation and mitigated the recombination rate (Zeng et al. 2019a).

The Bi<sub>2</sub>S<sub>3</sub>/MoS<sub>2</sub> revealed the highest photocatalytic activity for red phenol degradation up to 83.4% in 60 min compared to the pristine MoS<sub>2</sub> nanosheets and Bi<sub>2</sub>S<sub>3</sub> nanorods (Vattikuti and Byon 2016). This was due to the outstanding suppression of charge recombination rate and increase in charge carrier lifetime, which reinforced the redox reaction. They explained the phenol red photodegradation over  $Bi_2S_3/$ MoS<sub>2</sub> binary composite. When Bi<sub>2</sub>S<sub>3</sub>/MoS<sub>2</sub> was exposed to visible light, electrons are leaped to the conduction band with forming positive holes in the valence band of  $Bi_2S_3$ and MoS<sub>2</sub>. Then, the excited electrons in Bi<sub>2</sub>S<sub>3</sub> conduction band migrated to MoS<sub>2</sub> conduction band (Jiang et al. 2016; Long et al. 2016), while positive holes transferred to the valence band of  $Bi_2S_3$  from the valence band of  $MoS_2$ . This electron separation mechanism suppressed the charge recombination rate and rose the charge carrier's lifetime and thereby enhanced the phenol red photodegradation(Vattikuti and Byon 2016).

Also, the  $WS_2/MoS_2/BiOCl$  achieved 99.36% of methylene blue degradation in 240 min (Qi et al. 2021). The construction of a heterojunction between  $WS_2$ ,  $MoS_2$ , and BiOCl improved light-harvesting performance, created a narrow band gap, and facilitated charge transfer and separation, resulting in this outstanding efficiency.

The precipitation–deposition process was utilized to prepare PbS/MoS<sub>2</sub> binary nanocomposites with various PbS molar proportions (0.5%, 1.0%, and 1.5%) and investigated it for the methylene blue dye photodegradation under visible light. 1% PbS-MoS<sub>2</sub> achieved the highest activity for methylene blue removal and reached 83% in 180 min. The findings of characterization techniques indicated that 1% PbS-MoS<sub>2</sub> exhibited the largest surface area and the highest electron–hole pair separation efficiency, which explains its outstanding photocatalytic behavior (Raja et al. 2017).

The electrospinning method used to make MoS<sub>2</sub>/Cd<sub>8</sub>/ TiO<sub>2</sub> ternary nanocomposites deposited on carbon nanofibers followed by calcination under nitrogen (Pant et al. 2019). This nanocomposite showed outstanding efficiency for methylene blue removal compared to the bare TiO<sub>2</sub> nanofibers. This was due to the high absorption efficiency of carbon nanofibers and their good synergy with other components. They explained the adsorption and removal mechanism of methylene blue dye over MoS<sub>2</sub>/Cd<sub>5</sub>/TiO<sub>2</sub>. The heterojunction between MoS<sub>2</sub>, CdS, and TiO<sub>2</sub> distributed on carbon fibers extended the light absorption capacity to the visible light region. When the ternary nanocomposite was exposed to the visible light, the electrons are leaped to the conduction band with generating positive holes in the valence band in each component. The excited electrons in the CdS conduction band migrated to the TiO<sub>2</sub> conduction band mean, while positive holes transferred from the CdS valence band

to the MoS<sub>2</sub> valence band. This electron transfer mechanism prolonged the lifetime of charge carriers and decreased their combination. These photogenerated electrons reacted with oxygen to generates  $O_2^-$ , and the holes reacted with OH<sup>-</sup> and generated OH. These radicals ( $O_2^-$ , and OH) degraded methylene blue dye to CO<sub>2</sub> and H<sub>2</sub>O (Pant et al. 2019).

The binary composite consists of MnS and MoS<sub>2</sub> nanostructures and tested it for the photocatalytic degradation of methylene blue dye (Chen et al. 2019a). The MnS/MoS<sub>2</sub> nanocomposite exhibited the highest performance compared to the bare MnS and MoS<sub>2</sub>. Due to the difference in the conduction band and valence band energies of both MnS and MoS<sub>2</sub>, the excited electrons in the MnS conduction band migrated to the MoS<sub>2</sub> conduction band. However, holes at MoS<sub>2</sub> valence band transferred to the MnS valence band. This movement of charge carriers inhibited the charge recombination and thereby enhanced the photocatalytic efficiency (Chen et al. 2019a). A way for the wastewater purification and synchronous generation of valuable chemicals such as hydrogen was opened by (Zhang et al. 2017a). They investigated the photocatalytic efficiency of  $MoS_2/ZnIn_2S_4$ @reduced graphene oxide for the degradation of methylene blue, rhodamine B, fulvic acid, eosin Y, and p-nitrophenol, and it showed photodegradation performance 98.5%, 98.8%, 92.2%, 98.6%, and 91%, respectively. This was due to reduced graphene oxide's efficient role in facilitating electron transfer, and a large number of active sites were provided by MoS<sub>2</sub>. The highest amount of hydrogen (45 µmol) was obtained during rhodamine B removal (Zhang et al. 2017a).

Heavy metal contamination has become a global problem. The ecosystem is significantly harmed by industrial wastewater containing heavy metals such as chromium Cr(VI). Carbon nanotubes/MoS<sub>2</sub>/SnS<sub>2</sub> hydride nanotubes composite was prepared and explored it for the Cr(VI) reduction under visible light subjection (Dong et al. 2019). The carbon nanotubes/MoS<sub>2</sub>/SnS<sub>2</sub> composite demonstrated 100% removal of Cr(VI) solution containing 50-mg/L in 90 min, while SnS<sub>2</sub> and carbon nanotubes/MoS<sub>2</sub> exhibited 96.3% and 80%, respectively, under the same circumstances. Besides, within 90 min, carbon nanotubes/MoS<sub>2</sub>/SnS<sub>2</sub> completely eliminated Cr(VI) from a solution containing 120 mg/L. They proposed a reduction mechanism of Cr(VI) over carbon nanotubes/  $MoS_2/SnS_2$  composite under visible light subjection. The p-n heterojunction formed by  $MoS_2$  (p-type) and  $SnS_2$ (n-type) increased and decreased the Fermi energy level of MoS<sub>2</sub> and SnS<sub>2</sub> responsibly, respectively, and reached the same Fermi energy level (Swain et al. 2018; Bagherzadeh and Kaveh 2018). Under visible light illumination, the electrons in MoS<sub>2</sub> and SnS<sub>2</sub> are leaped to the conduction band, leaving positive holes in the valence band (Hu et al. 2018a; Zhang et al. 2018b; Zhang et al. 2018c).  $MoS_2$  has a more

negative conduction band potential than  $SnS_{2}$ , and thus, the excited electrons in the  $MoS_2$  conduction band transferred to the  $SnS_2$  conduction band. Meanwhile, the positive holes migrated from the  $SnS_2$  valence band to  $MoS_2$ , leading to excellent charge separation performance. These electrons reduced the adsorbed Cr(VI), and holes oxidized water to generate  $O_2$ .

 $MoS_2/Co_3S_4$  core-shell dispersed on nanofiber aerogel by (Qiu et al. 2020). This nanocomposite reduced Cr(VI) with excellent efficiency reached 90% after 50 min. The MoS<sub>2</sub>/ SnS<sub>2</sub> with Mo/Sn ratio of 7.5% demonstrated the highest efficiency for Cr (VI) reduction up to 99.9% and 96.5% for methylene blue removal when subjected to visible light (Qiang et al. 2021). This outstanding performance due to the Z-Scheme and the heterojunction construction facilitated the charge transfer process and inhibited the charge carrier reunion rate. Further, the 2-Cu<sub>2</sub>S-MoS<sub>2</sub> achieved the rapid Cr(VI) photoreduction performance which was 0.0058 min<sup>-1</sup> when subjected to visible light (Zhang et al. 2020b), which was about 8.3- and 2.9-fold greater than pristine MoS<sub>2</sub> and Cu<sub>2</sub>S, respectively. They studied the Cr(VI) photoreduction mechanism in-depth. Due to the difference in the energy levels of the conduction band and valence band of  $MoS_2$  and  $Cu_2S$  and the formation of  $\Pi$ -type alignment, the photoexcited electrons transferred from Cu<sub>2</sub>S conduction band to MoS<sub>2</sub> conduction band, while positive holes migrated to MoS<sub>2</sub> valence band from Cu<sub>2</sub>S valence band under visible light illumination. This phenomenon mitigated the charge carriers reunion rate and prolonged their lifetime. These electrons in MoS<sub>2</sub> conduction band reduced Cr(VI) to Cr(III); meanwhile, the positive holes in the valence band of  $Cu_2S$  oxidized water to generate  $O_2$  (Zhang et al. 2020b).

### MoS<sub>2</sub>-based nanocomposites for supercapacitors

Currently, the amalgamation of energy demand with the depletion of only accessible power and energy resources is triggering scientists to look for novel, clean, low-cost, and environmental energy outputs and storage devices with superior performance (Xia et al. 2018). Electrochemical capacitor shows a growing role in providing the demand for high-rate production, storing, and conveying electrical energy. As a result, the necessity for high-power, ever-present, and high-energy-density storage has increased (Simon and Gogotsi 2020). Owing to their swift charge/discharge rate, high-power density, ultra-long cycle life, relatively low-cost, environmental, and safe operation environments, supercapacitors exhibit superiority over traditional electrostatic capacitors and batteries (Yin et al. 2020). As a result, according to the Statista database, the automotive supercapacitors market worldwide is predicted to rise to 7 billion US \$ by 2028, related to ~0.5 US \$ in 2018. According to the Scopus database, the number of "MoS<sub>2</sub> in energy storage" publications compared with "MoS<sub>2</sub> supercapacitors" from 2013 till 2020 is increased concern to MoS<sub>2</sub> as a likely material for energy storage strategies in general and supercapacitors in specific.

### Principle of energy storage in electrochemical capacitors

Supercapacitors primarily obey two charge storage mechanisms based on supercapacitors' working mechanism: (1) electrochemical double-layer capacitors, EDLCs, and (2) pseudo-capacitors. The first mechanism is charge separation at the interface sandwiched between the electrode and the electrolyte (EDLCs), where energy is stored via the accumulation (electrostatic) of charges at the interface. The second one, up through redox reactions, endures a Faradaic process (pseudo-capacitors). Pseudo-capacitors allow high specific capacitance than EDLCs due to the high density of charge storage done in the redox process. Systematically energy is deposited near or at the electrode's surface by the electro-sorption and/or reversible redox reactions (Salanne et al. 2016).

In EDLCs, energy stored via charge adsorption at the electrode surface is deprived of faradaic reactions. Throughout the progression of charge–discharge, current resulted from the prearrangement of charges in the two oppositely charged layers (Helmholtz double layer). The EDLCs can bring energy swiftly, and the sum of the stored energy is restricted and much lower than that of pseudo-capacitors due to the endurance of the electrode surface. Electrochemical double-layer capacitance ( $C_{dl}$ ) and the response current (I) are described in the following equations (Zhang and Zhao 2009; Conway et al. 1997):

$$C_{dl} = \frac{Q}{V} = \frac{\varepsilon_r \varepsilon_o A}{d} \tag{1}$$

$$I = \frac{\mathrm{d}Q}{\mathrm{d}t} = C_{\mathrm{d}l}\frac{\mathrm{d}V}{\mathrm{d}t} \tag{2}$$

where Q,  $\varepsilon_o$ ,  $\varepsilon_r$ , A, d, t are the total charge transferred at potential V, the dielectric constant of vacuum, the dielectric constant of the electrolyte, the electrode surface area, the charge separation distance, and the charge time, respectively. Generally, carbon and carbon-based materials occupied most of the electrode materials of EDLCs due to their first-rate electric conductivity and their large specific surface area. However, EDLCs' carbon-based electrodes meet a limitation in commercial application from a high energy density point of interest (Thakur et al. 2017; Lamberti 2018; Zhao et al. 2018).

Energy storage concerning pseudo-capacitance displays the transitional electrochemical behavior between solid-state diffusion and pure electrostatic EDLCs controlled by Faradaic reactions in bulk electrode materials. Faradic mechanisms is divided into: (1) underpotential deposition, in which ions are placed on a metal/electrolyte boundary at positive potentials to their reversible redox potentials (e.g., H<sup>+</sup> on platinum or Pd<sup>2+</sup> on gold)(Sudha and Sangaranarayanan 2002). (2) Redox pseudo-capacitance, where there is some range of change in reduced species on the electrode surface or within a slight shallow surface region of oxidized species (or vice versa) in a Faradaic redox system (e.g., or MnO<sub>2</sub>, and conducting polymers) (Makino et al. 2015; Lang et al. 2011). (3) Intercalation pseudo-capacitance, in which ions intercalation into a redox-active material occur without any change in the crystallographic phase and in a timescale near to that of EDLCs (e.g., Nb<sub>2</sub>O<sub>5</sub>) (Kong et al. 2014; Kong et al. 2015). Many kinds of research work are intensive on transition metal oxide and sulfide-based materials as pseudocapacitors, especially metal sulfides. This is because the interaction between the Li<sup>+</sup>, for example, as a guest ion and the sulfide mesh should be weakened compared to oxides.

Additionally, this faded interaction should lead to swift ion passage through the lattice.  $MoS_2$  is an attractive material for pseudo-capacitive electrode due to their large van der Waals gap (6.2 Å) in  $\mu$ -sized samples that touch (6.9 Å) for nanostructured systems. This large van der Waals space will be reflected on the guest–host interaction by reduction, making  $MoS_2$  a perfect pseudo-capacitive material (Liang et al. 2011; Hwang et al. 2011).  $MoS_2$  has another advantage; that is, lithium inset into the semiconducting (2H phase) boosts a phase transition to the metallic (1 T phase) of  $MoS_2$  (Cook et al. 2017).

### Supercapacitors' electrode materials

Capacitors performance was mastered by the electrode materials, which commonly studied electrode materials: (1) carbon materials (e.g., carbon nanotubes, carbon nanofibers, activated carbon, graphene, carbon aerogel). They show a high specific surface area, making them a good choice for EDLCs electrodes. Unfortunately, they are imperfect in their minimal energy density and low specific capacitance. (2) Conducting polymers, the most common (polypyrrole and polyaniline that covered some defects of  $MoS_2$  as well as could maximize the electrochemical performances). (3) Transition metal oxides (such as  $RuO_2$ ,  $NiO_x$ ,  $MnO_x$ , and iron oxides) which show 10 to tenfold (100) times superior specific capacitance than previously mentioned carbon materials. Inappropriately, conducting polymers were subjected to exhaustive degradation on swelling and shrinking through several charge/discharge cycles. (4) Metal dichalcogenides (e.g.,  $MoS_2$  and  $MoSe_2$ ) are other electrode materials that will be covered in this work.

MoS<sub>2</sub>-based electrodes offer a tunable morphology, structure, and surface chemistry of supercapacitors electrode materials (Yang et al. 2015). Thus, MoS<sub>2</sub> exhibits high capacitance because, firstly, MoS<sub>2</sub> has a dual charge storage potency rendered by the double-layer structure and the faradic action taking place at its daggling edge and defects at the surface (da Silveira Firmiano et al. 2014; Soon and Loh 2007; Zhang et al. 2015). Secondly, the wide oxidation state ranges (+2 up to +6) drive participation in a redox reaction (Chhowalla et al. 2013). Then, the non-stop redox reactions eliminate dead time. The redox-reaction activity and the charge separation efficiency are predominately particular by the accessibility of the active surface area and the nature of surface chemistry. Henceforth, refining the active surface area of MoS<sub>2</sub> will meaningfully raise its specific capacitance when utilized as an electrode for supercapacitors applications (Zhu et al. 2015). Additionally,  $MoS_2$  can store charges by both mechanisms (i.e., EDLCs and pseudo-capacitance within both negative and positive windows, respectively). Therefore, MoS<sub>2</sub> can act as cathode and anode (mixed-type) materials for supercapacitors (Sun et al. 2015; Wang et al. 2014a).

### Electrochemical performance of unsupported MoS<sub>2</sub>

Owing to  $MoS_2$ ' high specific capacitance,  $MoS_2$  is highly fortunate for supercapacitors. For instance,  $MoS_2$  in both forms (homogenous ultrathin and petal-like structure) was stated to display a good specific capacitance of over 575  $Fg^{-1}$  at (5 mV s<sup>-1</sup>, scan rate) (Karade et al. 2016) and 811  $Fg^{-1}$  at (0.1 A.g<sup>-1</sup>, current density) (Mishra et al. 2018). Although  $MoS_2$  displayed an excellent specific capacitance, its performance (electrochemical) is restricted by its intrinsic restacking feature. Previously reported specific capacitances

| Material structure   | Current density, $(A \cdot g^{-1})$ | Potential range (V) | Specific capaci-<br>tance, $(F \cdot g^{-1})$ | Refs.                        |  |
|--|-------------------------------------|---------------------|---|------------------------------|--|
| MoS <sub>2</sub> nanosheets                                  | 1                                   | -0.6: 0.4 V         | 34.6  | (Thangappan et al. 2016)     |  |
| MoS <sub>2</sub> nanosheets                                  | 1                                   | -0.8: -0.2 V        | 192.2   | (Huang et al. 2014a)         |  |
| Sphere-like MoS <sub>2</sub>                                 | 0.5 (mA. Cm <sup>2</sup> )          | −0.2: −0.5 V        | 92.85   | (Krishnamoorthy et al. 2014) |  |
| Spherically clustered MoS <sub>2</sub>                       | 1                                   | −0.5: −0.5 V        | 122   | (Ilanchezhiyan et al. 2015)  |  |
| Layered MoS <sub>2</sub>                                     | 1                                   | -1:0 V              | 120   | (Huang et al. 2013a)         |  |
| Layered MoS <sub>2</sub>                                     | 1                                   | −0.8: −0.2 V        | 149   | (Huang et al. 2014b)         |  |
| MoS <sub>2</sub> nanowall films                              | 1                                   | -0.2: -0.7 V        | 100   | (Soon and Loh 2007)          |  |
| Flower-like MoS <sub>2</sub>                                 | 1                                   | -0.8: -0.2 V        | 118.9   | (Huang et al., 2015b)        |  |
| Flower-like MoS <sub>2</sub>                                 | 1                                   | -0.9: -0.2 V        | 168   | (Wang et al. 2014a)          |  |
| Layer expanded MoS <sub>2</sub> nanorods                     | 1                                   | -1:0 V              | 231   | (Xiao et al. 2017b)          |  |
| Metallic 1 T phase MoS <sub>2</sub> petal-like nanostructure | 0.1<br>10.0                         | -                   | 811<br>400                                    | (Mishra et al. 2018)         |  |
| Layer expanded $MoS_2$ nanorods                              | 0.5<br>1.0                          | -                   | 275<br>231                                    | (Xiao et al. 2017b)          |  |

Table 1 Comparison of supercapacitor performances of different forms of unsupported molybdenum disulfide nanostructures

and cyclic stabilities of diverse morphologies of  $MoS_2$  are tabulated in Table 1.

Among these structures, layered  $MoS_2$ , which bids a great charge storage affinity as a result of its inherent ionic conductivity as well as ions intercalation within the layers, permits an effective absorption of these ions on the  $MoS_2$  exterior (Ramadoss et al. 2014; Zheng et al. 2003). Since the morphology is crucial for making effective supercapacitors, a plethora of effort laid to propose an enhanced morphology of  $MoS_2$  for improved capacitance, such as microspheres, nanospheres, nanowires, nanorods, and nanofibers (Ma et al. 2008; Nagaraju et al. 2007; Li et al. 2003; Tian et al. 2005; Tang et al. 2013).

Consequently, a bit incompact arrangement of  $MoS_2$ nanosheets might enhance capacitance since the enlarged active surface area (Xiao et al. 2017b). Incorporating  $MoS_2$ with materials (electrically active) such as carbon materials, conductive polymers, transition metal oxides, and transition metal sulfides produces hybrids and/or composites possess excellent electrochemical features as electrode material. These materials could improve the conductivity as well as provide a supportive mate to  $MoS_2$ . This may be reflected in the enhanced structural stability and electrochemical performance (Xiao et al. 2017b; Radhakrishnan et al. 2021).

### Electrochemical performance of carbon-based hybrids of MoS<sub>2</sub>

For instance, carbon nanotubes, carbon aerogel, graphene, as examples of carbon-based materials, have a high surface area, controlled surface functionality, morphology, and excellent electrical conductivity, putting them together as promising candidates as electrode materials for supercapacitors. Still, low-energy storage capacity restricts them for use in practical applications. Molybdenum disulfide can boost conductive features and afford support to expand the hybrid's electrochemical performance and structural firmness.

Many researchers seek to fascinate the supercapacitors' electrode materials, especially those based on  $MoS_2/carbon$  composites. In turn, hybridization of the previously mentioned materials with  $MoS_2$  outcomes in amended morphology and  $MoS_2$  eases the interconnected network of carbon materials. Table 2 shows the electrochemical performances of yet tested  $MoS_2/carbon$  hybrids.

Graphene, a representative of the most exciting carbon material, has drawn widespread consideration due to its physical/chemical features. It has a notable sizeable surface area, conductivity, good thermal tolerance, besides its robust mechanical strength (Liu et al. 2019; El-Kady and Kaner 2013; Guo and Dong 2011; Wu et al. 2013). The harmonizing action between  $MoS_2$  and graphene ( $MoS_2$ /graphene) hybrids, which adjusts each material's imperfections, progresses the electrochemical performance, improves the conductivity, provides more active sites, and hastens the charges (electrons) transport as well as diffusion of the electrolyte inside the electrode material (Sarkar et al. 2019).

Precisely, the upgrading of the  $MoS_2/graphene's$  electrochemical performances composites can be due to three main factors: Electron transportation from  $MoS_2$  to graphene, besides structural constancy of  $MoS_2$  hybrids, results from C-O–Mo interfacial interaction; this leads to remarkable rate capacity and reversible capacity (Teng et al. 2016). Secondly, the coupling between  $MoS_2$  and highly conductive graphene leads to a hybrid ( $MoS_2/graphene$ ) with enhanced electrochemical performances. In this hybrid, graphene is robust to accumulate and delivers a large surface area to  $MoS_2$  mounting. Hence, a homogenous electrode structure

|  |   |  |                              |                  | -  |  |                         |
|--|---|--|------------------------------|------------------|--|--|-------------------------|
| Material structure   | Electrolyte/Elec-<br>trode composi-<br>tion, mass ratio | Specific<br>capacitance,<br>F. g <sup>-1</sup> | Current density, A. $g^{-1}$ | Number of cycles | Specific capaci-<br>tance retained,<br>% | Energy density,<br>Wh. Kg <sup>-1</sup> /Power<br>density, kW.kg <sup>-1</sup> | Refs.                   |
| MoS <sub>2</sub> /carbon<br>aerogel                            | 1 M Na <sub>2</sub> SO <sub>4</sub>                     | 260  | 1                            | 1500             | 92.4                                     |  | (Huang et al., 2015b)   |
| MoS <sub>2</sub> /graphene                                     | 1 M Na <sub>2</sub> SO <sub>4</sub>                     | 243  | 1                            | 1000             | 92.3                                     | 73.5/19.8  | (Huang et al. 2013a)    |
| MoS <sub>2</sub> /carbon nanotubes                             | 1 M Na <sub>2</sub> SO <sub>4</sub>                     | 108  | 0.1                          |                  |  | 7.4/3.7  | (Khawula et al. 2016)   |
| MoS <sub>2</sub> /carbon nanotubes                             |   | 231  | 0.1                          |                  |  | 26/6.443   |                         |
| Reduced gra-<br>phene oxide/<br>MoS <sub>2</sub>               | -   | 334.21   | 5 mV/s                       | 500              | 90                                       | -  | (Murugan et al. 2017)   |
| Graphene<br>wrapped carbon<br>nanotubes /<br>MoS <sub>2</sub>  | -   | 498  | 1                            | 10,000           | 94.3                                     | -  | (Sun et al. 2017)       |
| Carbon nanotubes<br>/MoS <sub>2</sub>                          | 1 M Na <sub>2</sub> SO <sub>4</sub>                     | 350.6  | 1                            | 10,000           | 85                                       | -  | (Sun et al. 2017)       |
| Electrospun<br>MoS <sub>2</sub> /carbon<br>nanofiber           | 6 М КОН   | 355.6  | 5 mV/s                       | 2000             | 93                                       | -  | (Kumuthini et al. 2017) |
| MoS <sub>2</sub> /three-<br>dimensional<br>graphene<br>network | 3 М КОН   | 1972.58  | 1                            | 4000             | 110.57                                   | -  | (Zhou et al. 2017)      |
| MoS <sub>2</sub> /graphene nanobelts                           | -   | 445.71   | 0.8                          | 1000             | 96.75                                    | 38.6/0.4   | (Jia et al. 2017)       |
| Carbon/MoS <sub>2</sub><br>nanosphere                          | 3 M KOH   | 1000   | 20                           | 20,000           | 93                                       | -  | (Luo et al. 2018)       |

 Table 2
 Previously reported electrochemical performance of carbon-based hybrids of MoS<sub>2</sub>

and adjusted frame of  $MoS_2$  will result during the cycling progression (Teng et al. 2016; Yu et al. 2014; Sun et al. 2016; Liu et al. 2014b). Finally, the conductive voids and channels shaped inside the  $MoS_2$ /graphene hybrids increased surface area and numerous active sites. Thus, afford continuous pathways for ions intercalations and electrochemical reactions and, in turn, enhance the electrode's reaction kinetics and elevate the hybrid's electrocatalytic performance (Paul et al. 2019; Huang et al. 2013b; Liu et al. 2020b).

As known, maximizing the capacitance is a challenge. The MoS<sub>2</sub> micro-flowers were prepared via a cost-effective hydrothermal method and further electrospunned over carbon nanofibers forming a three-dimensional network for robust charge transfer (Rajapriya et al., 2020). The hybrid shows a capacitance ( $\approx$  900 F g<sup>-1</sup>, at 1 A g<sup>-1</sup>) and only loss ( $\approx$  5%) in efficiency at 5×10<sup>3</sup> cycles in 1 M potassium chloride as an electrolyte (Rajapriya et al., 2020). The effect of MoS<sub>2</sub> concentration via microwave heating as a facile method to deposit MoS<sub>2</sub> with different concentrations over reduced graphene oxide was considered. The best result was for low concentration MoS<sub>2</sub> (MoS<sub>2</sub>/ reduced graphene oxide) achieved a specific capacitance 1316 F g<sup>-1</sup>. This electrode displays that an energy density was 63 Wh.kg<sup>-1</sup> and good cyclic stability (>90%) of the specific capacitance retained after 1000 cycles (da Silveira Firmiano et al. 2014).

The large volume change of  $MoS_2$  and the depressed electrical conductivity is another challenge. An active encapsulation approach is applied to preparing a core–shell  $MoS_2/$  mesoporous hollow carbon spheres MHCS as a nanocomposite (Zheng et al. 2019). MHCS controlled the development of  $MoS_2$  and upgraded both conductivity and structural stability. The electrode brings a reasonably elevated (capacitance > 610 F g<sup>-1</sup>, at 1 A g<sup>-1</sup>) with respectable (rate performance > 350 F g<sup>-1</sup>, at ten A g<sup>-1</sup>) and excellent cycle performance aqueous supercapacitors. More significantly, an ultrahigh (specific energy density > 200 Wh kg<sup>-1</sup>, at 200 W kg<sup>-1</sup>) is confirmed for Li-ion capacitors in which the nanocomposite is the anode (Zheng et al. 2019).

Another challenge is maximizing the gravimetric and volumetric capacitances still another challenge. From that, the hybridization of  $MoS_2$  with hollow carbon nanobowls is studied by (Wang et al. 2020a). The semi-concave shape of  $MoS_2$  encourages rapid electrolyte penetration and offers

an excellent conductive path for both the tested electrode as a supercapacitor, the MoS<sub>2</sub> nanosheets inside hollow carbon nanobowls named MoS<sub>2</sub>/hollow carbon nanobowls confirmed outstanding gravimetric capacitance and volumetric capacitance equal (560 F  $g^{-1}$  at 0.2 A  $g^{-1}$  and 874 F cm<sup>-3</sup>), respectively, and cycling performance of 94.4% capacitance retention next 5,000 cycles which is considerably higher than hollow carbon nanobowls/MoS2 in which hollow carbon nanobowls' surface covered by two-dimensional MoS<sub>2</sub> nanosheets (Wang et al. 2020a). Hollow carbon-MoS<sub>2</sub>-carbon nanoplatelets synthesized with excellent stability and dispersibility in water merit electrical conductivity based on morphology enhancement. The hollow nanoplate can provide a high surface area of 543  $m^2 g^{-1}$  with a total pore volume of 0.677 cm<sup>3</sup> g<sup>-1</sup>. The symmetric supercapacitors device exhibited a specific capacitance of 248  $F/g^{-1}$  at 0.1 A  $g^{-1}$ , signifying that the prepared nanoplates are talented candidates for supercapacitors (Quan et al. 2019).

Now, a new challenge directs the researchers into environmental, economic, and high performances electrodes for supercapacitors. In particular, lots of efforts made to yield low-cost and environmental carbons. For fascinating the outcome of performance accompanied by environmentally available material, a simplistic process to prepare MoS<sub>2</sub>/graphene system based on an improved, environmental-friendly, and cost-effective, scalable ball milling process that resulted in MoS<sub>2</sub>/graphene-based inks with few-layer MoS<sub>2</sub> is presented by (Wang et al. 2020b). This ink was used for fabricating two-dimensional sandwiched supercapacitor electrodes. The electrodes displayed a (specific capacitance >  $390 \text{ F g}^{-1}$ , at 5 mV s<sup>-1</sup>) and depressed (equivalent resistance  $\approx 0.40 \Omega$ ), which outpaces the features of graphene electrodes. The specific capacitance of a two-dimensional printed electrode using the as-prepared composite's ink was ( $\approx 76 \text{ F g}^{-1}$  (at the same scan rate) with (capacitance  $\approx$  of 0.058 µF cm<sup>-2</sup>, at 0.77 mg cm<sup>-2</sup>) signifying high energy storage potentiality. The MoS<sub>2</sub>/graphene composites' performance and their inks highlight their capacity as suitable electrodes for energy storage devices (Wang et al. 2020b).

Seeking for enhancing the performance with an environmental approach to add more active points and excellent conductance properties, (Zhao et al. 2020) succeeded in synthesizing (MoS<sub>2</sub>/carbon) using cornstalks as a biocarbon source with a large surface area that showed a high ( $\approx 0.340 \ \mu F \ g^{-1}$  as specific capacitance) and good stability as the anode in supercapacitors (Zhao et al. 2020). Molybdenum disulfide/activated carbon is prepared in which carbon is derived from corncob (Wang et al., 2020c). The nanoflower-like MoS<sub>2</sub> is developed on the nanoflakes biomass-derived carbon to increase the specific surface area and thus enhanced its performance and maximized its (specific capacitance  $\approx 0.333 \ \mu F \ g^{-1}$ , at a current density of 0.001  $\mu A \ g^{-1}$ ) with the capacitance retention loss ( $\approx 20\%$ )

over 7000 cycles, which is 16-fold and fourfold that of activated carbon and molybdenum disulfide, respectively. The as-assembled MoS<sub>2</sub>/activated carbon "symmetric supercapacitor" owns (specific capacitance and energy density  $\approx$  $800 \ \mu F g^{-1}$  and 7.6 W h kg<sup>-1</sup>), respectively. One-step and solvent-free ball-milling approach is to synthesize  $MoS_2/$ reduced graphene oxide tidy composite by (Ji et al. 2019). The prepared electrode delivers specific capacitance approximately twice that of pure  $MoS_2 \approx 300 \text{ F g}^{-1}$  at 0.5 A g<sup>-1</sup>; current density) (Ji et al. 2019). An innovative, highly flexible, environmental, lightweight, and all-solid-state supercapacitor nanocellulose-derived carbon nanosphere fibers/ MoS<sub>2</sub>/reduced graphene oxide aerogel nanocomposite is proposed by (Lv et al. 2019) that is derived from nanocellulose fibers in one-step pyrolysis tailed by freeze-drying. The electrode exhibited an excellent energy density and power density touches of 57.5  $\mu$ W h cm<sup>-2</sup> (28.8 W h kg<sup>-1</sup>) and 29.1 mW cm<sup>-2</sup> (14.5 kW kg<sup>-1</sup>), with an excellent capacitance of 1114 F  $g^{-1}$  at 2 mV  $s^{-1}$  and stability loss (less than 2%) after  $10 \times 10^3$  cycles in an electrolyte made of H<sub>2</sub>SO<sub>4</sub>/ polyvinyl alcohol gel (Lv et al. 2019).

Maximum utilization of the available sources, as well as waste management, succeeded achieved by (Sangeetha and Selvakumar 2018). Firstly, they used biomass–Tendu leaves as a source for activated carbon. The synthesized composite ( $MoS_2/activated$  carbon) was used for supercapacitors. The activated carbon displayed both micro/mesopore structures with (specific surface area of 1509 m<sup>2</sup> g<sup>-1</sup>). 0.261 mF g<sup>-1</sup> and 0.193 mF g<sup>-1</sup> are the specific capacitance values for the tested symmetric and hybrid supercapacitors, respectively (Sangeetha and Selvakumar 2018). Secondly, they used polyethylene terephthalate bottles as an activated carbon source with a high specific surface area ( $\approx$  900 m<sup>2</sup> g<sup>-1</sup>). The sponge-like activated carbon network with a minor layer of molybdenum disulfide–carbon displayed a power density up to 469 W kg<sup>-1</sup> (Sangeetha et al. 2020).

## Electrochemical performance of polymeric hybrids of MoS<sub>2</sub>

Two-dimensional  $MoS_2$  considered an auspicious electrode material for supercapacitors, owing to its good morphology (exposed surface area), outstanding electrical features, and attractive physical properties. Nevertheless, its bulk suffers from low capacity resulting from the layers' overlaying and poor electric conductivity.

The combination of conductive polymers with  $MoS_2$  resulted in integrating pseudo-capacitive behavior of conductive polymers and interactive features of  $MoS_2$  to frame highly stable electrodes with good performance (electrochemical) such as astonishing capacitance and decent cycling stability. Reversible transport of ions within electrolyte related to the multilayered  $MoS_2$ , while conductive

Material Preparation Electrolyte Specific capaci-Cycling Current density, Capacitance, Refs.  $A.g^{-1}$  $F.g^{-1}$ method tance retained, stability,  $cycles \times 10^3$ % MoS<sub>2</sub>/polyaniline Solvothermal 496 79 1 M H<sub>2</sub>SO<sub>4</sub> 6 (Meng et al. 2015) 1 in situ oxida-0.5 552 79 6 (Ren et al. 2015) tive polymerization MoS<sub>2</sub>/polypyr-553.7 90 0.5 Hydrothermal 1 M KCl 1 (Ma et al. 2013) and in situ role oxidative polymerization In situ oxidative 0.5 695 85 4 (Tang et al. 2015) polymerization MoS<sub>2</sub>/polyani-Chemical 1 M H<sub>2</sub>SO<sub>4</sub> 1 mV s - 1678 80 10 (Yang et al. 2016) line/carbon exfoliation and oxidative polymerization 5 1H-MoS<sub>2</sub>/ Hot-injection 1 M Na<sub>2</sub>SO<sub>4</sub> 0.37 50.65 mF cm<sup>-2</sup> 100 (Savjani et al. oleylamine thermolytic 2016) decomposition

 Table 3 Electrochemical performance of polymeric hybrids of MoS<sub>2</sub>:

polymers cover these layers, will increase the specific surface area (Wazir et al. 2019). Table 3 shows the electrochemical performances of some conductive polymers (such as polyaniline and polypyrrole) that were previously studied and indicated that conductive polymers– $MoS_2$  hybrids are actually suitable supportive candidates for supercapacitor applications (Huang et al. 2013c; Ren et al. 2015; Ma et al. 2013; Tang et al. 2015; Savjani et al. 2016).

For polyaniline– $MoS_2$  hybrids, multifunctional  $MoS_2$ / polyaniline pseudo-supercapacitor electrodes was proposed by (Zhu et al. 2015).  $MoS_2$  nanosheets and polyaniline nanoarrays were fabricated via a large-scale approach.



**Fig. 1** Molybdenum disulfide crystal structure: octahedral, trigonal prismatic, and trigonal prismatic that abbreviated (1 T), (2H), and (3R), respectively. Reprinted with permission of John Wiley and sons from (Han and Hu 2016)

Capacitance retention retained for 4000 cycles ( $\approx 91\%$ ). High energy density achieved ( $\approx 0.106 \times 10^3$  Wh.kg<sup>-1</sup> at  $\approx 106 \text{ kW kg}^{-1}$ ; power density) (Zhu et al. 2015). Other MoS<sub>2</sub>/polyaniline nanocomposites reported by (Huang et al. 2013c) proved the positive synergistic effect of the conductive polymer (polyaniline) on molybdenum disulfide through the enhancement of specific capacitance ( $\approx 0.575 \text{ mF g}^{-1}$ at 1 A  $g^{-1}$ ) with an outstanding long-term cyclic stability. Polyaniline-MoS<sub>2</sub> hybrid offers a larger specific surface area "contact" for the protons' intercalation/deintercalation resulting from the MoS<sub>2</sub> nanohybrid with graphene-like form which was assisted as an excellent two-dimensional conductive skeleton that affords an extremely electrolytic accessible surface area of redox-active (polyaniline) and runs a straight pathway for electrons (Huang et al. 2013c). Optimized method of the capacitive performance through a controlled process of progress of polyaniline nanowires arrays on the tubular molybdenum disulfide surface proposed by (Ren et al. 2015). MoS<sub>2</sub>/polyaniline hybrid showed both high specific capacitance ( $\approx 0.55 \text{ mF g}^{-1}$  at 0.5 A g<sup>-1</sup>) and an excellent rate capability (only loss = 18%) from (0.5 to 30 A  $g^{-1}$ ).

Recently, (Zeng et al. 2019b) stated that the covalent linking MoS<sub>2</sub> with conducting polymers would boost the electrochemical performance and overcome the drawbacks. So, (Zeng et al. 2019b) synthesized MoS<sub>2</sub>–NH<sub>2</sub>/polyaniline via in situ growth of polyaniline over MoS<sub>2</sub>–NH<sub>2</sub> patterns and found that the as-prepared composite revealed a high (capacitance  $\approx 0.326$  mF g<sup>-1</sup>, at 0.5 A g<sup>-1</sup>), with low rate retention loss ( $\approx 27\%$ ) as current intensity elevated from (0.5 to  $1 \times 10^3$  A. g<sup>-1</sup>) in the three-electrode model, while, in the symmetric supercapacitor devices, cycling stability retained



Fig.2 a Zigzag structure of  $MoS_2$  and b both square and cylinder nanotube. Reprinted with permission of Elsevier from (Zhang et al. 2021)

at 96.5% (subsequent 10,000 cycles at 5 A  $g^{-1}$ ). This is also in agreement with the good impact of conducting polymers on MoS<sub>2</sub> and its capability as promising electrode materials for energy storage devices (Zeng et al. 2019b).

Another category of nanostructured polyaniline hybrids and polyaniline hydrogels has superior features such as flexible durability, good electrical conductivity, and astonishing electrochemical reactivity. So, (Das et al. 2019) used  $MoS_2$  quantum dot and *N*, *N*'-dibenzoyl-l-cystine via in situ polymerization to make  $MoS_2$ /polyaniline hydrogel as a solid-state elastic supercapacitor electrode. The covalently linked hybrid achieved an enhanced energy storage performance and showed an excellent specific capacitance ( $\approx$ 791 F g<sup>-1</sup> at 1 A g<sup>-1</sup>) and ( $\approx$  331 F g<sup>-1</sup> at 1 A g<sup>-1</sup>) for the three-electrode and the stretchy all-solid-state supercapacitor device, respectively. Additionally, the energy and power densities were ( $\approx 29.4$  Wh kg<sup>-1</sup> and 398 W kg<sup>-1</sup>), respectively, with capacitance retention ( $\approx 84.2\%$  after 10,000 cycles). A tandem supercapacitor model consists of 4 (charged) solid-state supercapacitors connected together and linked to power different colored diode bulbs for a lengthy period, indicating their good capability as a storage device (Das et al. 2019).

According to MoS<sub>2</sub>/polypyrrole hybrids, (Ma et al. 2013) reported a facile approach to synthesize MoS<sub>2</sub>/polypyrrole as an electrode for high-performance supercapacitors. Firstly, a hydrothermal treatment was used to synthesize flower-like MoS<sub>2</sub> (graphene-like) and then in situ oxidation polymerization of polypyrrole in MoS<sub>2</sub> nanosheets suspension. The MoS<sub>2</sub>/polypyrrole nanocomposite revealed a specific capacitance ( $\approx 5.5 \times 10^2$  F g<sup>-1</sup> at 1 A g<sup>-1</sup>; current density) and (capacitance loss 10% after  $5 \times 10^2$  cycles) (Ma et al. 2013). The polypyrrole ultrathin film gowns on two-dimensional  $MoS_2$  monolayer synthesized by (Tang et al. 2015). The hybrid MoS<sub>2</sub>/polypyrrole exhibited a high specific capacitance reached ( $\approx 700 \text{ F g}^{-1}$ , at 0.5 A g<sup>-1</sup>; discharge current) and  $(5 \times 10^2 \text{ F g}^{-1})$ , at 10 A g<sup>-1</sup>; discharge current density). This signified the admirable rate of performance (Tang et al. 2015).

Also, (Savjani et al. 2016) synthesized high-quality and pure  $MoS_2$  nanosheets covered by oleylamine through hot-injection thermolysis (one-pot synthetic route).  $MoS_2/$ oleylamine showed (0.05 F cm<sup>-2</sup>; specific capacitance, at 0.37 A g<sup>-1</sup>). The cycling stability was excellent as it retained as much as 100% (up to 5000 cycles) (Savjani et al. 2016).

A comprehensive study between graphene oxide/polypyrrole and MoS<sub>2</sub>/polypyrrole is fabricated via an easy and fast one-pot chronoamperometry procedure. The hybrids used to fabricate additive-free, scalable, and binder-free supercapacitors electrodes. Both the electrodeposited hybrids (graphene oxide-polypyrrole and molybdenum disulfide-polypyrrole) electrodes exhibited specific capacitance (nearly equal  $\approx 2.7 \times 10^2$  F g<sup>-1</sup> and  $1.3 \times 10^2$  F g<sup>-1</sup>, at 1 A g<sup>-1</sup>; current density), respectively. Reduced graphene oxide in polypyrrole mate presented high capacitance, while molybdenum disulfide upgraded the structural stability and a noticeable (2000 cycles; cycling stability). MoS<sub>2</sub>/polypyrrole retains 82%, and graphene oxide/polypyrrole retains 64% of their initial capacitance (Prasankumar et al. 2019).

A facile strategy for in situ integrating two-dimensional molybdenum disulfide nanosheets into a three-dimensional polypyrrole network was proposed by (Tian et al. 2020). This was achieved via intercalation between MoS<sub>2</sub> nanosheets and (dodecylbenzene–sulfonate anions), allowing direct growth of polypyrrole in an ordered manner. The resulting orderly self-standing films of polypyrrole chains delivered a good areal capacitance and volumetric capacitance ( $\approx$ 1.2 F cm<sup>-2</sup> and 325 F cm<sup>-3</sup>), respectively, indicating the **Fig. 3 a–f** Scanning electron microscope images, **g** mapping images for Red phosphorus coating  $MoS_2@$  reduced graphene oxide. Reprinted with permission of Elsevier from (Bai et al. 2018), showing the curly layers where the graphene oxide works as a scaffold to resulting in anchoring and stabilizing for the nanostructured sheets of  $MoS_2$  and Red phosphorus and affirmed a consistent distribution of elements



Fig. 4 Scanning electron microscope images of **a** pure  $MoS_2$ , **b**-**f** different ratios of  $MoS_2$ in  $MoS_2$ /carbon nanofibers composite (0.1–0.5, step=0.1). Reprinted with permission of Elsevier from (Liang et al. 2020)



superiority of  $MoS_2$  synergism effect with polypyrrole over pure polypyrrole and, as a result, imparting good applicability for stretchable supercapacitors with excellent performances (Tian et al. 2020).

Recent studies focus on ternary composites to cover the previously stated hybrids' defects, enhancing the composite characters and fascinating the electrode capacitance. In the same context, (Yang et al. 2016) synthesized ( $MoS_2/$  polyaniline @carbon) ternary composite formed of  $MoS_2$  (1 T phase) monolayers on which carbon shell-coated polyaniline grown up. The  $MoS_2$ /polyaniline/carbon composite

electrode with a (~3.00 nm; carbon shell) and unveiled a notable specific capacitance ( $\approx 678$  F g<sup>-1</sup> at 1.0 mV s<sup>-1</sup>), reserved only retention loss ( $\approx 20\%$  after 10,000 cycles), and 19% at 10 mV s<sup>-1</sup>, as good rate performance as a result of the combined effects of both 1 T MoS<sub>2</sub> substrates with polyaniline nanostructure and the protective cap of carbon shell (Yang et al. 2016).

Another research trend focused on inexpensive starting materials with the environmental manner; (Ma et al. 2014) succeeded to synthesize  $MoS_2$  (flower-like) via sodium alginate as an additive for the annealing process via a facile route

(hydrothermal). The resulted  $MoS_2$  was hexagonal phases with hierarchical morphology built on  $MoS_2$  nanosheets. For the electrode for supercapacitors, the synthesized microsphere brought a good specific capacitance( $\approx 145$  F g<sup>-1</sup>, at 3 A g<sup>-1</sup>) as well as exhibited good cycle stability (Ma et al. 2014).

Natural resources such as lignin were used by (Wang et al. 2019) as a renewable source for carbons. Laser irradiation and pyrolysis were the methods used to obtain tetrahedral amorphous carbon and graphitic carbon, respectively. They also mixed MoS<sub>2</sub> into the lignin/polyacrylonitrile hybrid polymers to optimize the capacities. Lignin/polyacrylonitrile compared to lignin/polyacrylonitrile doped with MoS<sub>2</sub> was found to fascinate the areal specific capacitance twice from (6.7 mF cm<sup>-2</sup> (0.9 F cm<sup>-3</sup>); at 10 mV s<sup>-1</sup>) to (16 mF  $cm^{-2}$  (2.2 F cm<sup>-3</sup>); and at 10 mV s<sup>-1</sup>) (Wang et al. 2019). Also, (Ge et al. 2017) demonstrated a free-standing bendable MoS<sub>2</sub>-based supercapacitor electrode. The poly (3,4-ethylene dioxythiophene)/poly (styrene sulfonate) highly conductive polymer was combined with robust MoS<sub>2</sub>. The volumetric capacitance was ( $\approx 1.41 \times 10^2 \,\mathrm{F \, cm^3}$ ), volumetric energy density was ( $\approx$ 4.9 mWh cm<sup>3</sup>), and capacitance retention was ( $\approx 98.6\%$ ; after 5 × 10<sup>3</sup> cycles). The main reason for these enhanced results is that the fabricated film possesses remarkable mechanical features such as Young's modulus (=2.0)GPa) and fracture strength of 18.0 MPa) (Ge et al. 2017).

### Electrochemical performance of metal-based hybrids of MoS<sub>2</sub>

Metal oxides (Ni, Co, and iron oxides) are abundant, environmental, chemically stable and have high theoretical capacitance. Besides, metal-MoS<sub>2</sub> hybrids/composites can be ascribed to their improved architecture and atomically sharp heterojunctions (Wazir et al. 2019). Transition metal oxides such as  $(Co_3O_4, Co(OH)_2, RuO_2, NiO, and NiCo_2O_4)$ can maximize specific capacities and perform swift redox kinetics. Therefore, they likely act as electrode materials for supercapacitors. Nevertheless, these oxides typically have a low surface area. Some have a poor electrical conductivity that increases the intrinsic resistance, hindering ions and electrons transfer, and restricted practical use. On the flip side, the transition metal oxides and sulfides engage a reversible faradaic reaction to stock charges. Their capacitance capabilities and energy densities are superior to those of carbon-based materials. Defects in commercial applications may result from their poor cycling stability from distortion in their microstructures and their original shape. So, the progress of highly porous transition metal oxides nanostructures having an excellent electrochemical performance is crucial.

Incorporating  $MoS_2$  in  $MoS_2$ -transition metal oxides hybrids nanostructured will fascinate the energy-storage performances associated with a high-rate capability. MoS<sub>2</sub>-transition metal oxides hybrids are expected to have the following merits: low-cost, environmental, scalable, and facile synthesis approach with compatible and tunable morphologies. These heterostructures prevent restacking of the MoS<sub>2</sub> that will permit abundant active sites to be added due to enhanced ions permeability and electron interactions. The insertion of porous transition metal oxides (e.g.,  $Co_3O_4$ , NiO, and  $Fe_2O_3$ ) into two-dimensional MoS<sub>2</sub> nanosheets using a facile strategy is studied by (Wang et al. 2017c). The resulting hybrid positively impacted enhanced electronic/ionic transport and confirmed an astonishing pseudo-capacitive performance (over  $1 \times 10^3$  at 1 A g<sup>-1</sup> and retained 101.9% after 9000 cycles at 2 A g<sup>-1</sup>). MoS<sub>2</sub>-NiO// MoS<sub>2</sub>-Fe<sub>2</sub>O<sub>3</sub> asymmetric supercapacitor achieved a high energy density ( $\approx 40.0 \text{ W h kg}^{-1}$ ) (Wang et al. 2017c).

Another study presented by (Chai et al. 2018) used an in situ redox etching reaction to fabricate  $MnO_2$  (hollow nanospheres) on a molybdenum disulfide (nanospheres) as a sacrificial matrix. The supercapacitor electrode verified (95.2%; capacitance retention after  $5 \times 10^3$  cycles; at  $5.0 \text{ A g}^{-1}$ ) and (394 F g<sup>-1</sup>; specific capacitance, at 1.0 A g<sup>-1</sup>) (Chai et al. 2018).

Ternary composites will aid to cover the defects in the previously studied hybrids. Low-cost  $MoS_2/graphene$  coated on mesoporous  $MnO_2$  nanocomposites that reveal (up to 527.0, 727.0, and 1160.0 F g<sup>-1</sup>; specific capacitance) escorted by continuous cyclic stability was fabricated by (Ramalingam et al. 2018).

Microwave-assisted, facile, and one-step methods are used to synthesize  $MoS_2/MoOx$  nanocomposites that are grown on activated carbon (Sari and Ting 2018). The resulted composite supports the ions intercalation:  $MoO_{3-x}$ , monoclinic  $MoO_2$ , the conductive activated carbon. The cloth provides swift electron transport. On the contrary, molybdenum disulfide nanosheets/ $MoO_{3-x}$  nanoparticles will expand capacitance. Briefly,  $MoS_2/MoO_x$ -activated carbon cloth displayed an excellent specific capacitance ( $\approx 230$  F g<sup>-1</sup>, at 5.0 mV s<sup>-1</sup>) and showed steadiness over 125% and capacitance retention after 1500 cycles (Sari and Ting 2018).

The synergistic effect of Fe<sub>3</sub>O<sub>4</sub>, MoS<sub>2</sub>, and reduced graphene oxide was considered by (Salarizadeh et al. 2020). The synthesized nanocomposite via a 2-step hydrothermal way demonstrated a respectable specific capacity ( $\approx$  527 F g<sup>-1</sup>, at 0.5 mA cm<sup>-2</sup>). This confirms that MoS<sub>2</sub> with iron oxides offers electroactive sites for electrolyte accessibility and faradic processes, and reduced graphene oxide provides conductivity (Salarizadeh et al. 2020).

The metal sulfides  $(NiS_x, CoS_x, CuS_x, and FeS_2)$  considered novel and suitable electrodes for supercapacitors because they have minor electronegativity and developed

electrochemical activity reflecting positively on specific capacities and energy/power densities. Specifically, metal sulfides-based hybrids can afford better redox reactions than monometal sulfides, expressing superior specific capacity. However, their poor conductivity retards rater capability and cycling stability. Introducing MoS<sub>2</sub> could reduce the previous defects, facilitate electron transport, and boost the electrochemical features (Li et al., 2020a). Owing to their low cost, good electrical conductivity, their activity, especially with their electrochemical stability, and the proper architecture of composites' metal sulfides is supposed to be very operative for abundantly exploiting their merits and breaking through their confines of the low-rate capability and lesser cycling stability in supercapacitors applications. The metal sulfides are widely tested and developed for supercapacitors with astonishing electrochemical performances.

This study presented a facile (in situ hydrothermal) approach to making high-performance binder-free electrodes (Zhao et al. 2020). The NiS<sub>2</sub>/MoS<sub>2</sub> composite fabricated by (Yang et al. 2021) using a hydrothermal approach. Then the NiS<sub>2</sub>/MoS<sub>2</sub> was decorated by graphene nanosheets. The obtained composite electrode owned imposing electrochemical performances such as a high specific capacity (over 230 F g<sup>-1</sup>; at 1 A g<sup>-1</sup>) with first-rate rate capability (over 60%; at  $1 \times 10^2$  A g<sup>-1</sup>) (Yang et al. 2021).

Additionally, other metal-MoS<sub>2</sub> hybrids that enhance electrode performance have been reported. For instance, (Wang and Xie 2020) designed an electro-active hybrid based on FeS<sub>2</sub>/MoS<sub>2</sub>. The hybrid tested theoretically and presented a high density of states (Fermi level) and a narrow bandgap. The hybrid revealed higher specific capacitance  $(394 \text{ mF cm}^{-2})$  linked to that of MoS<sub>2</sub> (218.1 mF cm<sup>-2</sup>) and that of FeS<sub>2</sub> (286.5 mF cm<sup>-2</sup>) at 1.0 mA cm<sup>-2</sup> in 0.5 M Na<sub>2</sub>SO<sub>4</sub>. The capacity retention enhanced from 58 and 73% for MoS<sub>2</sub> and FeS<sub>2</sub>, respectively, to be 76% for the hybrid in the same electrolyte. The cycling capacity retention for FeS<sub>2</sub>/  $MoS_2$  was 100.7% (5×10<sup>3</sup> cycles; at 5.0 mA cm<sup>-2</sup>). For the asymmetric device, the anode was FeS<sub>2</sub>/MoS<sub>2</sub>, the cathode was exfoliated graphite carbon paper, and the electrolyte was NaMoO<sub>4</sub>-Na<sub>2</sub>SO<sub>4</sub>-poly(vinyl alcohol) gel. The performance was 112.8 mF cm<sup>-2</sup> (at 1.0 mA cm<sup>-2</sup>) and 56.56 mWh cm<sup>-2</sup> for the specific capacitance and the energy density. Capacity retention lowered that ideal by 2% after (5000 cycles, at  $5.0 \text{ mA cm}^{-2}$ ) (Wang and Xie 2020).

Another strategy to improve the electrochemical performance and good stability and cyclability is fabricating a ternary composite based on metal sulfide and carbon materials along with MoS<sub>2</sub>. Recently, (Li et al., 2020a) fabricated a ternary composite (MoS<sub>2</sub>/NiCo<sub>2</sub>S<sub>4</sub>/carbon) composed of carbon-coated MoS<sub>2</sub>/NiCo<sub>2</sub>S<sub>4</sub> urchin-like micro-spheres via a self-template approach that achieved a high ( $\approx$ 250 mAh g<sup>-1</sup>; specific capacity at 2 A g<sup>-1</sup>) besides capability ( $\approx$  91.1%; at 40 A g<sup>-1</sup>). The asymmetric device with the as-prepared composite as positive electrode and AC as negative electrode displayed an energy density of ( $\approx 53.01$  Wh kg<sup>-1</sup>) at power density ( $\approx 4.20$  kW kg<sup>-1</sup>) and stability of nearly ninety percent after ten thousand cycles at (10 10 A g<sup>-1</sup>; current density) (as presented in Fig. 5) (Li et al., 2020a).

Reprinted with permission of Elsevier from(Li et al., 2020a). Among the studied electrodes, the discharging time of the  $MoS_2/NiCo_2S_4/C$  is the longest, which is in agreement with the cyclic voltammetry curves. Also, the  $MoS_2/NiCo_2S_4/C$  displays a lower equivalent series resistance than that of  $MoS_2/NiCo_2S_4$  and  $NiCo_2S_4/C$ .

The synergistic effect of molybdenum disulfides with nickel sulfides on carbon nanotubes as a supportive mate was studied by (Yang et al. 2017). The composite (nickel sulfides/carbon nanotubes) was fabricated via a one-step hydrothermal approach. The asymmetric device assembled as nickel sulfides/carbon nanotubes achieved a specific capacitance over 107 F g<sup>-1</sup> at 0.5 A g<sup>-1</sup> with 100% cycling stability after ten thousand cycles. The network affords accessibility to the electrolyte and nickel sulfides nanoparticles encouraged the diffusion of ions onto the electrode surface, and nickel sulfides voids tolerate changes in volume while redox process (Yang et al. 2017).

The NiCo<sub>2</sub>S<sub>4</sub>-C-MoS<sub>2</sub> composite structure was fabricated via hydrothermal and solvothermal techniques by (Wang et al., 2018). In the three-electrode system, the as-prepared electrode showed a specific capacitance of 1601 F g<sup>-1</sup> at 0.5 A g<sup>-1</sup>, and the asymmetric device exhibited (energy density = 27.7 Wh kg<sup>-1</sup>) at (power density = 400 W kg<sup>-1</sup>) after one thousand cycles at 2 A g<sup>-1</sup> (Wang et al., 2018).

### MoS<sub>2</sub>-based nanocomposites for batteries

### Lithium-ion batteries

Lithium-ion batteries played a master role in the past few years from both academic and industrialized energy storage societies because of their distinctive importance as the safest, low-cost, and widespread power/energy source for most portable electronics such as smartphones, digital cameras, laptop computers, and also as a talented power source for hybrid/electric vehicles(Scrosati et al. 2011). However, the hindrance is facing the current rechargeable batteries and their relatively low energy density, low stability, and sluggish charging rate (Xu et al. 2020). Therefore, discovering and tailoring innovative electrode materials are essential for improving the batteries' performance. However, the currently commercialized graphite anode in lithium-ion batteries is restricted by its theoretically low specific capacity and capacity fading over long-standing charge/discharge processing, which does not satisfy the request of high energy/power densities (Shen et al. 2018).

**Fig. 5** a Cyclic voltammetry curves of the studied electrodes at 10 mVs<sup>-1</sup>. b Galvanostatic charge–discharge curves of the studied electrodes at 10 A g<sup>-1</sup>. c Specific capacities of the studied electrodes at different current densities. d Nyquist plots of the studied electrodes. e Cycling stability of the studied electrodes at 10 A



Moreover, the electrode volume will suffer from the increase in size during the lithiation/delithiation course in lithium-ion batteries, affecting the battery performance. In this regard, the energy storage field has witnessed a dramatic growth in the research efforts that are going on to accomplish new electrode materials for lithium-ion batteries. Owing to its remarkable properties and extensive potential applications, two-dimensional (graphene-like structure) materials have long been studied intensively (Cao et al. 2018). In this regard, the attractive advantages of rich abundance and low-cost transition metal sulfides play an essential part in the progress of electrode materials for batteries along with their energy-related performance. Among the two-dimensional transition metal sulfides, MoS<sub>2</sub> attracted the most attention due to its natural abundance and suburban stabilities (Wang et al. 2015). The layered-structure  $MoS_2$  has a tremendous theoretical capacity of 0.67 Ah  $g^{-1}$  depending on the following lithiation storage response:

 $MoS_2 + 4Li^+ + 4e^- \leftrightarrow Mo + 2Li_2S$  (Xing et al. 2020).

This lithiation mechanism is characterized by a fast diffusion rate of lithium ions, excluding volume expansion (Xing et al. 2020; Li et al., 2020b).

Practically, the low electrical conductivity of pristine  $MoS_2$  inhibits the kinetic of electronic transfer, which impacts the behavior of lithium-ion batteries (Hu et al. 2015). Additionally, the bulk  $MoS_2$  reveals slow kinetics of redox reaction, which decreases its electrochemical reactivity. Additional, poor cycle stability arises during the lithiation/delithiation process. Therefore, for practical application, pristine  $MoS_2$  has drawback concerning with its cycling stability and conductivity. In this regard, structural modifications, including composite tailoring and/or atom doping, are often suggested to improve the desired features of  $MoS_2$ -based electrodes successfully.

Based on the layered structure of  $MoS_2$  with sufficient interlayer distance, which allows for effective ion diffusion, (Teng et al. 2016) prepared nanosheets of molybdenum disulfide on the graphene sheets within a carbon–O–Mo bond via a feasible hydrothermal method. The growth of MoS<sub>2</sub> on the graphene layers improved the mechanical stability and the electrical conductivity of the designed composite anode material for lithium-ion batteries, delivering outstanding rate capability and extensive cycle stability. The threefold electrode acquired additional advantages; for example, (1) the O-containing groups act as "connectors/collectors" leading to MoS<sub>2</sub> nanosheets to be spread vertically over the aligned graphene layers and thus provides frequent active edge sites for lithium reactivity as well as lessens the distance required for diffusion of both Li<sup>+</sup> ions and electrons. (2) C-O-Mo bonds resulted in a stable MoS<sub>2</sub>/graphene hybrid and an excellent path for electrons between the hybrid subunits. (3) Limited volume expansion is as a result of the robust graphene sheets. The previously mentioned features made MoS<sub>2</sub>/graphene anodes have an astonishing performance.

Three dimensional-ordered microporous structure of  $MoS_2$  combined with carbon cloth to impede the restacking of  $MoS_2$  layers and regulate lithiation/delithiation volume expansion (Zhang et al. 2019a). The obtained electrode material maintains its structure even after 100 cycles.

Carbon-based/MoS<sub>2</sub> nanocomposite onion-like construction as an active material for the as-prepared anode electrode of lithium-ion batteries was designed by (Wang et al. 2014b). The nanocomposite showed a specific capacity ( $\approx$  853 mAh g<sup>-1</sup>, at 50 mA g<sup>-1</sup>; current density) and can deliver for the first cycle an excellent coulombic efficiency of 97.6% (Wang et al. 2014b). More advance, (Wang et al. 2016b) have successfully prepared nanoleaves MoS<sub>2</sub> upon graphene nanosheets. This can not only stop the restacking of graphene layers but also improve the growth of MoS<sub>2</sub>. The obtained electrode exhibited a specific capacity of 1277 mAh g<sup>-1</sup> at 100 mA g<sup>-1</sup> current density. Also, it can keep a capacity of 1109 mAh g<sup>-1</sup> after even 100 consecutive cycles, reflecting its excellent cycling performance.

Other electrical active materials such as metal oxides (Pan et al. 2017), Mxene (Li et al. 2019b; Wu et al. 2017), and metal sulfides (Jiang et al. 2017) have been hybridized with MoS<sub>2</sub>, in addition to carbon materials, to improve their lithium storage capacity. The synergistic effect between each part can improve favored the electrochemical performance of the prepared hybrids and/or composites by scheming the structure of the binary combinations rationally. Also, (Chen et al., 2014a) have prepared a MoS<sub>2</sub> with the help of a tiny Fe<sub>3</sub>O<sub>4</sub> nanoparticle, using a two-step hydrothermal method. In the Fe<sub>3</sub>O<sub>4</sub>/MoS<sub>2</sub> hybrid, spacers Fe<sub>3</sub>O<sub>4</sub> inhibited MoS<sub>2</sub> nanosheets restacking, while MoS<sub>2</sub> prevented Fe<sub>3</sub>O<sub>4</sub>/MoS<sub>2</sub>-fabricated anodes showed superior capacities ( $\approx$ 224 and 1033) mAhg<sup>-1</sup> at current densities ( $\approx$ 10 and 2) A g<sup>-1</sup>, respectively.

Further, (Chen et al., 2014b) have prepared a composite anode material with great potential made from,  $SnO_2/MoS_2$ , with different ratios, where  $SnO_2$  nanoparticles are used to

preclude the restacking of  $MoS_2$  nanolayers, whereas  $MoS_2$  nanolayers act as a substrate to provide accommodations with the  $SnO_2$  nanoparticles. Four composites with different ratios of  $SnO_2/MoS_2$  are prepared. One of them,  $SnO_2/MoS_2$  composite with a mass ratio of 2: 1, achieved the best performance as anode material, providing the maximum and most stable reversible capacity within 230 cycles and a current density ( $\approx 10^2$ :  $10^4$  mA g<sup>-1</sup>).

The Sn/SnO<sub>2</sub>/C/MoS<sub>2</sub>, as a novel anode material for lithium-ion batteries, contained nanosheets of Sn/SnO<sub>2</sub>/C that combined with MoS<sub>2</sub> synthesized by (Huang et al. 2016). The composite revealed pronounced enhancement in the electrochemical response. They deliver outstanding cycling stability (exceeded 840.0 mAh g<sup>-1</sup> at 1.0 A g<sup>-1</sup>, after  $4 \times 10^2$  cycles) and excellent rate capability (over 450 mAh g<sup>-1</sup> at 10.0 A g<sup>-1</sup>) to their practical combined effect among MoS<sub>2</sub> and Sn/carbon nanosheets.

Also, (Chen et al. 2019b) have fabricated the heterostructure of  $MoS_2$ -SnO<sub>2</sub> encapsulated inside carbon nanofibers and tested it as a negatively binder-free anode material ( $MoS_2$ -SnO<sub>2</sub>/carbon nanofibers) for lithiumion batteries. Such innovative architecture produced a 983 mAh g<sup>-1</sup> discharge capacity at 200 mA g<sup>-1</sup> after 100 cycles and 710 mAh g<sup>-1</sup> after 800 cycles at 2000 mA g<sup>-1</sup>.

Lately, (Li et al. 2019b) proposed synthesizing of molybdenum disulfide on Mxene structures via in situ sulfidation of  $Mo_2TiC_2T_x$ -Mxene designed for lithium storage (Li et al. 2019b). Mxene increased the electrical conductivity of  $MoS_2$  and improved Li and polysulfide adsorption, which helped to enhance Coulombic efficiencies and cyclic performance. Molybdenum disulfide/TiO<sub>2</sub> nanotubes hybrid nanostructures are fabricated in a twophase way. The prepared hybrid has demonstrated excellent lithium storage capacity and rate capabilities as an electrode in lithium-ion batteries (Xu et al. 2014).

The easy in situ conversion was used to transform molybdenum dioxide into  $MoS_2MoO_2$  three-dimensional sulfur architectures (Xu et al. 2017). The obtained architectures from  $MoO_2/MoS_2$  show explicitly increased Li<sup>+</sup> storage and cycling capacity. The optimized composition was (91: 9%) of  $MoS_2$  and  $MoO_2$ , respectively; the architectures of the  $MoO_2/MoS_2$  are ready to have a reversible capacity of 1167 g<sup>-1</sup> at the 2<sup>nd</sup> cycle of 1016 mAh g<sup>-1</sup> after 2000 cycles.

Besides carbonaceous and metal oxides' electrodes, other electroactive electrode materials such as conducting polymers have gained a huge interest owing to their comparatively high energy density, inexpensive, facile manufacturing, and environmentally safe. However, the main challenge of conducting polymers lies in fading their performance after long-term cycling because of the swelling/shrinkage process of their bulk and consequent material destruction during the charging/discharging of ions. As a result, they are often mixed with other electroactive materials such as carbon materials and/or metal oxide and/or sulfide. For example, nanosheets  $MoS_2$  decorated polyvinylpyrrolidone as a surfactant (Liang et al. 2013), porous  $MoS_2$ /polyaniline composite (Liu et al. 2015) as the template, and quasi-hollow hierarchical  $MoS_2$  microspheres coated by monodisperse polystyrene sulfonates synthesized by (Wan et al. 2014). The polystyrene sulfonates have been working as a good template for carbon/MoS<sub>2</sub> micro-shell preparation. The carbon/MoS<sub>2</sub> microspheres, as prepared as an anode material, showed excellent cycling stability and high rates of performance (95% of the capacity retained after 100 cycles).

Three-dimensional hierarchical MoS<sub>2</sub>/polyaniline nanoflowers composite was fabricated using a feasible hydrothermal route (Hu et al. 2014). The as-prepared electrode of three-dimensional MoS<sub>2</sub>/polyaniline showed suburb electrochemical performance. Moreover, the annealing of MoS<sub>2</sub>/polyaniline may lead to the development of threedimensional hierarchical MoS<sub>2</sub>/C nanoflowers, as shown in Fig. 6. The produced MoS<sub>2</sub>/C sample revealed superior electrochemical performance (Fig. 7), more reversible capacity ( $\approx$ 888.0 mAh g<sup>-1</sup>), with the coulombic efficiency preserved with only a loss of 10% from the initial cycle, at a current density of 10<sup>2</sup> mA g<sup>-1</sup>.

Also, (Yang et al., 2013b) integrate nanosheets of  $MoS_2/$  polyaniline nanowires, showing adequate capacity and respectable cyclability, demonstrating promising anode material for lithium-ion batteries. The gained nanowires of  $MoS_2/polyaniline$  with the optimum ratio of  $(MoS_2/polyaniline)$  which was equal (66.7: 33.1%), respectively, show a high charge capacity of 1063.9 mAh g<sup>-1</sup> at 100 mA g<sup>-1</sup>, holding over 90% of the initial capacity even after fifty cycles.



**Fig. 7** Cycling performance and Coulombic efficiency of threedimensional hierarchical  $MoS_2$ /polyaniline and  $MoS_2$ /C nanoflowers. Reprinted with permission of American Chemical Society from (Hu et al. 2014). Notably, both the  $MoS_2$ /polyaniline and  $MoS_2$ /C nanoflowers exhibit excellent cycling stability with high reversible specific capacities of 801.2 and 888.1 mAh g<sup>-1</sup> after 50 cycles, respectively

### **Sodium-ion batteries**

Besides its low redox potential and its outstanding rate capability, the vast abundance of sodium in nature lets the researchers more intensively interest sodium-ion batteries in being the coming generation of energy storage systems' market (Chen et al. 2020).

Nevertheless, the ionic radius (r) of  $(Na^+ = 1.02 \text{ Å})$ , whereas  $(Li^+ = 0.76 \text{ Å})$  (Li et al., 2020b); sodium usually displays a slow reaction rate due to its relatively large radius. In this regard, it is important to examine new host electrode materials capable of accelerating and permitting sodiation/ desodiation kinetics (Hwang et al. 2017). The large interlayer spacing of molybdenum disulfide allows sodium ions to intercalate/deintercalate the layered arrays and offers a

Fig. 6 Scanning electron microscopy with different magnifications imaged of three dimensional  $MoS_2$ /polyaniline **a**, **b** and  $MoS_2$ /carbon **d**, **e** with two photographs **c**, **f** of natural roses. Reprinted with permission of American Chemical Society from (Hu et al. 2014). The figure demonstrates that the hierarchical flower-like structures of the  $MoS_2$ /polyaniline are successfully prepared



larger surface area for Na<sup>+</sup> absorption, enhancing the electrochemical performance of sodium-ion batteries (Mao et al. 2018).

In this regard, (Hu et al. 2018b) developed a network structure constructed from a hybrid carbon base/MoS<sub>2</sub> composite as active electrode material for both Li-ion batteries and Na-ion batteries. This construction helps the accommodation of volume enlargement and facilitates the diffusion of ions in/out the layers during battery operation.

The composite of  $MoS_2$ /graphene microspheres was obtained by (Choi et al. 2015). The layers of  $MoS_2$  have homogeneously surrounded the graphene microspheres. As a consequence of graphene microspheres porosity and the layered structure of  $MoS_2$ , the diffusion process of Na<sup>+</sup> has been boosted.

The high coulombic efficiency value ( $\approx 99.98\%$ ) was attained after 600 repeated cycles. The MoS<sub>2</sub> nanosheet have been growth on carbon paper (Nan et al. 2021). The obtained hierarchical structure of MoS<sub>2</sub>/carbon is favorable for the electrode/electrolyte interaction, reducing the electron transfer resistance. The obtained electrode exhibited an initial capacity of 0.556 and 0.442 Ah g<sup>-1</sup> for discharge and charge. Moreover, it delivered an excellent initial coulombic efficiency of 79.5% compared to 38.3% for the pristine carbon paper.

Nanosized petals of  $MoS_2$  micro-flowers for sodium-ion batteries display 0.595 Ah g<sup>-1</sup> after 50 cycles (Kumar et al. 2015).

Also, (Kong et al. 2017) synthesized a new composite formed from ultrathin  $MoS_2$  vertical nanosheets arrays with iron oxide (Fe<sub>3</sub>O<sub>4</sub>) that allowed growth over the surface of graphite paper and used it as an anode for sodium-ion batteries. The as-prepared anode of Fe<sub>3</sub>O<sub>4</sub>/MoS<sub>2</sub> delivered 468 and 0.231 Ah g<sup>-1</sup> at 100 and 3.2 A g<sup>-1</sup>, respectively, and 72.5% of its original capacitance retained after 300 cycles.

Poly(ethylene oxide)/intercalated  $MoS_2$  nanocomposites were synthesized via a simple exfoliation/restacking route and evaluated as electroactive anode material for sodium-ion batteries (Li et al. 2015). The prepared anode revealed a specific capacity of 0.225 A h g<sup>-1</sup> of 0.05 A g<sup>-1</sup> current density, double that of commercial  $MoS_2$ , and displayed better rate capability due to the enhancement of Na<sup>+</sup> ion diffusivity.

A nanostructure of nanoplates Sb anchored the ultrathin layered structure of  $MoS_2$  ( $MoS_2/Sb$ ) and tested it as anode material for sodium-ion batteries (Li et al., 2018b). The fabricated sodium-ion batteries delivered a superb reversible capacity of 0.666 Ah g<sup>-1</sup> and 0.454 Ah g<sup>-1</sup> at current densities of 0.1 A g<sup>-1</sup> and 10 A g<sup>-1</sup>, respectively, indicating its excellent cyclability and good rate performance.

### Lithium-sulfur batteries

The economic sulfur cathode, respectable theoretical capacity (1.672 A h g<sup>-1</sup>), and high energy density (1.672 kW h g<sup>-1</sup>) (Xiang et al. 2019) have attracted much interest for lithium–sulfur batteries as a prospective energy storage market candidate. However, some problems face lithium–sulfur batteries, such as the non-conductivity of sulfur and its discharging products (Li<sub>2</sub>S<sub>2</sub> and Li<sub>2</sub>S), leading to a slow operating and low capacity (Chen et al. 2019c).

During the charging/discharging operations, polysulfide was formed as an intermediate product, which is easily soluble in electrolyte material and freely migrates between the two electrodes of lithium–sulfur batteries (Yuan et al. 2019). If the reactive lithium polysulfide is missing during the cycling process, it will lead to fast capacity fading. This problem is called "shuttle effects" (Zhang et al., 2020). Moreover, the shuttle effect will cause passivation to the lithium anode and induce low-rate behavior and sulfur consumption.

A device fabricated in which  $MoS_2$  combined with a Celgard separator in lithium–sulfur batteries displayed a high conductivity and rapid diffusion rate of lithium (Zhang et al. 2019b). This separator can impede the diffusing rate of polysulfide. Therefore, the shuttle could be inhibited, which enhanced the battery's performance, keeping a capacity of 0.401 Ah g<sup>-1</sup> after 600 cycles and sustained 99.5% coulombic efficiency. An efficient protective coating layer of  $MoS_2$ protects lithium metal anode from producing high-efficiency lithium–sulfur batteries (Cha et al. 2018).

### **Bibliometric analysis**

Search methodology for TOPIC: ("MoS<sub>2</sub>" or "Molybdenum disulphide") AND TOPIC: (capacitor OR wastewater OR "energy storage" OR "Water remediation" OR "MoS<sub>2</sub>-based hybrids" OR "supercapacitors"). Timespan: All years from 1970 till 2021.

Figure 8a, b illustrates the bibliometric mapping created from the Web of Science core collection, where Fig. 8a shows the network visualization and Fig. 8b depicts the density visualization. Initially, the data from the web of science (2022 results) were exported and then plotted using VOS viewer software. The co-occurrence analysis was used in this study, including all keywords in the literature from 1970 till 2021, as well as the fractional counting method with a minimum number of occurrences of five keywords. Direct clusters connect identifiable keywords to broad topics such as molybdenum disulfide, wastewater, and supercapacitor in energy storage. This allowed for the visualization of the majority of the significant keywords associated with the use of  $MoS_2$  in water remediation and energy storage



**Fig. 8** The bibliometric mapping of  $MoS_2$  utilization in water remediation and energy storage applications **a** network visualization and **b** density visualization maps. The bibliometric analysis was carried out in the timespan of 1970–2021

applications in publications from 1970 to 2021. Figure 8a, b clearly demonstrates that keywords such as supercapacitors, high capacity, composites, electrode material, nanosheet, electrochemical performance, molybdenum disulfide, and transition metal dichalcogenides had seen a momentous increase in popularity and, as a result, progress in keyword research. Besides, other associated keywords have shown in the bibliometric analysis, such as graphene and lithium-ion batteries. This implies that the utilization of  $MoS_2$  in the energy storage route is at a mature stage in the research and development of water remediation application, as shown by the prominence of literature keywords over more than fifty years

On the other hand, the water treatment application of  $MoS_2$  is still progressing and would require research and development in the near future. For instance, areas related to  $MoS_2$  in water treatment include one-step synthesis, adsorbents, desalination, separation, and the mechanism. While bibliometric mapping is also shown in Fig. 8a, b, cyclic stability, asymmetric supercapacitors, pseudo-capacitance, flexible electrode, and stability are areas for  $MoS_2$  energy storage application that need further investigation.

### Conclusion

In this review, we critically reviewed the recent literature investigating molybdenum disulfide (MoS<sub>2</sub>) material as a subclass of transition metal dichalcogenides, possessing a unique two-dimensional layered structure. This unique structure has granted MoS<sub>2</sub> promising electronic, physicochemical, optical, and electrical characteristics. These properties have attracted a lot of researchers' interests, directing them to investigate the versatile applications of these materials. Two of the main focus areas are environmental (water remediation) and energy storage applications (supercapacitors and ion batteries). As presented, MoS<sub>2</sub> can be prepared via many different synthetic approaches that can be divided into two main routes: topdown and bottom-up methods, through which their properties can be precisely tuned, giving researchers a significant advantage in how they are constructed. In addition, density-functional theory calculations can be used to analyze many electronic properties of MoS<sub>2</sub> materials, including their density of state, bandgap, HOMO-LUMO, charge density profiles, and work function. Then, we outlined the promising potential of MoS<sub>2</sub>-based hybrids (MoS<sub>2</sub>-carbon, MoS<sub>2</sub>-metal oxides, and MoS<sub>2</sub>-metal sulfides) to be employed as photocatalysts and absorbent materials due to their exceptional surface uptake, cost-effectiveness, and their small bandgap. MoS<sub>2</sub>-based composites can be potential substitutes to complete the ongoing efforts toward clean accessible water due to the ease of conjugation with other active materials (small bandgap metal oxide semiconductors). Moreover, they can be used to satisfy the continuously increasing energy demand due to their outstanding electrical characteristics by acting in supercapacitors and ion batteries to save energy. This can potentially be achieved due to their high power density,

fast charge/discharge rates, and long cycle life. However, more investigations revealing and outlining their potential hybrids, subsequent properties, and available applications are still required.

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### Declarations

**Disclaimer** The views and opinions expressed in this review do not necessarily reflect those of the European Commission or the Special EU Programmes Body (SEUPB).

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