

Review

Exploration of Molybdenum Oxide Compounds-A Review

Jyoti Bhattacharjee, Subhasis Roy *

Department of Chemical Engineering, University of Calcutta, 92 A. P. C. Road, Kolkata- 700009, India;
E-Mails: jyotibhattacharjee651@gmail.com; subhasis1093@gmail.com; srchemengg@caluniv.ac.in;
ORCID: 0009-0006-6835-2899; 0000-0003-4197-535X

* **Correspondence:** Subhasis Roy; E-Mails: subhasis1093@gmail.com; srchemengg@caluniv.ac.in;
ORCID: 0000-0003-4197-535X

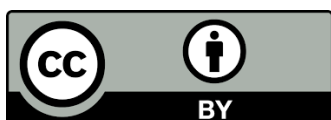
Academic Editor: Placidus B. Amama

Catalysis Research
2024, volume 4, issue 3
doi:10.21926/cr.2403011

Received: February 17, 2024
Accepted: July 04, 2024
Published: August 09, 2024

Abstract

The evolution of nanomaterials has been critical in modifying materials at the nanoscale for specialized uses. Carbon nanotubes were initially viewed as promising for electronics, but their inability to discriminate between semiconducting and metallic phases led to the creation of quasi-two-dimensional (Q-2D) materials. Molybdenum nanoparticles are utilized as alloy additions in corrosive and high-vacuum environments. Their characteristics differ significantly from those of their bulk counterparts. This review analyses the use of molybdenum oxide compounds in electrical devices, sensors, and memory devices. Their fascinating electrical conductivity and programmable characteristics give prospects for developing innovative electronic components. Furthermore, their performance in new technologies, such as flexible electronics and wearable devices, is evaluated. Molybdenum oxide compounds are incredibly versatile and can be used in various applications, including energy storage, electronics, and catalysis. Their essential use for tackling current materials science and technology issues has been discussed. The classifications, structural variations, and basic properties of molybdenum oxide compounds are covered in this paper, which offers a solid basis for comprehending the range of applications for these compounds. This review paper explores the catalytic processes, the challenges, and their critical significance in enabling environmentally remedial and sustainable chemical transformations.



© 2024 by the author. This is an open access article distributed under the conditions of the [Creative Commons by Attribution License](https://creativecommons.org/licenses/by/4.0/), which permits unrestricted use, distribution, and reproduction in any medium or format, provided the original work is correctly cited.

Keywords

Molybdenum oxides; catalysis; versatility; nanoscience; thermal stability

1. Introduction

1.1 History

Since the 20th century, environmental and energy challenges have escalated, prompting increased focus from scientists on developing new materials that can address or mitigate these issues. One class of materials that garnered significant attention is transitional metal oxides, known for their favorable performance in energy storage, photocatalysis, and fuel cells [1]. Molybdenum oxide clusters, Mo_mO_n ($m = 1-6$; $n = 1-3m$), a specific type of metal oxide with n-type semiconducting properties and a non-toxic nature, have emerged as a promising candidate due to its diverse functionalities. The effectiveness of MoO_x material is mainly contingent on its composition and structure. For instance, it alters the stoichiometric ratio of molybdenum oxide from 1:3 to 1:2, resulting in distinct physicochemical properties. Regarding optical characteristics, MoO_3 typically exhibits white, while MoO_2 displays dark blue or black hues, enabling varied light absorption. Oxygen vacancies in the MoO_x crystal induce changes in electrical conductivity and a controllable band gap within the 2.8–3.6 eV [2, 3].

Furthermore, the structural versatility of MoO_x facilitates extensive applications in energy conversion and storage, such as in lithium-ion batteries or as catalysts for the hydrogen evolution reaction (HER). MoO_x where 'x' can range from 2 to 6, also finds utility in gas sensors and photodevices due to its localized surface plasmon resonance (LSPR) effect. Consequently, considerable efforts have been directed towards tailoring the properties of MoO_x materials by manipulating their sizes, crystalline phases, morphologies, and even components to enhance their suitability for catalysts, gas sensing, energy conversion, and photodevice applications [3]. Molybdenum is a fascinating class of compounds with the general formula MoO_x , where 'x' can range from 2 to 6, exhibit a broad range of versatile characteristics, and have substantial potential for various applications across numerous industries. These compounds comprise molybdenum atoms bound to oxygen atoms in varying stoichiometric ratios, resulting in different chemical compositions and structural arrangements. Molybdenum trioxide (MoO_3) and molybdenum dioxide (MoO_2) are the most prevalent molybdenum oxides. Molybdenum oxides are typically yellow or brown solids insoluble in water [4]. Molybdenum oxides have demonstrated their versatility in electronics, energy storage, catalysis, and optoelectronics applications. The primary source of molybdenum is molybdenite, primarily found in regions such as China North and South America [5]. Molybdenite is typically obtained as a by-product of copper mining in Chile, where the ores contain around 0.5% molybdenum. MoS_2 is extracted from surrounding minerals through flotation, resulting in a concentration of approximately 85% MoS_2 . Subsequent roasting at 600°C yields MoO_3 from this concentrated material. The production of molybdenum and its alloys involves techniques such as powder metallurgy, electron-beam melting, or vacuum-arc melting. The powder metallurgical process is widely favored for its notable advantages and is the primary method for producing alloys like molybdenum doped with La_2O_3 or Y_2O_3 . This study also emphasizes the ability of molybdenum

oxides to transition between various oxidation states and accommodate different ions, making them well-suited for energy storage applications such as supercapacitors and batteries, enhancing performance and durability [6, 7]. Additionally, their catalytic properties find applications in chemical processes, environmental cleanup, and sustainable energy production through processes like water splitting. This characteristic is harnessed in intelligent windows, LEDs, displays, light, heat sensors, and multiferroic thin films, opening up new avenues for responsive and energy-efficient devices. The paper delves into recent advancements in molybdenum oxides, comprehensively exploring their synthesis, properties, and diverse applications [8].

This discussion deals with information about heterostructures, specifically MoS₂ heterostructures and an instance of a 2D-3D heterostructure involving MoS₂/MoO₃. Combining different nanomaterials in heterostructures offers various applications in various fields, such as photovoltaics, medicine, and optoelectronics [9]. The example of MoS₂/MoO₃ heterostructure highlights the use of molybdenum trioxide (MoO₃) as an n-type semiconductor with a wide band gap, showcasing its potential to enhance the conductive and insulating properties of transistors due to its electrical properties and stability as a transition metal oxide [10]. Despite numerous efforts to introduce defects into 2D materials, the mechanism of implantation remains incompletely understood. Therefore, a diverse array of techniques, encompassing both theoretical and instrumental analysis, is crucial for gaining insight into the structure of 2D materials. This paper also highlights a case study on the MoO₃ complex [11]. Figure 1 illustrates the number of publications vs. years on the morphological evolution of molybdenum oxide substances. These films exhibit reversible color changes upon electrochemical stimulation, making them ideal candidates for electrochromic devices such as bright windows, rearview mirrors, and displays.

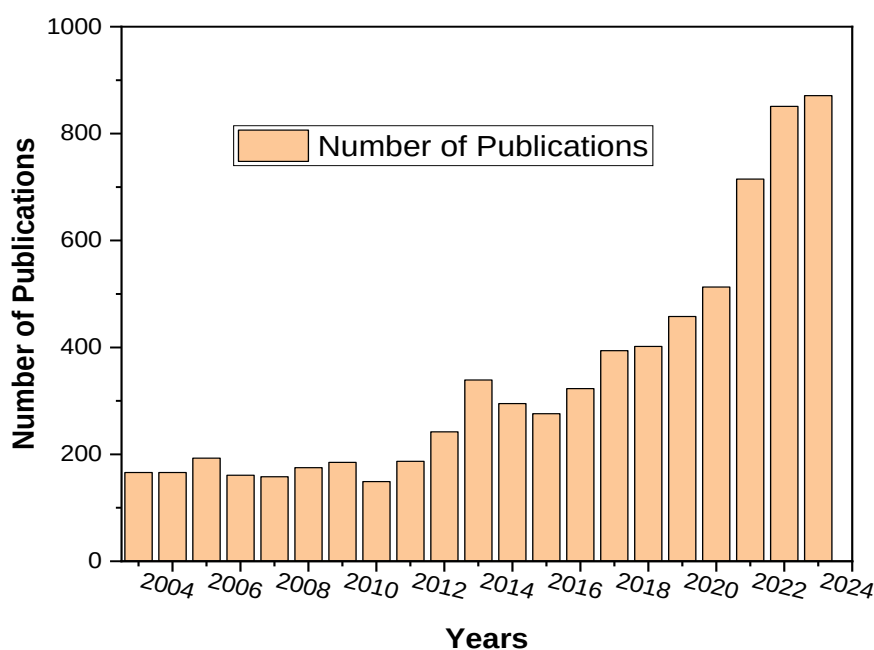


Figure 1 Schematic representation of the number of publications based on the evolution of molybdenum oxides year-wise. (Data input from ScienceDirect.com).

1.2 Classification Of Molybdenum Oxides

Molybdenum oxides are a class of chemical compounds composed of molybdenum (Mo) and oxygen (O) atoms. These compounds can display a variety of molybdenum oxidation states, resulting in a diverse set of characteristics and applications. Molybdenum oxides are classed based on their stoichiometry, crystal structure, and oxidation state. Among the most common classifications are:

1.2.1 Molybdenum Trioxide (MoO_3)

This is a well-known molybdenum oxide with the stoichiometry MoO_3 . It has polymorphic forms with diverse structures, such as orthorhombic -MoO_3 , hexagonal -MoO_3 , and in three forms in nature: α -orthorhombic (α), β -monoclinic (β), and h-hexagonal (h). others. Molybdenum oxide is an n-type semiconductor featuring a large band gap ($E_g \sim 3.20 \text{ eV}$) [12].

1.2.2 Dimolybdenum Tetraoxide (Mo_2O_4)

This oxide comprises two molybdenum and four oxygen atoms. It has fascinating electrical characteristics and is utilized in catalysts [13-15]. Molybdenum tetraoxide and pentoxide, for instance, create multilayer structures with various degrees of oxygen shortage. On the other hand, molybdenum oxides in a lower oxidation state tend to have more compact structures, such as the rutile structure of molybdenum dioxide.

1.2.3 Molybdenum Blue Compounds

These are reduced heteropolymolybdate complexes containing molybdenum in both +5 and +6 oxidation states and a heteroatom such as phosphorus or silicon.

Reduced isopolymolybdate complexes: These are polyoxometalates containing molybdenum in +5 and +6 oxidation states, which form when molybdenum (VI) solutions are reduced. Due to its extensive application, the term "heteropoly-molybdenum blues" is commonly used in analytical chemistry and catalysis. Additionally, the formation of "isopoly-molybdenum blues" is notable for producing an intense blue color, which serves as a sensitive test for the presence of reducing agents [14, 15].

Bronzes with the general formula H_xMoO_3 : In the context of photochromism, these bronzes exhibit color changes when exposed to light. The introduction of hydrogen into molybdenum trioxide (MoO_3) forms H_xMoO_3 , leading to these photochromic properties.

Bronzes with the general formula Me_xMoO_3 : Here, 'Me' represents alkali metals such as lithium (Li), potassium (K), or sodium (Na). These bronzes demonstrate electrochromic properties, meaning they change color when an electric field is applied. Incorporating alkali metal ions into the MoO_3 structure, forming Me_xMoO_3 , facilitates these electrochromic characteristics [15, 16].

1.2.4 MoO_x Compounds

Molybdenum bronze compounds are complex oxides with distinctive electrical and catalytic characteristics. MoO_x nanoparticles were employed to create very effective water-splitting photocatalysts. This could pave the way for developing new techniques for providing clean water. Figure 2 presents the various types of molybdenum oxide compounds.

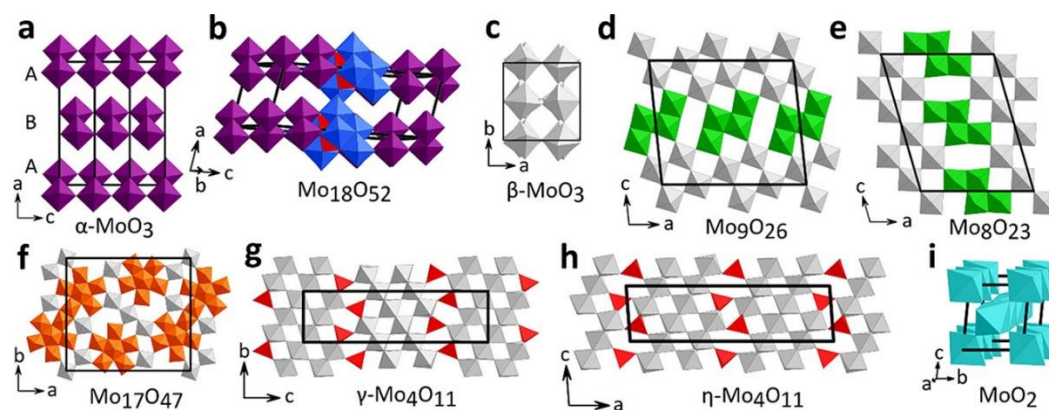


Figure 2 The crystal structures of molybdenum oxides, MoO_x , can be represented as different Mo–O polyhedra arrangements. These include a) Layered $\alpha\text{-MoO}_3$, where MoO_6 octahedra are arranged in zig-zag chains along the b direction, b) Triclinic $\text{Mo}_{18}\text{O}_{52}$, characterized by crystallographic shear planes containing MoO_4 tetrahedra, c) Metastable $\beta\text{-MoO}_3$ with a ReO_3 -type structure, d) Mo_9O_{26} with crystallographic shear planes, e) Mo_8O_{23} , f) $\text{Mo}_{17}\text{O}_{47}$ featuring pentagonal columns, g) $\gamma\text{-Mo}_4\text{O}_{11}$ at high temperature, h) $\eta\text{-Mo}_4\text{O}_{11}$ at low temperature, i) MoO_2 with a distorted rutile-type structure [17-18]. (Reproduced with permission).

Figure 2(a) shows the edge-sharing $[\text{MoO}_6]$ octahedra form zig-zag chains that connect via corners, creating slabs with AB stacking in the $[100]$ direction. Van der Waals interactions hold together these slabs. Removing oxygen and partially reducing Mo (VI) leads to crystallographic shear, maintaining the layer structure while forming triclinic $\text{Mo}_{18}\text{O}_{52}$ ($x = 2.889$, Figure 2b). Although $\text{Mo}_{18}\text{O}_{52}$ is presumed to be a pseudo-1D conductor based on its crystal structure, there is limited evidence beyond note on its electrical conductivity. Additionally, a monoclinic high-temperature modification Mo_9O_{26} (Figure 2d) is observed for the same composition, derived from the metastable ReO_3 -type modification $\beta\text{-MoO}_3$ (Figure 2c) by introducing crystallographic shear, as described by Magnéli. This phase represents the homologous series $\text{MonO}_{3(n-1)}$ with $n = 9$, and calculations suggest its thermodynamic stability. Another series member is monoclinic $\text{Mo}_{18}\text{O}_{33}$ ($x = 2.875$), differing in the distance between crystallographic shear planes (Figure 2e). Further reduction yields the pentagonal column (PC) phase $\text{Mo}_{17}\text{O}_{47}$ (Figure 2f, $x = 2.765$), where the PC structural motif contains an unusual terminating oxygen atom within tunnels. Another reported PC phase, Mo_5O_{14} ($x = 2.800$), is considered a metastable intermediate during $\text{Mo}_{17}\text{O}_{47}$ formation. Although not stable in the binary Mo–O system, Mo_5O_{14} can be stabilized by substituting Mo with V, Ti, Nb, or Ta, with W showing no influence on stability. In the orthorhombic γ (Figure 2g) and monoclinic η (Figure 2h) modifications of Mo_4O_{11} ($x = 2.750$), ReO_3 -type slabs are interconnected by $[\text{MoO}_4]$ tetrahedra. Both γ and η modifications exhibit low-temperature transitions around 100 K, interpreted as charge density wave (CDW) formations in these pseudo-2D conductors [18].

2. Overview of Molybdenum Oxides

2.1 Importance of Molybdenum Oxides

This paper explores the function of different oxidation states of molybdenum in these catalytic processes, offering a road map for constructing efficient catalysts for varied reactions.

2.1.1 Catalysis

Due to their redox characteristics, molybdenum oxides are essential catalysts for various chemical processes. For instance, in the selective oxidation of methanol to formaldehyde, -MoO_3 is a catalyst. Nano- MoO_x sensors can detect gases such as ammonia, nitrogen dioxide, and volatile organic compounds (VOCs) and have applications in environmental monitoring and industrial safety [19]. The flaky molybdenum nanorod structures are confirmed by (Tunneling Electron Microscopy) TEM pictures. With a maximum capacitance of 1080 F and a current density of 2 Ag^{-1} , the nanorod structure ensures good cyclic behavior for photocatalysis [20]. The latest research from a group of researchers has focused on examining a specific type of material called $\text{MoO}_x/\text{Fe}_2\text{O}_3$, aiming to understand the behavior of the Mo species on the active surface of the material. Qing and colleagues [16] have verified the presence of segregated Mo in these core-shell structures using TEM-EDX studies. Analyzing the EDX line profiles shows that Mo tends to accumulate at the surface, potentially at the expense of Fe, as shown in Figure 3.

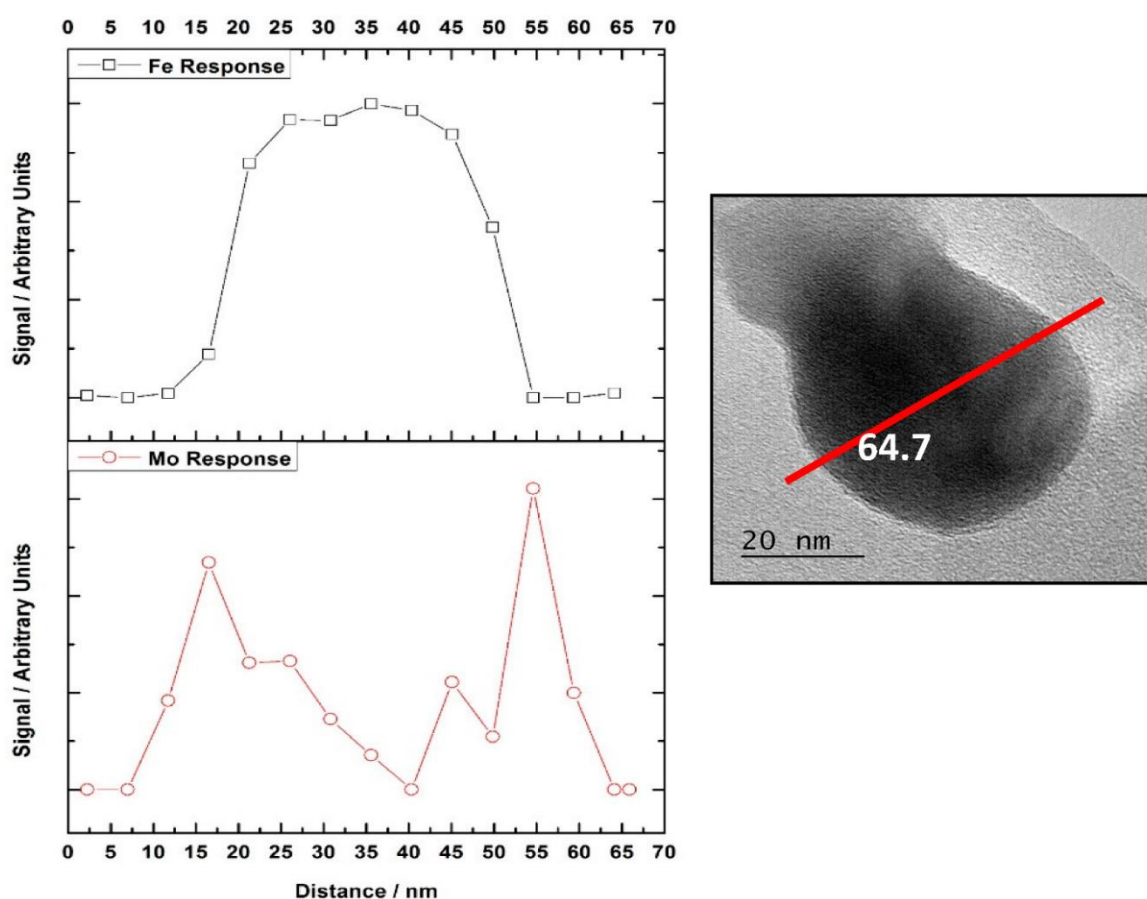


Figure 3 Representation of TEM picture and corresponding EDX line scan of a particle from 3 ML $\text{MoO}_x/\text{Fe}_2\text{O}_3$ following calcination at 500°C (right) [21]. (Reproduced with permission).

2.1.2 Devices with Electrochromic Properties

Electrochromic windows and displays employ molybdenum oxides. Electrochromic materials change color when a voltage is applied, making them suitable for energy-efficient windows and

intelligent mirrors. These applications frequently make use of molybdenum blue compounds [22]. Molybdenum substance electrodes have been used to develop new batteries with higher energy densities and longer lifetimes. This could lead to the development of more powerful and longer-lasting portable electronic devices.

2.1.3 Storage of Energy

Due to their high capacitance and outstanding electrochemical characteristics, molybdenum compounds are being researched for potential use in energy storage devices such as supercapacitors, magnetic levitation, and batteries. Nano-MoO_x can selectively oxidize hydrocarbons and alcohols, making it helpful in synthesizing delicate compounds and pharmaceuticals [23].

2.1.4 Photocatalysis

Some molybdenum oxides have photocatalytic activity, which can be used for water splitting, pollutant degradation, and hydrogen production. Molybdenum oxides having semiconducting characteristics are used in electrical and optoelectronic devices. MoO₃, for instance, is employed as a hole transport layer in organic solar cells. Nickel-doped molybdenum oxides are a renewable substitute for platinum in dye-sensitized solar cells [23]. Using MoO_x nanoparticles to fabricate highly efficient photocatalysts for water splitting holds promise for innovative techniques to deliver clean water.

2.1.5 Molybdenum Bronze Films

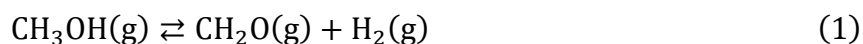
Molybdenum films are being investigated for various biomedical applications, such as drug delivery, tissue engineering, and imaging. These films change color with temperature and are utilized in applications such as temperature indicators and intelligent fabric. They can be used as protective coatings to improve the corrosion resistance of materials [24-26]. As seen in solar panels and optical lenses, nano-MoO_x coatings can be applied to surfaces to reduce reflection and enhance light absorption.

2.2 Fundamental Properties of Molybdenum Oxides

The discovery of molybdenum oxides dates back to the early 18th century when Swedish chemist Carl Wilhelm Scheele extracted molybdenum trioxide (MoO₃) from the mineral molybdenite. MoO₃, a yellow solid, is soluble in water and acids [27]. Scheele's work was furthered by Peter Jacob Hjelm, who named the new element "molybdenum," deriving from the Greek word "molybdos," meaning "lead." Throughout the early 19th century, several prominent scientists, including Martin Heinrich Klaproth, Joseph Louis Gay-Lussac, and Humphry Davy, conducted extensive research on molybdenum oxides and chemical composition and properties of crystals. Their investigations were instrumental in establishing molybdenum as a valuable industrial metal. By the late 19th and early 20th centuries, molybdenum oxides and crystals had been found to have an increasing application in various industries, including high-temperature furnaces, light bulbs, and steel alloys [28]. In addition to these developments, researchers identified molybdenum disulfide as a significant layered transition metal dichalcogenide with essential applications in electronics, catalysis, and energy storage [29]. This review paper looks into several synthesis processes, including sol-gel,

hydrothermal, and chemical vapor deposition procedures. It investigates how these approaches can produce nanoparticles, nanowires, and thin films of molybdenum oxides with regulated sizes and morphologies. Beyond their intrinsic properties, molybdenum oxide compounds exhibit fascinating catalytic activity, catalyzing many chemical transformations with high efficiency and selectivity. From hydrogen evolution reactions to oxygen reduction reactions, molybdenum oxide-based catalysts facilitate sustainable energy conversion and environmental remediation efforts. Industrial production of formaldehyde (CH_2O) involves the selective oxidation of methanol using an iron molybdate catalyst that contains excess molybdenum oxide [30]. This procedure, called the Formox process, uses a multitubular reactor to process nitrogen as a carrier gas while methanol, water, and oxygen are delivered into the system. The reactor maintains a temperature of 200–250°C while operating at a pressure close to the atmosphere. Owing to the exothermic reaction and the solid nature of the reactor, it produces a temperature hotspot that ranges from 350 to 400°C [31]. This high temperature makes it easier for methanol to convert to formaldehyde, with yields usually ranging from 88% to 92%. Furthermore, their versatility extends to heterogeneous catalysis, where molybdenum oxide compounds serve as robust and effective catalyst supports for various catalytic systems, as shown in equation 1 [32–34]: Iron molybdate catalysts are known for their high catalytic activity in the oxidation of methanol to formaldehyde. They facilitate the efficient conversion of methanol to formaldehyde, leading to high yields of the desired product.

- Selectivity: Iron molybdate catalysts demonstrate good selectivity towards forming formaldehyde, minimizing the formation of undesired by-products. This selectivity is crucial for maximizing the efficiency of the formaldehyde production process.
- Thermal Stability: Iron molybdate catalysts exhibit thermal stability under the high temperatures required for the methanol oxidation reaction. This stability ensures that the catalyst remains active and effective over extended periods of operation.
- Iron molybdate catalysts are known for their high catalytic activity in methanol oxidation to formaldehyde. They facilitate the efficient conversion of methanol to formaldehyde, leading to high yields of the desired product.
- Selectivity: Iron molybdate catalysts demonstrate good selectivity towards forming formaldehyde, minimizing the formation of undesired by-products. This selectivity is crucial for maximizing the efficiency of the formaldehyde production process.
- Thermal Stability: Iron molybdate catalysts exhibit thermal stability under the high temperatures required for the methanol oxidation reaction. This stability ensures that the catalyst remains active and effective over extended periods of operation, as shown in equations 1, 2, and 3 [32–34]. The catalysts help achieve a more balanced interaction between support and catalyst an effective oxygen renewal on the catalyst surface. This is crucial for improving catalysts selectivity, stability, and longevity. This review explores recent developments in the catalytic behavior of iron molybdate in formaldehyde production, emphasizing a comprehensive understanding of the catalyst and its pivotal role in these processes. Researchers attributed the enhanced catalytic performance to the formation of interactions between MoO_3 and Al_2O_3 , which facilitated the bonding of molybdenum to the support and the creation of robust acidic sites. However, this improvement was tempered by a reduction in specific surface area. The study concludes that developing stable catalysts utilizing MoO_3 presents a promising avenue for converting oils containing high levels of free fatty acids into valuable products [33].



Molybdenum oxides and compounds have diverse electrical and optical properties that can be tailored by adjusting their composition, structure, and morphology.

2.2.1 Electrical Properties

Depending on their content and structure, molybdenum oxides can be conductors or insulators. For instance, Molybdenum trioxide (MoO_3) has a band gap of 2.8 eV and is a semiconductor, but MoS_2 is a conductor. Doping molybdenum oxides with other elements like tungsten or nitrogen can also influence their electrical conductivity. MoO_3 exhibits electrochromic behavior, changing color when an electric field is applied. This property finds applications in bright windows and displays [33].

2.2.2 Optical Properties

Molybdenum oxides and compounds offer a wide range of optical properties, including a high refractive index, substantial absorption in the visible and infrared ranges, and photoconductivity. The optical properties of molybdenum oxide compounds are attractive for applications such as electrochromic devices and intelligent windows. As a result of these qualities, they are appropriate for a wide range of applications, including sensors and solar cells. Some molybdenum oxide compounds exhibit resistive switching behavior, which can be utilized in non-volatile memory devices [34]. Nanostructured molybdenum oxides can be used in photocatalytic applications for water splitting and pollutant degradation. Table 1 summarizes the electrical and optical properties and comparison of their refractive index, gap, and absorption efficiency in visible light of some common molybdenum oxides and compounds:

Table 1: Tabular presentation of various characteristics of Molybdenum oxide Compounds.

Material	Electrical Conductivity	Bandgap(eV)	Refractive Index	Absorption in Visible Light	Photoconductivity	References
MoO_3	Semiconductor	2.8	2.6	High	Yes	[35]
MoS_2	Conductor	1.8	2.1	Low	Yes	[36]
MoTe_2	Semiconductor	0.8	2.7	High	Yes	[36, 37]
Mo_2C	Conductor	0.7	2.9	Low	Yes	[37]
$\text{MoO}_3\text{-Bi}_2\text{O}_3$	p-n heterojunction	2.4	2.3	Medium	Yes	[37, 38]
MoO_3/WO_3 High	Heterojunction	2.8	2.1	High	Yes	[39]

2.2.3 Mechanical Properties

Hardness. Molybdenum oxide compounds are generally hard materials with different degrees of hardness based on their composition and crystal structure. Distributing molybdenum oxide nanoparticles into polymers or ceramics creates composites with increased strength, toughness, and thermal stability. This is especially useful in producing aerospace, automotive, and construction components [39, 40].

Elastic Modulus. The elastic modulus of molybdenum oxide compounds varies, but they are generally stiff materials. As highlighted in the subsequent papers, the strength of molybdenum oxide compounds is determined by crystal shape and defect density. They might be of moderate to high strength, such as Ammonium di-molybdate, a thermally stable compound [40].

Catalytic Properties. Molybdenum oxides are efficient catalysts for removing sulfur from petroleum products via hydrodesulfurization (HDS). Since sulfur damages the environment and human health, this is a crucial application of molybdenum oxides in the petroleum sector. Ammonium Heptamolybdate ((NH₄)₆Mo₇O₂₄) is a precursor to various molybdenum oxide catalysts. It can be used for catalytic applications in the synthesis of organic compounds and in the petrochemical industry. Molybdenum oxides can also remove oxygen from petroleum products using hydrodeoxygenation (HDO). This is beneficial in the production of cleaner fuels and other products. Molybdenum oxides can transform hydrocarbons into nitriles and amines by ammoxidation. This is a valuable reaction for synthesizing various compounds, including polymers and medicines [41]. Molybdenum incorporation into vanadium oxide complexes can improve their catalytic characteristics. These compounds have been studied in processes such as selective oxidation and dehydrogenation. Molybdenum doping of titanium oxide frameworks can boost photocatalytic and catalytic performance in activities like water splitting and organic pollutant degradation.

Ammonia Oxidation. This reaction creates nitric acid, which is employed in various industrial applications. Molybdenum oxides are effective ammonia oxidation catalysts used in multiple nitric acid factories [42].

Olefin Metathesis. This reaction creates various compounds, including polymers and medicines. Molybdenum oxides are active catalysts for olefin metathesis and are employed in multiple industrial applications and perovskite solar cells.

Catalytic Reforming. This reaction transforms petroleum fractions into petrol and other products. Molybdenum oxides are being studied as catalysts for catalytic reforming since they can potentially improve process efficiency. Catalytic dehydrogenation eliminates hydrogen from molecules. Molybdenum oxides have the potential to manufacture a wide range of compounds from fossils [43].

2.3 Case Study on MoO₃

Molybdenum trioxide (MoO₃) has recently attracted much attention due to its unique qualities and broad applications. This thorough analysis examines the many uses of MoO₃, from energy storage and catalysis to optoelectronics and sensing. Furthermore, the review highlights \ the

potential of MoO_3 for further innovation and improvement in materials science and technology, and it addresses current research trends and prospects for the material [44].

In 2003, Wang and colleagues achieved the preparation of single-crystal $\alpha\text{-MoO}_3$ nanowires without the need for a catalyst or template. Few researchers improved the electrochemical properties of these nanowires by synthesizing lithiated $\alpha\text{-MoO}_3$ nanowires, a first in the field. They achieved this by subjecting the nanowires to a secondary reaction with a LiCl solution, maintaining their crystal structure and surface morphology. This information, along with the morphology, is depicted in Figure 4. In 2011, a few researchers developed a technique utilizing atmospheric conditions and no catalyst to substrates rapidly synthesize flower-like arrays of $\alpha\text{-MoO}_3$ nanowires on various substrates. They successfully controlled the growth rate, morphology, and density of nanowire coverage on the substrate [45].

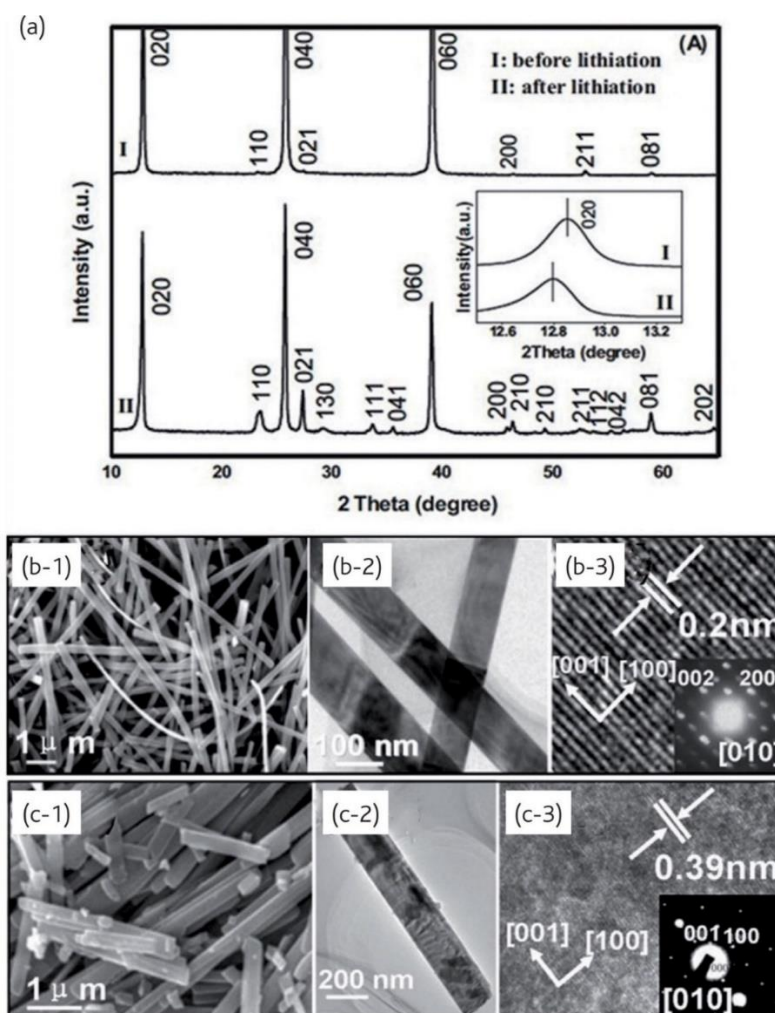


Figure 4 (a) The X-ray diffraction (XRD) profiles of a MoO_3 nanowire before and following lithiation are depicted, with a focus on the (020) diffraction peak as shown in the inset. (b-1 to 3) and (c-1 to 3) Illustration of the scanning electron microscopy (SEM), transmission electron microscopy (TEM), and high-resolution transmission electron microscopy (HRTEM) analyses of the nanowire before and after lithiation, respectively. The insets in the HRTEM images exhibit the corresponding selected area electron diffraction (SAED) patterns [46]. (Reproduced with permission).

As a transition metal oxide with fascinating characteristics, molybdenum trioxide is a prospective option for many applications. An outline of MoO_3 , including its synthesis techniques, characteristics, and crystal structure, is given in this section. It also highlights the significance of comprehending uses and possibilities of MoO_3 in the future for advancing technological breakthroughs [47]. MoO_3 has exceptional catalytic activity; it can selectively and efficiently catalyze various processes. This case study also addresses ways to improve the catalytic performance of MoO_3 and goes over the fundamental mechanisms controlling its catalysis. Due to its distinct electrochemical characteristics, MoO_3 is a viable option for energy storage systems, such as lithium-ion batteries and supercapacitors. MoO_3 electrodes have been applied in high-performance battery systems in real-world scenarios, enhancing capacity, cycling stability, and safety. In addition, we investigate the incorporation of MoO_3 into developing battery technologies, including potassium- and sodium-ion batteries, emphasizing its potential to meet future energy storage needs [48]. When identifying different gases, volatile organic compounds (VOCs), and biomolecules, MoO_3 has exceptional sensing qualities. Case studies demonstrate its application in gas sensors for industrial safety, medical diagnostics, and environmental monitoring.

Additionally, we talk about developments in MoO_3 -based sensing platforms, such as creating flexible and wearable sensors and incorporating MoO_3 with complementary metal-oxide-semiconductor (CMOS) technology for scalable sensor arrays. MoO_3 research and applications have advanced significantly, but several issues, such as scalability, affordability, and environmental sustainability, still need to be resolved. The possible approaches to surmount these obstacles include sophisticated synthesis methods, innovative device designs, and environmentally friendly production procedures. In addition, we describe new directions in application fields, including artificial intelligence and quantum technologies, as well as the combination of MoO_3 with cutting-edge materials like perovskites and 2D materials. These developments present stimulating prospects for further study and advancement [49].

3. Applications

Molybdenum oxide compounds have sparked considerable interest due to their broad and unique uses in various disciplines. The diverse features of these compounds make them excellent for use in electronics, catalysis, energy storage, sensors, and other fields. The following papers dive into the exciting realm of molybdenum oxide compounds, presenting instances of their inventive applications and emphasizing their distinct properties.

3.1 Electronics

Molybdenum oxide compounds have applications in electronics and optoelectronics due to their semiconducting and conductive characteristics. One noteworthy instance is molybdenum trioxide (MoO_3), a transparent conductor in thin-film transistors, displays, and solar cells. Its remarkable transparency in the visible spectrum and moderate electrical conductivity make it an ideal contender for transparent electrodes [50].

3.2 Catalysis

Molybdenum oxide compounds are frequently used as catalysts in various chemical processes. Molybdenum oxide-based catalysts have good redox characteristics and high thermal stability. For instance, MoO_3 is used in the petroleum sector for refining procedures such as hydrodesulfurization and hydrodenitrogenation. These catalysts aid in removing sulfur and nitrogen contaminants from crude oil and, thus, improve fuel quality. Molybdenum trioxide is used as a catalyst in the hydrodesulfurization (HDS) of petroleum, which removes sulfur from the fuel. XPS investigation of a $\text{MoO}_x/\text{Fe}_2\text{O}_3$ composite revealed synergistic effects, improving its photocatalytic efficiency [51].

3.3 Energy Storage

Molybdenum oxide compounds have shown promise in energy storage applications, particularly rechargeable batteries and supercapacitors. Due to its unusual layered structure, MoO_3 is excellent as an anode material in lithium-ion batteries. Molybdenum oxide nanowires have been integrated into field-effect transistors (FETs) with high electron mobility, which could pave the way for smaller, more efficient electronic components [52]. Molybdenum oxide compounds have the potential to be integrated into flexible and elastic electronic devices, allowing for the development of wearable sensors and electronic fabrics, such as conductive inks based on molybdenum oxide have been used to print flexible strain sensors that may be embedded in garments to monitor body movements and offer vital data for sports and rehabilitation [53].

3.4 Gas Sensing

Due to the sensitivity of molybdenum oxide compounds to various gases, they are used in gas-sensing devices. MoO_3 , for instance, has been used as a gas sensor to detect gases such as nitrogen dioxide, ammonia (NH_3), and carbon monoxide (CO). Due to the changes in electrical conductivity caused by gas exposure, these compounds can operate as excellent gas sensors for environmental monitoring and industrial safety [54]. Molybdenum oxide nanoparticles have been integrated into the interlayer of wearable devices such as nano-belts that detect volatile organic compounds (VOCs) in real-time, allowing for personalized air quality evaluation and potential early warning of pollutant exposure.

3.5 Photocatalysis

Molybdenum oxide compounds have photocatalytic characteristics that can be used for environmental remediation and solar fuel generation. MoO_3 , when correctly adjusted, can aid in the breakdown of organic contaminants in water via photocatalytic reactions. Another area of interest is using nano-molybdenum oxides in photoelectrochemical cells for water splitting. These cells have the potential to generate clean hydrogen fuel using solar energy [55].

3.6 Thermochromic Materials

Certain molybdenum oxide compounds display thermochromic behavior, changing color in response to temperature changes. MoO_3 -based materials have been used in "smart windows" that can control the quantity of sunlight that enters buildings. As the temperature fluctuates, the material

transitions between transparent and colored states, helping to energy-efficient building designs. Molybdenum oxides, particularly MoO_3 and its derivatives, have been extensively studied for their thermochromic behavior. At different temperatures, these materials undergo structural or electronic changes that manifest as alterations in their optical absorption or reflection properties, leading to observable changes in color. The thermochromic properties of molybdenum oxides are attributed to reversible phase transitions or electronic transitions induced by temperature changes. For instance, MoO_3 can exhibit reversible color changes between yellow and blue as it transitions from orthorhombic to monoclinic structures at specific temperatures.

3.7 Nanomaterials and Nanotechnology

Molybdenum oxide compounds can be synthesized into nanomaterials with customized characteristics, paving the way for nanotechnology applications. Owing to their biocompatibility and capacity to transport therapeutic substances to specific areas in the body, molybdenum oxide nanoparticles, for instance, can be functionalized and utilized in drug delivery systems. Given their sensitivity to acidity and alkalinity variations, molybdenum oxide thin films have shown potential in pH sensing. These sensors are used in environmental monitoring, medical diagnostics, perovskite cells, and industrial activities [56]. Molybdenum oxide compounds have been included in 3D printing materials, enhancing the potential for generating practical and customized things with enhanced qualities. For instance, molybdenum-based powders have been utilized in additive manufacturing procedures to build heat-resistant components for aerospace and automotive applications.

3.8 Lubrication and Wear Resistance

Molybdenum disulfide (MoS_2), a molybdenum oxide compound, has excellent lubricating qualities. It is a solid lubricant to minimize friction and wear between moving parts in various applications, including automotive engines and industrial machinery [57]. Molybdenum oxide coatings have been applied to steel structures and components in coastal areas to mitigate corrosion and extend the lifespan of infrastructure.

3.9 Biological Applications

Molybdenum oxide compounds have biological and medicinal applications. Molybdenum oxide nanoparticles, for instance, have been studied for their possible antibacterial characteristics. Molybdenum-based nanoparticles have been investigated as contrast agents for X-ray and Computed Tomography (CT) imaging, potentially improving imaging capabilities for disease diagnosis. Molybdenum oxides can create nanomaterials with various properties, such as high surface area, tunable electronic and optical properties, and biocompatibility, such as molybdenum oxide nanoparticles used in medicine. While molybdenum oxide compounds exhibit many promising applications, several challenges must be addressed. Molybdenum oxides can be used to create drug delivery systems, sensors for medical diagnostics, and implants with improved biocompatibility. These include improving synthesis methods to control material properties, enhancing stability in harsh environments, and optimizing performance for specific applications [58]. A comprehensive depiction of the applications of molybdenum oxides has been shown in Figure 5.

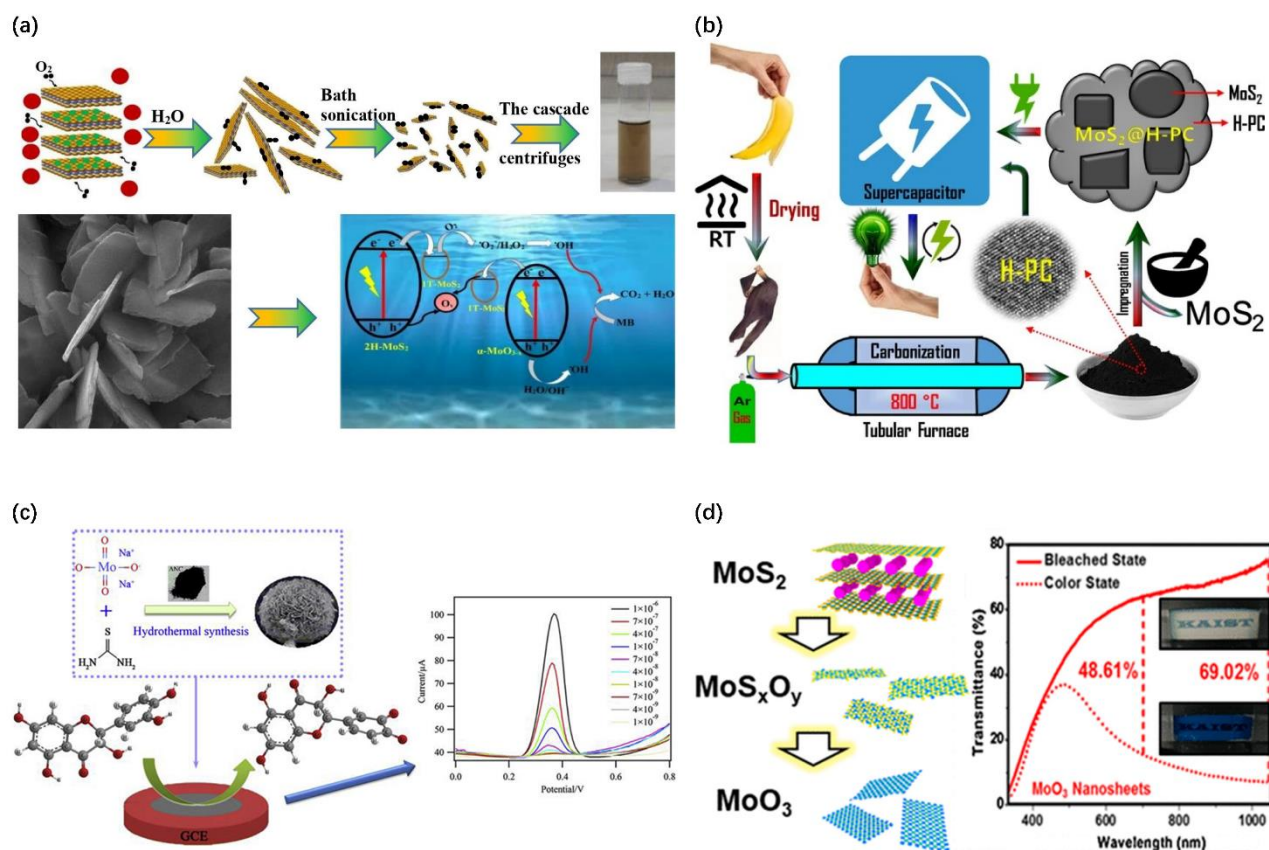


Figure 5 (a) Nanosheets of a Single Layer Heterojunction of MoS_2 - MoO_{3-x} Exhibiting Both Photoluminescence and Co-Photocatalytic Properties Simultaneously [54]; (b) Scheme of simple synthesis of heteroatom-doped porous carbon decorated with molybdenum disulfide for energy storage applications [55]; (c) Development of a susceptible electrochemical platform based on molybdenum sulfide for detecting taxifolin in Chinese medicine [56]; (d) 2D MoO_3 nanosheets produced through exfoliation and oxidation of MoS_2 for high-contrast, fast-response electrochromic devices [57]. (Reproduced with permission).

Additionally, within living organisms, molybdenum plays a vital role as a cofactor for various enzymes, assisting in metabolic processes and facilitating essential physiological functions like protein synthesis. One auspicious antibacterial material is MoO_3 . Its antibacterial action occurs when it comes into contact with water, leading to a dissolution process that generates an acidic environment and produces hydronium (H_3O^+) and molybdate (MoO_4^{2-}) ions. The infiltration of hydronium ions through bacterial cell walls disrupts their pH balance, enzyme activity, and transportation systems, creating an inhospitable environment for bacterial growth. This acidic condition induced by MoO_3 nanoparticles has proven effective against various bacterial strains, including those resistant to conventional antibiotics. The penetration of hydroxonium ions through cell membranes inhibits bacterial and fungal proliferation by affecting their enzymes and transportation systems, ultimately slowing their growth, as shown in Figure 5. Previous research has shown that incorporating molybdenum trioxide nanoparticles (NPs) into polyacrylonitrile (PAN) has been effective in speeding up wound healing and managing the gradual release of silver ions to fight bacteria [57, 58] as shown in Figure 6.

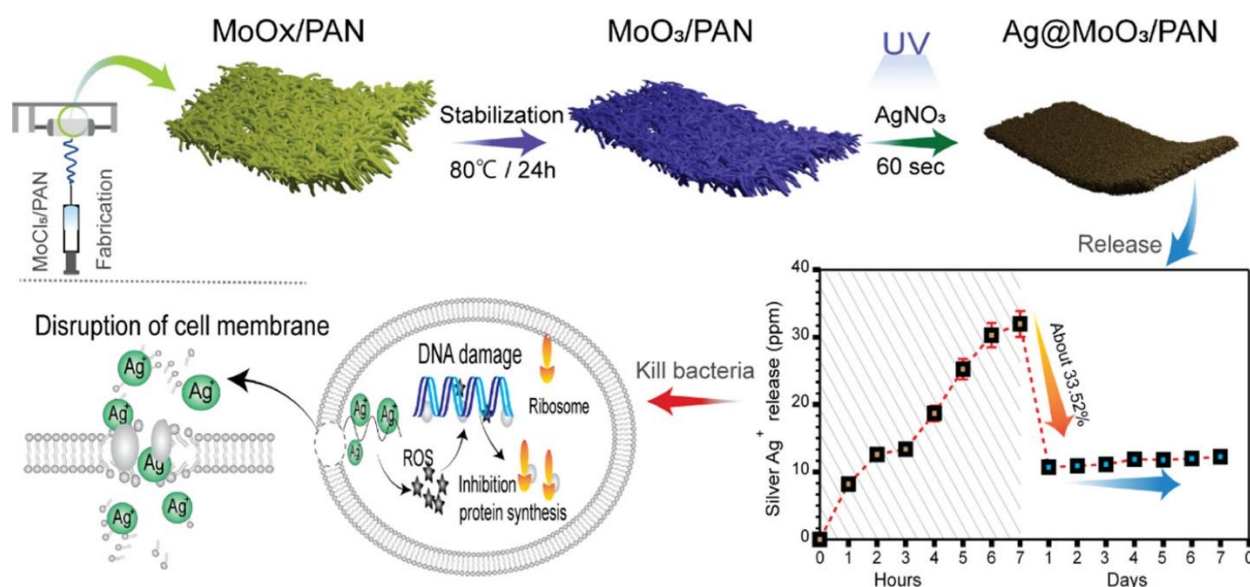


Figure 6 Pictorial representation of silver nanoparticles inserted into the MoO₃/PAN composite membrane, as well as how silver ions are released with time. There is also a scheme showing how the presence of these silver ions affects and eventually kills bacterial cells [58] (Reproduced with permission).

4. Challenges

Molybdenum oxides are a monument to the limitless possibilities that result from the convergence of chemistry, physics, and materials science. Molybdenum crystals are a class of molybdenum and oxygen-containing chemical compounds with many uses, including steelmaking, electronics, and catalysts. Molybdenum oxide compounds present several obstacles and dangers. A few cases are outlined below:

4.1 Environmental Effect

Molybdenum oxides can be hazardous to human health if inhaled or swallowed. They can cause respiratory difficulties such as coughing, wheezing, and liver and kidney damage. A fire at a molybdenum processing plant in China in 2012 blasted dangerous chemicals into the air, causing neighboring people to evacuate. Molybdenum oxides can harm the environment if released into the air or water. They can cause acid rain and harm plants and animals [59]. Inhalation of molybdenum trioxide (MoO₃) dust can result in respiratory irritation, coughing, and difficulty breathing. Prolonged exposure might lead to chronic respiratory diseases.

4.2 Environmental Impact

Improper disposal or discharge of molybdenum oxide compounds into the environment can contaminate soil, water, and air. This contamination has the potential to destabilize ecosystems and destroy aquatic life. For instance, industrial wastewater containing molybdenum compounds can contaminate neighboring water bodies, impacting marine organisms and potentially entering the food chains [60].

4.3 Occupational Dangers

Workers involved in manufacturing, handling, and processing molybdenum oxide compounds may be exposed to occupational hazards such as airborne particle inhalation and skin contact [61]. For instance, employees in a metal processing factory who come into direct contact with molybdenum oxide compounds may get skin irritation or dermatitis. A few years back, a study by the Environmental Protection Agency found that molybdenum oxides can contribute to acid rain. A new technique of Mo doping to boost the low-temperature Selective catalytic reduction (SCR) efficiency of CeSi_2 demonstrated superior SO_2 and molybdenum dioxide resistance [62].

4.4 Chemical Reactivity

Molybdenum oxide complexes can be chemically reactive, potentially reacting unexpectedly with other materials, gases, or chemicals. Molybdenum trioxide, for instance, can combine with reducing agents to form volatile molybdenum compounds, releasing hazardous gases. Occupational exposure limits (OELs) for molybdenum oxide compounds govern the maximum permitted concentration in working air to protect worker health.

4.5 Legislative Adherence

Manufacturers and consumers of molybdenum oxide composites must follow some rules and regulations concerning worker safety, environmental protection, and chemical handling. In the United States, the Occupational Safety and Health Administration (OSHA) establishes workplace exposure limits and safety practices for molybdenum oxide compounds [63].

4.6 Supply Chain Disruptions

The supply chain of molybdenum oxide compounds can be disrupted by challenges in sourcing raw materials, such as molybdenum ores, due to geopolitical factors, mining regulations, and fluctuations in global demand. Disruptions in the production process, including equipment failures, labor strikes, or natural disasters, can impact the supply chain of molybdenum oxide compounds, leading to delays in manufacturing and distribution. Ensuring consistent quality and purity of molybdenum oxide compounds throughout the supply chain can be challenging, requiring stringent quality control measures and testing protocols. Fluctuations in the prices of molybdenum oxide compounds due to market volatility, currency exchange rates, or changes in production costs can impact the profitability of manufacturers and suppliers. [64].

4.7 Trash Management

Proper disposal of trash containing molybdenum oxide compounds is critical to preventing environmental contamination and ensuring compliance with legislation. Due to the possible toxicity of molybdenum oxide compounds, waste from semiconductor manufacturing operations must be treated as hazardous waste [65].

4.8 New Risks

As new applications and uses for molybdenum oxide compounds emerge, unexpected concerns may arise, demanding constant risk evaluation and management. For instance, developing molybdenum oxide-based nanomaterials for medical imaging may pose health and environmental hazards that must be carefully considered. The high processing temperatures required for some molybdenum oxide composites might cause thermal deterioration of the matrix or phase changes. Fabricating molybdenum alloy TZM (Mo, 0.5% Ti, 0.1% Zr), reinforced ceramic composites where the sintering temperature exceeds the ceramic oxides, resulting in phase transitions [64, 65].

Protective coatings can be applied to MoO_3 and molybdenum composites to improve their corrosion resistance. They can be coated with a layer of yttria-stabilized zirconia (YSZ), a very corrosion-resistant material. This paper provided a comprehensive resource that helps the collective understanding of this fascinating field of study by combining theoretical insights with practical applications for the future. Molybdenum oxide composites, their tunable properties, various states, and applications are also addressed in this paper. Several challenges and hazards are encountered when handling these chemical compounds mentioned in the latter papers; hence, when choosing molybdenum oxide composites for a specific application, these challenges and roadblocks must be carefully examined [66]. Recent advances in the synthesis and engineering of molybdenum oxide nanostructures have created new potential in photocatalysis, photothermal treatment, and optoelectronics. Researchers can accurately regulate the optical, electrical, and thermal properties of molybdenum oxide nanostructures by adjusting their morphology, size, and composition, opening the door to novel applications in solar energy conversion, cancer treatment, and next-generation electronic devices. With continued advances in materials synthesis, characterization techniques, and computational modelling, we are on track to realize the full potential of molybdenum oxide compounds across a wide range of scientific and technological domains [67].

5. Types of Synthesis Methods

The synthesis of molybdenum oxide nanoparticles offers a sustainable approach to producing these materials, which are vital for energy conversion and storage applications.

5.1 Hydrothermal Synthesis

Hydrothermal synthesis involves crystallizing substances from high-temperature aqueous solutions at high vapor pressures.

- Example: Synthesis of MoO_3 Nanorods
- Procedure: Molybdenum trioxide (MoO_3) nanorods can be synthesized by reacting molybdenum powder with hydrogen peroxide (H_2O_2) to form a precursor. This solution is then transferred to a stainless-steel autoclave and heated at 180°C for 24 hours [64-68].
- Outcome: The resulting product is MoO_3 nanorods, which can be washed and dried for further use.

5.2 Sol-Gel Method

The sol-gel method involves the transition of a solution system from a liquid "sol" into a solid "gel" phase.

- Example: Preparation of MoO_3 Thin Films
- Procedure: A sol is prepared by dissolving molybdenum alkoxide in ethanol, hydrolysis, and polycondensation. The resulting sol is then spin-coated onto a substrate and heat-treated to form MoO_3 thin films.
- Outcome: Uniform thin films of MoO_3 are obtained, which can be used in applications such as electrochromic devices, as shown in Figure 7.

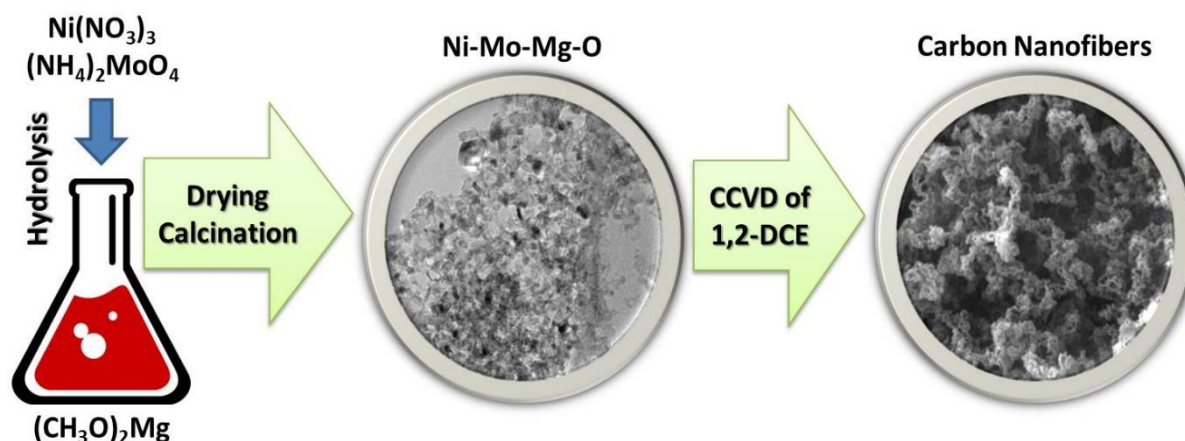


Figure 7 Presentation of sol-gel-prepared Ni-Mo-Mg-O system for catalytic transformation [68]. (Reproduced with permission).

5.3 Chemical Vapor Deposition (CVD)

CVD is a process used to produce high-purity, high-performance solid materials, typically under vacuum.

- Example: Deposition of MoO_3 Nanostructures
- Procedure: A volatile molybdenum precursor such as molybdenum hexacarbonyl ($\text{Mo}(\text{CO})_6$) is decomposed in a CVD reactor at high temperatures (typically 600-800°C) in the presence of oxygen to form MoO_3 nanostructures [68, 69].
- Outcome: This method yields highly crystalline MoO_3 nanostructures with controlled morphology.

5.4 Precipitation Method

Precipitation involves the formation of a solid in a solution during a chemical reaction.

- Example: Synthesis of $\alpha\text{-MoO}_3$ Microplates
- Procedure: Ammonium heptamolybdate is dissolved in distilled water and acidified with nitric acid. The solution is then heated to induce precipitation of MoO_3 , which is collected by filtration, washed, and dried.
- Outcome: The product is $\alpha\text{-MoO}_3$ microplates, which can be used for photocatalytic applications.

5.5 Thermal Decomposition

This method involves the thermal breakdown of a precursor compound to form the desired oxide.

- Example: Formation of MoO₂ Nanoparticles
- Procedure: Molybdenum pentachloride (MoCl₅) is thermally decomposed in an inert atmosphere at around 500°C to produce MoO₂ nanoparticles.
- Outcome: This results in MoO₂ nanoparticles that can be used in catalysis and battery electrodes [69, 70].

5.6 Electrochemical Deposition

This method involves the reduction of metal ions from a solution onto a conductive substrate.

- Example: Deposition of MoO₃ on Conductive Substrates
- Procedure: A solution of molybdenum salt, such as ammonium molybdate, is used as the electrolyte. By applying a potential, MoO₃ is deposited onto the conductive substrate.
- Outcome: This method can produce MoO₃ films with controlled thickness and morphology.

5.7 Laser-induced Method

Formation of molybdenum oxide induced by laser pulses at low energy (nJ) and high repetition rates (MHz) of femtosecond duration has been demonstrated. Researchers have utilized femtosecond laser pulses to create controlled molybdenum oxide layers on surfaces, enhancing their catalytic activity. For instance, studies have shown that laser-induced oxide formation on molybdenum surfaces can create catalytically active sites for various chemical reactions, such as hydrogenation or oxidation reactions in organic synthesis. In nanotechnology, femtosecond laser pulses have been employed to deposit thin films of molybdenum oxides with precisely controlled thickness and morphology. This technique offers a way to fabricate nanostructured materials for applications in sensors, energy storage devices, and optoelectronics [71].

5.8 Low-temperature Plasma Atomic Layer Etching Method

The new way of making molybdenum oxide films without chemical reagents is a big step forward in materials science. This method uses a particular low-temperature plasma that helps create high-quality molybdenum oxide films more precisely and cleanly. It is like giving the movie a detailed and careful makeover using unique energy instead of traditional chemicals. By not using chemical reagents, the new method keeps the synthesis process cleaner and more eco-friendly. This change reduces the use of harmful chemicals, making it easier to manage waste and reducing the risk of contamination. Operating at lower temperatures saves energy and allows for a broader range of materials to be used. This means that molybdenum oxide films can now be applied to materials sensitive to heat, opening up new possibilities in electronics and photonics. The Atomic Layer Precision (ALE) technique ensures that the films are uniform and precise in thickness, providing exact control over their properties. This level of accuracy is crucial for applications like semiconductor devices that require specific material characteristics [72].

6. Molybdenum Oxides in Batteries

The passage highlights molybdenum oxides, specifically MoO₃, in novel batteries, mainly rechargeable lithium-sulfur (Li-S) batteries. Here is a breakdown of the key points mentioned below:

1. Challenges with Li-S Batteries: Li-S batteries offer high theoretical energy density, natural abundance, and nontoxicity. However, cyclic stability and specific capacity reduction during cycling are observed due to the insulating nature of sulfur, polysulfide dissolution, and high-volume expansion [73-75].
2. Role of Metal Oxides and Sulfides: Metal oxides and sulfides, including MoO_3 , are being explored as sulfur hosts in Li-S batteries due to their strong interaction with lithium polysulfides. MoO_3 , in particular, shows promising binding strength with lithium polysulfides, making it an ideal material for anchoring these species and improving battery performance [68-75].
3. Novel Interwoven Scaffold-like MoO_3 @CNT Interlayer: Researchers have developed a novel interwoven scaffold-like MoO_3 @CNT (carbon nanotube) interlayer to address the challenges in Li-S batteries. This interlayer effectively blocks the shuttle effect and immobilizes sulfur species, enhancing cycling stability and capacity retention [73-76].
4. Battery Performance: The Li-S battery assembled with the MoO_3 @CNT interlayer demonstrates significant performance improvements. It achieves a capacity of 755 mA h g^{-1} after 200 cycles at a rate of 0.3°C and 655 mA h g^{-1} at 3°C , surpassing the performance of a CNT-based sulfur cathode. Overall, the integration of sulfur host material in Li-S batteries, along with innovative interlayer designs like MoO_3 @CNT, shows promise in overcoming the challenges associated with sulfur cathodes, enhancing battery performance, and advancing the development of high-energy-density storage solutions, as shown in Figure 8.

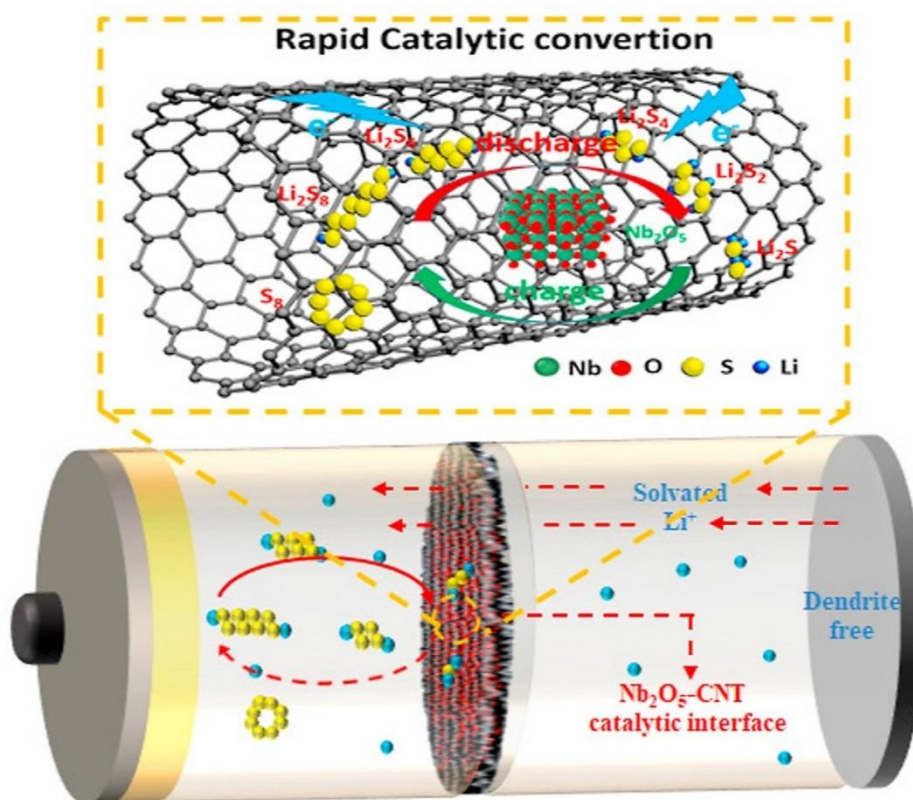
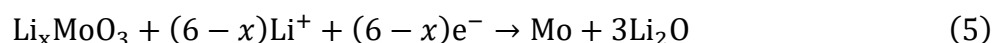
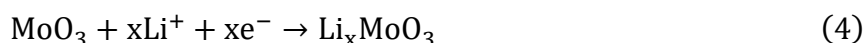


Figure 8 Schematic illustration of the multifunctional Nb_2O_5 -CNT catalytic layer. The layer directly traps and rapidly converts lithium polysulfides, enhancing battery performance. [75]. (Reproduced with permission).

The diagram (niobium pentaoxide) describes the design and fabrication of the Nb₂O₅-carbon nanotube catalytic interface for advanced lithium-sulfur batteries. The points are explained in the following lines: - The designed multifunctional catalytic interface composed of Nb₂O₅ and CNT is applied to the separator of the Li-S battery. Li₂S Nucleation and Dissolution Regulation: It regulates Li₂S nucleation and dissolution. The Nb₂O₅-CNT interface-supported sulfur cathode can provide an initial discharge capacity of 1286 mAh g⁻¹.

After 100 cycles at 0.2C, it still sustained a capacity of 992 mAh g⁻¹. Its capacity retention was 77.0%, while the capacity decay is very low, at 0.23% per cycle. This is a novel strategy toward improvement in terms of efficiency and lifetimes of Li-S cells because they usually suffer from problems associated with polysulfide trapping and conversion.

Lithium-ion batteries (LIBs) stand out as one of the leading energy storage solutions due to their superior storage capacity and power density compared to other rechargeable batteries. The surge in portable electronic devices and electric vehicles has driven the demand for LIBs with high energy and power densities. Consequently, there is a pressing need to develop high-capacity electrode materials for these batteries. Since its introduction by Sony Corporation, graphite has been the standard anode material for LIBs [77-79]. However, its relatively low theoretical capacity (372 mAh g⁻¹ and 850 mAh cm⁻³) falls short of meeting the needs of large-scale energy applications. To overcome this limitation, researchers are continuously exploring alternative anode materials. Transition metal oxides (TMOs), including NiO, MnO₂, TiO₂, Fe₃O₄, and MoO₂, are promising candidates due to their abundance, low cost, and high theoretical specific capacity (around 500–1200 mAh g⁻¹) resulting from their conversion reaction upon lithiation. Among these, molybdenum oxides with various oxidation states (such as MoO₃, MoO_{3-δ}, MoO_{3n-1}, and MoO₂) exhibit a wide range of electrical properties, from the semiconducting nature of MoO₃ to the metallic character of MoO₂, making them attractive anode materials for LIBs. Their specific capacities are significantly higher than that of graphite. In particular, MoO₃, which has an orthorhombic crystal structure, is thermally stable, abundant, cost-effective, and safe. It offers a theoretical capacity of 1117 mAh g⁻¹ and a typical discharge potential plateau around 0.45 V. These reactions can be described by the following equations [78-81]:



Its unique layered structure facilitates rapid lithium diffusion. The initial lithiation process of MoO₃ involves two stages: lithium insertion at potentials greater than 1.5 V up to approximately x ≈ 1.2 and a conversion reaction at potentials below 0.5 V up to approximately x ≈ 6.0.

7. Conclusions

This comprehensive analysis has emphasized various features and promising applications of molybdenum oxide compounds. Thanks to their flexible crystal structures and diverse functions, MoO_x materials have enormous potential across many areas. Numerous molybdenum oxide phases have been analyzed to understand their distinct features, such as MoO₃, β-MoO₃, MoO₂, and intermediate stages. Each phase has unique structural patterns and electrical properties, influencing their behavior and performance in various applications. The extraordinary sensing properties of

molybdenum oxide compounds have been extensively discussed, emphasizing their potential in gas sensing, biosensing, and environmental monitoring. Their sensitivity to target analytes, stability, and low cost make them ideal for constructing next-generation sensing platforms. Molybdenum oxide compounds have shown promise in biomedicine for drug administration, imaging, and theranostic uses. From catalysis to energy storage and beyond, molybdenum oxide compounds have demonstrated remarkable versatility and efficacy. Their biocompatibility, simplicity of functionalization, and controlled release qualities make them excellent candidates for targeted drug delivery systems and contrast agents in medical imaging.

Furthermore, their ability to generate reactive oxygen species (ROS) has applications in cancer therapy and photodynamic therapy (PDT), providing a holistic approach to cancer treatment. Further research and development efforts are warranted to unlock the full potential of molybdenum oxide compounds. Strategies focusing on synthesis optimization, structure-property relationships, and advanced characterization techniques that will drive innovation and enable the realization of novel applications have been portrayed in the paper. Additionally, interdisciplinary collaborations between researchers from chemistry, materials science, physics, and engineering will facilitate the translation of fundamental discoveries into practical solutions.

Acknowledgment

Author (S. Roy) would like to acknowledge 'Scheme for Transformational and Advanced Research in Sciences (STARS)' (MoE-STARS/STARS-2/2023-0175) by the Ministry of Education, Govt. of India for promoting translational India-centric research in sciences implemented and managed by Indian Institute of Science (IISc), Bangalore, for their support.

Author Contributions

J.B. conceived of the presented idea, wrote the article, and supervised the findings of this work and S.R. were involved in planning, encouraged and supervised the work. All authors discussed the results and contributed to the final manuscript.

Competing Interests

The authors have declared that no competing interests exist.

References

1. Vekariya RL, Dhar A, Paul PK, Roy S. An overview of engineered porous material for energy applications: A mini-review. *Ionics*. 2018; 24: 1-17.
2. Roy S, Majumder SB. Recent advances in multiferroic thin films and composites. *J Alloys Compd*. 2012; 538: 153-159.
3. Lv S, Du Y, Wu F, Cai Y, Zhou T. Review on LSPR assisted photocatalysis: Effects of physical fields and opportunities in multifield decoupling. *Nanoscale Adv*. 2022; 4: 2608-2631.
4. Bhattacharjee J, Roy S. A review on photocatalysis and nanocatalysts for advanced organic synthesis. *Hybrid Adv*. 2024; 6: 100268.

5. Gharibi Kharaji A, Shariati A. Performance comparison of two newly developed bimetallic (X-Mo/Al₂O₃, X = Fe or Co) catalysts for reverse water gas shift reaction. *China Pet Process Petrochem Technol.* 2016; 18: 51-58.
6. Sowmya B, John A, Panda PK. A review on metal-oxide based p-n and n-n heterostructured nano-materials for gas sensing applications. *Sens Int.* 2021; 2: 100085.
7. Datta S, Roy S. Simulated performance studies of thin film perovskite solar cell. *J Inst Eng India Ser C.* 2022; 103: 189-195.
8. Maitra S, Pal S, Datta S, Maitra T, Dutta B, Roy S. Nickel doped molybdenum oxide thin film counter electrodes as a low-cost replacement for platinum in dye-sensitized solar cells. *Mater Today Proc.* 2021; 39: 1856-1861.
9. Jones MM. State of Mo(VI) in acid solutions. *J Am Chem Soc.* 1954; 76: 4233-4234.
10. Bhattacharjee J, Roy S. Review on green resources and AI for biogenic solar power. *Energy Stor Conver.* 2024; 2: 457.
11. Gulomov J, Accouche O, Al Barakeh Z, Aliev R, Gulomova I, Neji B. Atom-to-device simulation of MoO₃/Si heterojunction solar cell. *Nanomaterials.* 2022; 12: 4240.
12. Brookes C, Bowker M, Wells PP. Catalysts for the selective oxidation of methanol. *Catalysts.* 2016; 6: 92.
13. Ding Y, Wang C, Zheng R, Maitra S, Zhang G, Barakat T, et al. Three-dimensionally ordered macroporous materials for photo/electrocatalytic sustainable energy conversion, solar cell and energy storage. *EnergyChem.* 2022; 4: 100081.
14. Zhou D, Yang L. Enhanced electrochromic properties of nanocrystalline molybdenum oxide films modified by dopamine. *Coatings.* 2023; 13: 1292.
15. van Deelen TW, Hernández Mejía C, de Jong KP. Control of metal-support interactions in heterogeneous catalysts to enhance activity and selectivity. *Nat Catal.* 2019; 2: 955-970.
16. Qing Y, Yang K, Chen Y, Zhu J, Li Y, Chen C, et al. Thermal stability, optical and electrical properties of substoichiometric molybdenum oxide. *Materials.* 2023; 16: 2841.
17. Kihlberg L. Studies on molybdenum oxides. *Acta Chem Scand.* 1959; 13: 954-962.
18. Kaiser F, Schmidt M, Grin Y, Veremchuk I. Molybdenum oxides MoO_x: Spark-plasma synthesis and thermoelectric properties at elevated temperature. *Chem Mater.* 2020; 32: 2025-2035.
19. Malik MI, Abatzoglou N, Achouri IE. Methanol to formaldehyde: An overview of surface studies and performance of an iron molybdate catalyst. *Catalysts.* 2021; 11: 893.
20. Ge F, Li X, Wu M, Ding H, Li X. A type II heterojunction α -Fe₂O₃/g-C₃N₄ for the heterogeneous photo-Fenton degradation of phenol. *RSC Adv.* 2022; 12: 8300-8309.
21. Brookes C, Wells PP, Cibir G, Dimitratos N, Jones W, Morgan DJ, et al. Molybdenum oxide on Fe₂O₃ core-shell catalysts: Probing the nature of the structural motifs responsible for methanol oxidation catalysis. *ACS Catal.* 2013; 4: 243-250.
22. Zeinidenov A, Mukametkali T, Ilyassov B, Aimukhanov A, Valiev D. The effect of MoO₃ interlayer on electro-physical characteristics of the perovskite solar cells. *Synth Met.* 2021; 281: 116903.
23. Mutta GR, Popuri SR, Wilson JJ, Bennett NS. Sol-gel spin coated well adhered MoO₃ thin films as an alternative counter electrode for dye sensitized solar cells. *Solid State Sci.* 2016; 61: 84-88.
24. Hermawan A, Septiani NL, Taufik A, Yulianto B, Suyatman, Yin S. Advanced strategies to improve performances of molybdenum-based gas sensors. *Nano-Micro Lett.* 2021; 13: 207.

25. Zhao Y, Heumueller T, Zhang J, Luo J, Kasian O, Langner S, et al. A bilayer conducting polymer structure for planar perovskite solar cells with over 1,400 hours operational stability at elevated temperatures. *Nat Energy*. 2022; 7: 144-152.
26. Peng X, Yu S, Chen M, Wang J, Yang B, de Mimérand YD, et al. Preparation of hexagonal boron nitride supported phosphomolybdic tungstic acid catalysts with different alkyl substituted imidazolium cations: Insight into hydrophobicity and electron transfer. *Fuel*. 2023; 333: 126424.
27. Tan W, Wang J, Cai Y, Li L, Xie S, Gao F, et al. Molybdenum oxide as an efficient promoter to enhance the NH_3 -SCR performance of CeO_2 - SiO_2 catalyst for NO removal. *Catal Today*. 2022; 397: 475-483.
28. Sun S, Zhang X, Cui J, Yang Q, Liang S. High-index faceted metal oxide micro-/nanostructures: A review on their characterization, synthesis and applications. *Nanoscale*. 2019; 11: 15739-15762.
29. Thomas N, Mathew S, Nair KM, O'Dowd K, Forouzandeh P, Goswami A, et al. 2D MoS_2 : Structure, mechanisms, and photocatalytic applications. *Mater Today Sustain*. 2021; 13: 100073.
30. Yang J, Song Z, Ma J, Han H. Toxicity of molybdenum-based nanomaterials on the soybean-Rhizobia symbiotic system: Implications for nutrition. *ACS Appl Nano Mater*. 2020; 3: 5773-5782.
31. Nagarajan T, Khalid M, Sridewi N, Jagadish P, Walvekar R. Microwave synthesis of molybdenum disulfide nanoparticles using response surface methodology for tribological application. *Nanomaterials*. 2022; 12: 3369.
32. Raun KV, Johannessen J, McCormack K, Appel CC, Baier S, Thorhauge M, et al. Modeling of the molybdenum loss in iron molybdate catalyst pellets for selective oxidation of methanol to formaldehyde. *Chem Eng J*. 2019; 361: 1285-1295.
33. Schulz P, Cowan SR, Guan ZL, Garcia A, Olson DC, Kahn A. $\text{NiO}_x/\text{MoO}_3$ Bi-layers as efficient hole extraction contacts in organic solar cells. *Adv Funct Mater*. 2014;24: 701-706.
34. Lukatskaya MR, Dunn B, Gogotsi Y. Multidimensional materials and device architectures for future hybrid energy storage. *Nat Commun*. 2016; 7: 12647.
35. Siao MD, Shen WC, Chen RS, Chang ZW, Shih MC, Chiu YP, et al. Two-dimensional electronic transport and surface electron accumulation in MoS_2 . *Nat Commun*. 2018; 9: 1442.
36. Deng Y, Zhao X, Zhu C, Li P, Duan R, Liu G, et al. MoTe_2 : Semiconductor or Semimetal? *ACS Nano*. 2021; 15: 12465-12474.
37. Xu H, Cen W, Tian Z, Zheng Q, Gao T, Liang Y, et al. A first-principles study of the surface electronic properties of Mo_2C . *Solid State Commun*. 2022; 353: 114867.
38. Hu Z, Zhou J, Zhang Y, Liu W, Zhou J, Cai W. The formation of a direct Z-scheme $\text{Bi}_2\text{O}_3/\text{MoO}_3$ composite nanocatalyst with improved photocatalytic activity under visible light. *Chem Phys Lett*. 2018; 706: 208-214.
39. Chary K. Structure and catalytic properties of molybdenum oxide catalysts supported on zirconia. *J Catal*. 2004; 226: 283-291.
40. Hu H, Wachs IE. Catalytic properties of supported molybdenum oxide catalysts: In situ raman and methanol oxidation studies. *J Phys Chem*. 1995; 99: 10911-10922.
41. Malik R, Joshi N, Tomer VK. Advances in the designs and mechanisms of MoO_3 nanostructures for gas sensors: A holistic review. *Mater Adv*. 2021; 2: 4190-4227.
42. Liu S, Zheng W, Fu J, Alexopoulos K, Saha B, Vlachos DG. Molybdenum oxide-modified iridium catalysts for selective production of renewable oils for jet and diesel fuels and lubricants. *ACS Catal*. 2019; 9: 7679-7689.

43. Hacatrjan S, Liu L, Gan J, Nakagawa Y, Cao J, Yabushita M, et al. Titania-supported molybdenum oxide combined with Au nanoparticles as a hydrogen-driven deoxydehydration catalyst of diol compounds. *Catal Sci Technol*. 2022; 12: 2146-2161.
44. Wu K, Zhan J, Xu G, Zhang C, Pan D, Wu M. MoO₃ nanosheet arrays as superior anode materials for Li- and Na-ion batteries. *Nanoscale*. 2018; 10: 16040-16049.
45. Rao PM, Cho IS, Zheng X. Flame synthesis of WO₃ nanotubes and nanowires for efficient photoelectrochemical water-splitting. *Proc Combust Inst*. 2013; 34: 2187-2195.
46. Mai LQ, Hu B, Chen W, Qi YY, Lao CS, Yang RS, et al. Lithiated MoO₃ nanobelts with greatly improved performance for lithium batteries. *Adv Mater*. 2007; 19: 3712-3716.
47. Bhattacharjee J, Roy S. Density functional waltz: Molecular theory of spin dynamics. *J Phys Opt Sci*. 2024; 6: 1-4. doi: 10.47363/JPSOS/2024(6)242.
48. Hu H, Chen N, Teng H, Yu R, Qu Y, Sun J, et al. Doping-driven topological polaritons in graphene/ α -MoO₃ heterostructures. *Nat Nanotechnol*. 2022; 17: 940-946.
49. Chen J, Han S, Zhao H, Bai J, Wang L, Sun G, et al. Robust wire-based supercapacitors based on hierarchical α -MoO₃ nanosheet arrays with well-aligned laminated structure. *Chem Eng J*. 2017; 320: 34-42.
50. Rasool A, Amiruddin R, Mohamed IR, Kumar MC. Fabrication and characterization of resistive random access memory (ReRAM) devices using molybdenum trioxide (MoO₃) as a switching layer. *Superlattices Microstruct*. 2020; 147: 106682.
51. De A, Bhattacharjee J, Chowdhury SR, Roy S. A comprehensive review on third-generation photovoltaic technologies. *J Chem Eng Res Updates*. 2023; 10: 1-17.
52. Gandeepan P, Ackermann L. Transient directing groups for transformative C–H activation by synergistic metal catalysis. *Chem*. 2018; 4: 199-222.
53. Huang C, Zhang W, Zheng W. The debut and spreading the landscape for excellent vacancies-promoted electrochemical energy storage of nano-architected molybdenum oxides. *Mater Today Energy*. 2022; 30: 101154.
54. Novak TG, Kim J, Tiwari AP, Kim J, Lee S, Lee J, et al. 2D MoO₃ nanosheets synthesized by exfoliation and oxidation of MoS₂ for high contrast and fast response time electrochromic devices. *ACS Sustain Chem Eng*. 2020; 8: 11276-11282.
55. Zhang X, Li D, Dong C, Shi J, Sun Y, Ye B, et al. Molybdenum sulfide-based electrochemical platform for high sensitive detection of taxifolin in Chinese medicine. *Anal Chim Acta*. 2020; 1099: 85-93.
56. Saadati M, Akhavan O, Fazli H. Single-layer MoS₂-MoO_{3-x} Heterojunction nanosheets with simultaneous photoluminescence and co-photocatalytic features. *Catalysts*. 2021; 11: 1445.
57. Kishore SC, Atchudan R, Perumal S, Edison TN, Sundramoorthy AK, Vinodh R, et al. Facile synthesis of molybdenum disulfide adorned heteroatom-doped porous carbon for energy storage applications. *J Nanostructure Chem*. 2023; 13: 545-561.
58. Farooq M, Bilal MI, Gohar S, Khalid M, Haider MK, Kim IS. Antibacterial activity of molybdenum oxide–Polyacrylonitrile composite membrane with fast silver ion reduction. *ACS Omega*. 2023; 8: 49467-49477.
59. Saliba M, Atanas JP, Howayek TM, Habchi R. Molybdenum disulfide, exfoliation methods and applications to photocatalysis: A review. *Nanoscale Adv*. 2023; 5: 6787-6803.
60. Cheng E, Notestein J. Molybdenum oxide and sulfide active sites for isobutane dehydrogenation with methanol as a probe molecule. *J Catal*. 2022; 413: 498-508.

61. da Silva Júnior MG, Arzuza LC, Sales HB, Farias RM, Neves GD, Lira HD, et al. A Brief Review of MoO_3 and MoO_3 -based materials and recent technological applications in gas sensors, lithium-ion batteries, adsorption, and photocatalysis. *Materials*. 2023; 16: 7657.
62. Bhattacharjee J, Roy S. Utilizing a variable material approach to combat climate change. *Mater Sci Res India*. 2024; 20: 141-145.
63. Wambach PF, Laul JC. Beryllium health effects, exposure limits, and regulatory requirements. *J Chem Health Saf*. 2008; 15: 5-12.
64. Martins RA, Carlos E, Kiazadeh A, Martins R, Deuermeier J. Low-temperature solution-based molybdenum oxide memristors. *ACS Appl Eng Mater*. 2024; 2: 298-304.
65. Gatzen C, Smokovych I, Scheffler M, Krüger M. Oxidation-Resistant environmental barrier coatings for Mo-based alloys: A review. *Adv Eng Mater*. 2020; 23: 2001016.
66. Chauhan I, Aggrawal S, Chandravati C, Mohanty P. Metal oxide nanostructures incorporated/immobilized paper matrices and their applications: A review. *RSC Adv*. 2015; 5: 83036-83055.
67. de Castro IA, Datta RS, Ou JZ, Castellanos-Gomez A, Sriram S, Daeneke T, et al. Molybdenum oxides – From fundamentals to functionality. *Adv Mater*. 2017; 29: 1701619.
68. Veselov GB, Karnaukhov TM, Bauman YI, Mishakov IV, Vedyagin AA. Sol-gel-prepared Ni-Mo-Mg-O system for catalytic transformation of chlorinated organic wastes into nanostructured carbon. *Materials*. 2020; 13: 4404.
69. Bhattacharjee J, Bhakta D, Roy S. Characteristics, applications, and limitations of nanocomposites in biosensing. In: *Smart and sustainable applications of nanocomposites*. Hershey, PA: IGI Global; 2024. pp. 161-191.
70. Bhattacharjee J, Roy S. Green remediation of microplastics using bionanomaterials. In: *Remediation of plastic and microplastic waste*. Boca Raton, FL: CRC Press; 2023. pp. 240-260.
71. Bhattacharjee J, Roy S. Significance of renewable energy in water management and irrigation. In: *Water Management in Developing Countries and Sustainable Development*. Singapore: Springer Nature Singapore; 2024. pp. 235-252.
72. Shao P, Chang Z, Li M, Lu X, Jiang W, Zhang K, et al. Mixed-valence molybdenum oxide as a recyclable sorbent for silver removal and recovery from wastewater. *Nat Commun*. 2023; 14: 1365.
73. Bhattacharjee J, Roy S. Smart materials for sustainable energy. *Nat Resour Conserv Res*. 2024; 7: 5536.
74. Ren L, Liu J, Zhao Y, Wang Y, Lu X, Zhou M, et al. Regulating electronic structure of Fe- N_4 single atomic catalyst via neighboring sulfur doping for high performance lithium-sulfur batteries. *Adv Funct Mater*. 2023; 33: 2210509.
75. Liu Y, Chen M, Su Z, Gao Y, Zhang Y, Long D. Direct trapping and rapid conversing of polysulfides via a multifunctional Nb_2O_5 -CNT catalytic layer for high-performance lithium-sulfur batteries. *Carbon*. 2021; 172: 260-271.
76. Vijaya Kumar Saroja AP, Sundara R. Core-shell cathode design with molybdenum trioxide as the electrocatalytic trapping layer for high-energy density room-temperature sodium sulfur batteries. *J Phys Chem C*. 2020; 124: 7615-7623.
77. Wang H, Li T, Hashem AM, Abdel-Ghany AE, El-Tawil RS, Abuzeid HM, et al. Nanostructured molybdenum-oxide anodes for lithium-ion batteries: An outstanding increase in capacity. *Nanomaterials*. 2022; 12: 13.

78. Kumari J, Basumatary P, Gangwar MS, Agarwal P. Molybdenum oxide (MoO_{3-x}) as an emitter layer in silicon-based heterojunction solar cells. *Mater Today Proc.* 2020; 39: 1996-1999.
79. Tang K, Farooqi SA, Wang X, Yan C. Recent progress on molybdenum oxides for rechargeable batteries. *ChemSusChem.* 2019; 12: 755-771.
80. Hairui X, Hu P, He C, Zhang X, Han J, Yang F, et al. Design of High-performance molybdenum alloys via doping metal oxide and carbide strengthening: A review. *J Mater Sci Technol.* 2023; 160: 161-180.
81. Shaikh AA, Bhattacharjee J, Datta P, Roy S. A comprehensive review of the oxidation states of molybdenum oxides and their diverse applications. *Sustain Chem Environ.* 2024; 7: 100125.