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2D Materials: Catalysis applications, opportunities, and challenges

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A B S T R A C T

It has been discovered that two-dimensional (2D) materials possess tunable electronic properties and abundant active sites, making them ideal for catalysis. This comprehensive review examines the use of 2D materials as catalysts and catalyst supports in energy conversion and environmental remediation. This field is characterized by the ability to enhance catalytic activity and selectivity through the engineering of defects, heterostructures, and hybrid composites. Despite these advances, challenges remain in scaling up synthesis, achieving structural stability under reaction conditions, and translating laboratory discoveries into industrial applications. By developing advanced characterization techniques and understanding structure-activity relationships, we can fully exploit the potential of 2D materials for catalysis.

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1. Introduction

A unique combination of structural and electronic characteristics has led to the emergence of 2D materials as an innovative class of catalysts [1]. Due to their atomic thin nature, these atomically thin catalysts have high surface-to-volume ratios, abundant active sites, and tunable electronic properties, making them ideal for a broad range of catalytic processes, from energy conversion to environmental remediation [2, 3]. The structure of 2D materials prendering them more efficient than bulk catalysts [2]. The catalytic potential of graphene, along with transition metal dichalcogenides (TMDs) like MoS_2 and WS_2, as well as other 2D materials such as black phosphorus and MXenes, has been extensively explored [4, 5]. These materials can act as catalysts themselves or in conjunction with atomic catalysts, making them versatile components of catalytic systems. Catalysts can be precisely designed and optimized using their well-defined atomic structures, allowing for the investigation of structure-function relationships [3, 6]. There has been significant progress in the electroreduction of CO_2 into valuable fuels and chemicals, aided by 2D materials for photocatalysis, electrocatalysis, and thermocatalysis [2]. As an example of enhanced catalytic activity, 2D MoS_2 has exposed edge sites and tunable electronic structures

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that can be further adjusted through doping and structural modulation [2, 3].

There are numerous potential applications of 2D materials, including energy conversion and environmental remediation. Although these developments are promising, translating 2D materials into practical catalytic systems still faces several challenges. Industry applications are limited by the inability of synthesis methods to scale up and be reproducible [7, 8]. Furthermore, to design rational catalysts, advanced characterization and theoretical modeling are required to understand the complex structure-activity relationships in multi-component 2D systems [8]. A wide range of 2D materials can be utilized in catalysis, from traditional chemical reactions to emerging fields such as sustainable energy conversion and environmental protection [9].

The versatility of these materials enables them to be functionalized and hybridized with other materials, extending their applicability across various applications. In order for multi-functional catalysts to realize their potential, advanced synthesis techniques, surface modifications, and multifunctional catalysts must be researched and developed [9, 10]. 2D materials have been extensively studied for their catalytic applications. Their unique properties and roles in various catalytic processes are discussed in this review. In addition to highlighting innovations and challenges, it encourages further research and industrial adoption of 2D catalysts by emphasizing opportunities and obstacles.

2. Catalytic properties of 2D materials

There are numerous examples of catalysis in nature and artificial chemical transformations that impact the chemical industry and shape our lives. This 2D material possesses a high specific surface area, making it ideal for catalysis [8, 11]. Due to their large lateral dimensions and atomic thickness, 2D materials provide ultrahigh surface areas, maximizing active sites and surface atoms, which accelerates the rate of reactions. In surface-related applications like catalysis, 2D materials hold significant potential [12]. A single-layer exfoliated layered double hydroxide (LDH) of NiFe and NiCo demonstrates higher catalytic activity during electrocatalytic oxygen evolution reactions (OER) than bulk NiFe or NiCo layers, primarily due to its enhanced electrochemical conductivity and active sites [13]. Another advantage of 2D materials is that their surface atoms are uncoordinated, allowing them to absorb more UV-visible light, while 3D bulk materials often face limitations due to light transmission and reflection [14, 15]. As a result of the 2D structure, photogenerated electrons and holes migrate much faster, reducing their recombination likelihood and potentially increasing the quantum yield [16]. The presence of more active sites may also enhance the performance of photocatalysts. Holy g-C_3N_4 nanosheets have been found to exhibit 20 times the photocatalytic activity for the hydrogen evolution reaction (HER) compared to bulk g-C_3N_4, attributed to improved light absorption, more exposed active sites, and increased separation efficiency of photoexcited electrons and holes [17]. The materials also exhibit excellent mechanical properties, allowing the catalyst to be durable and feature thermal conductivity, which facilitates heat diffusion during the exothermic reaction. Additionally, 2D materials possess tunable optical and electronic properties, making them ideal for catalysis [11, 17]. Currently, these materials are being researched for water splitting, degradation reactions, nitrogen fixation, hydrogenation, CO_2 reduction, and medical catalysis [18].

By modifying their surfaces, doping, engineering defects, and employing strain engineering, 2D materials will also be able to control their intrinsic properties at an atomic level, which is not possible with bulk materials [12, 19, 20]. Fig. 1 illustrates Properties of 2D Materials.

Fig. 1. Properties of 2D materials.

3. Applications of 2D catalysts

The unique physical and chemical properties of 2D catalysts, including their high surface area, dense active sites, active edges, enhanced conductivity, anti-photocorrosion properties, and chemical stability, have made them effective as sensors, conductive inks, environmental remediators, and energy storage products [21, 22]. Table 1 illustrates some of the applications and features of 2D catalysts.

3.1. Energy conversion

Energy storage and conversion benefit from various advantages [21]. 2D nanosheets can be utilized in numerous energy-conversion and storage applications, including supercapacitors, battery electrodes, electrocatalysis, and photocatalysis. An energy source, as well as a light source, can activate nanosheet processes [29, 30]. Photocatalysis can also be enhanced by trapping electrons or holes in vacancies to improve carrier separation. Numerous edges of nanosheets possess unsaturated coordination and dangling bonds, which facilitate the catalysis of biomolecules. Depending on the electronic structure, these catalytic sites can be tailored to enhance their catalytic activity [31].

MdS-Au/MoS_2 hybrid structures contain many active sites for hydrogen evolution within the MoS_2 layers. The hybrid structure also improves electron-hole separation by transferring electrons generated by CdS nanorods to the growing MoS_2 nanosheets and the Au metal surface [21]. As a potential fuel for transportation, this strategy may be an excellent option.

3.2. Environmental remediation

In recent years, single-atom catalysts (SACs) have gained enormous interest due to their rapid development. 2D SACs offer several unique advantages and can be utilized for environmental remediation [32]. Moreover, 2D supports can also serve as substrates for loading various single atoms, generating reactive species on both planes, which significantly enhances catalytic activity and capability [33, 34]. By stacking aromatic compounds on these readily available carbon supports (e.g., graphene, porous carbon, g-C_3N_4), we can improve the degradation or transformation of environmental pollutants, owing to the potential stacking interactions [33].

3.3. Sensors

It has been demonstrated that pristine graphene and its derivatives are highly sensitive to various gas molecules in an experimental setting. The high electron mobility, high conductance, and high surface area-to-volume ratio of a 2D graphene nanosheet all contribute to its superior chemical sensing performance, including high sensitivity and low noise [35]. Through micromechanical cleavage of graphite, Schedin et al. created microfabricated graphene devices for detecting common gases (NO_2, NH_3, H_2O, and CO).

They found that graphene exhibited a wide range of sensor properties, such as ultra-high sensitivity, fast response times, and linear responses to adsorbates [35, 36]. Surface doping with nanoparticles (which enrich the types of adsorbates at the surfaces) or introducing defects into graphene sheets can enhance adsorption sensitivity or enrichment [37].

There have been predictions regarding catalytic behavior based on gas adsorption studies. In Fig. 2, the catalytic behavior is primarily determined by the adsorption and dissociation of elements (or groups of chemical compounds) on a material's surface [38, 39].

4. Opportunities in 2D material catalysis

As technology advances, its rate of advancement may increase more rapidly in the 21st century than it has in centuries past. In the age of nanotechnology, new, environmentally friendly, economical, and sustainable materials are being discovered at an unprecedented rate [40]. Due to their abundance, two-dimensional (2D) materials can be used for a wide range of technical studies as well as various nano- and atomic-level applications [41]. A recent discovery of graphene has motivated considerable attention to the study of other novel 2D materials, called modern-day "alchemy," where scientists try to convert as many periodic table elements as possible into 2D material structures [42].

4.1. Novel applications

A heterostructure confers an appealing advantage over an isolated two in catalysis. Using 2D materials enhances the benefits of heterostructures. Among the tens of thousands of variations in electronic and structural elements, there are many opportunities to tune carrier distribution and mobility to enhance activity [43, 44].

Table 1
Applications and features of 2D catalysts.

2D catalyst type	Applications	Features/Advantages	Refs.
Graphene-based materials	• Energy storage • Sensors • Fuel cells	• High surface area • Tunable electronic structure • Active edges • High stability	[6, 8]
Transition metal dichalcogenides (TMDs, e.g., MoS_2, WS_2)	• Electrocatalysis • Fuel cells	• High surface area • Abundant active sites • Tunable bandgap • Exposed edges	[6, 10, 23]
Metal (Hydr)oxides	• Environmental catalysis	• High catalytic activity • Stability in aqueous media	[3]
MXenes (2D transition metal carbides/nitrides)	• Energy storage • Electrocatalysis (her, oer) • Batteries • Supercapacitors	• Conductivity • Hydrophilicity • Surface functionality	[24]
2D Metal-organic frameworks (MOFs)	• Energy conversion • Electrochemical catalysis	• Highly porous • Tunable active sites • Structural flexibility for selective catalysis	[25, 26]
2D Metal sulfides (e.g., SnS_2)	• Energy conversion • Electrochemical catalysis	• Stable catalytic performance • Enhanced electron density • High number of undercoordinated sulfur sites	[6]
Metallenes (2D metals)	• Electrocatalysis (HER, OER) • Energy conversion	• Atomically thin • High density of active sites	[24]
Graphitic carbon nitride (g-C_3N_4)	• Photocatalysis	• Chemical stability • Visible light absorption	[6, 27]
Hexagonal boron nitride (h-BN)	• Energy storage • Catalyst support	• Chemical stability • Wide bandgap • Insulating	[28]
Single-atom catalysts on 2D substrates	• Selective hydrogenation • Fuel cells	• Maximized active sites • High selectivity	[3]
Boron nitride (BN)	• Photocatalysis	• Chemical stability • Wide bandgap • High thermal conductivity	[4]

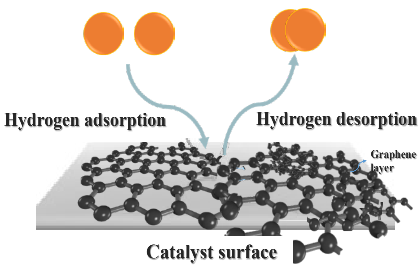

Fig. 2. Working principle of catalysis of elemental 2D materials.

Catalytic effects may also arise from defects and dislocations introduced during heterostructure formation [45]. Creating a microreactor will be possible at the interface between two components. Recent progress in designing and developing heterostructures based on 2D materials should stimulate more interest and efforts in research. In recent years, novel heterostructures have been designed using interesting 2D materials such as graphene, g-C_3N_4, and MoS_2 [44].

There are also various applications and industries that utilize 2D-material-based manufacturing devices, including high-quality, high-performance optical encoders. The functionalization of zero-BG 2D materials primarily addresses stability issues associated with their use in electronic devices [46]. BG Engineering has introduced a new set of potential candidates for electronic devices [42]. Investing in ultra-thin 2D p-n junctions can also be advantageous for light-sensing and harvesting applications in nanophotonics [47]. It has been demonstrated that 2D p-n junctions can function as photodetectors, and several material combinations exist, enabling the proposal of devices that operate effectively across wavelengths from infrared to ultraviolet [42].

4.2. Increased efficiency

It is common for 2D materials to exhibit excellent conductivity and stability during catalytic processes, leading to increased charge transfer and durability [2]. These properties often make 2D materials more effective than traditional catalysts for applications such as water splitting, CO_2 reduction, or hydrogen evolution [44, 48, 49].

4.3. Integration with other technologies

The integration of catalysts with 2D materials, such as nanoparticles, will enable a more effective use of 2D materials as catalysts by exploring innovative structures and hybrid systems [2, 50].

5. Challenges facing 2D catalysts

The development of ultrathin 2D materials for photocatalysis continues to face numerous challenges despite significant growth. A highly effective method exists for producing ultrathin photocatalysts with controlled thickness or crystal structure on a large scale [51, 52]. Given the potential commercial applications of ultrathin 2D photocatalysts, scalable manufacturing is critically important. As a result, greater attention should be directed toward cost-efficient production methods at scale [50, 52]. Lastly, atomic-scale thicknesses enable the utilization of ultrathin materials, along with simple electronic structure adjustments that enhance photocatalytic function [53]. Although defects are engineered, elements are doped, and other effective approaches are employed, such as modifying the tensile strain of the surface state to engineer the electronic structure, which greatly boosts photocatalytic activity [52]. It is still necessary to invest significant time and effort in developing suitable catalysts and reaction schemes for real-world applications, particularly those involving catalyst performance, selectivity related to yields and pollution, environmental friendliness, and cost-effectiveness [52, 54].

6. Conclusion

Catalysis can be significantly enhanced using 2D materials because of their large surface areas, tunable electronic properties, and atomically precise active sites. These materials present new pathways for energy conversion and sustainable chemical processes, including graphene, transition metal dichalcogenides, and beyond-graphene systems. Challenges remain in scaling up synthesis, maintaining stability under operational conditions, and integrating the catalytic system into a practical setting.

It is important to develop robust and scalable fabrication methods, enhance the stability and selectivity of 2D catalysts, and explore novel 2D materials and hybrid structures in the future. Developing next-generation catalysts will require advanced characterization and theoretical modeling to understand catalytic mechanisms and guide rational design. Overcoming these challenges will unlock the full potential of 2D materials, enabling their application in energy, environmental, and industrial catalysis on a large scale.

Author contributions

Bhekumuzi Sfundo Khanyile: Conceptualization, Writing – original draft, Writing – review & editing.

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Conflict of interest

The authors declare no conflict of interest.

Data availability

No data is available.

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