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Exploring the Photocatalytic and Photovoltaic properties of 2D Materials: A Comprehensive Review

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Abstract
Two-dimensional (2D) materials have emerged as highly promising candidates for advanced energy conversion technologies due to their unique optical, electronic, and surface properties. This review presents an in-depth examination of the photocatalytic and photovoltaic potential of various 2D materials, including transition metal chalcogenides (TMDs), MXene, black phosphorus, and layered perovskites. Key material attributes—such as bandgap tunability, light absorption efficiency, and charge carrier behavior—are discussed in relation to their roles in solar energy harvesting and photocatalytic water splitting. The paper further explores recent innovations in heterostructure engineering, surface modification, and material synthesis strategies designed to boost energy conversion performance. Challenges such as long-term material stability, large-scale production, and interfacial optimization are critically assessed. Additionally, the review highlights future research pathways that may help translate laboratory-scale success into practical applications. By integrating findings from both experimental investigations and theoretical modeling, this work aims to provide a well-rounded perspective on the role of 2D materials in next-generation renewable energy solutions.

Key words: Density Functional theory, Non equilibrium Green's function, 2D materials, Energy storage, Electron transport

Introduction
Background
In the recent past, two-dimensional (2D) materials have received a lot of attention because they possess unique physical properties, chemical properties as well as electronic properties. These mainly metallic or semiconducting materials

have electronic structures that are in a single or a small number of atomic layers and possess different and, in most cases, exceptional electronic properties from the bulk materials. Further, 2D materials can be categorized as materials with only one atomic layer in thickness; Graphene was discovered in 2004 and other layered materials including transition metal dichalcogenides (TMDs), hexagonal boron nitride (h-BN), and black phosphorus (BP) show potential for photocatalytic and photovoltaic applications. Photocatalysis – the technique by which one or more chemical reactions are driven by light- is a more substantial process that finds its use in environmental engineering and energy solutions. Photovoltaics, on the other hand, are systems that embrace the direct conversion of light directly into electricity which is the very basics of renewable power solutions. The characteristics that are intrinsic to 2D material such as high surface area, electronically addressable surface and high charge carrier mobility qualify these applications.
The presence of two-dimensional (2D) materials has changed many scientific and engineering fields because of their remarkable electronic, optical and catalytic characteristics. Of all these materials, graphene, transition metal dichalcogenides (TMDs), and black phosphorus materials have attracted interest in photocatalytic and photovoltaic applications. Geim and Novoselov's discovery in 2004 of a completely new form of carbon material, called graphene, opened a new epoch in material science as a new class of materials that are a layer of atoms thick are found to possess extraordinary electronic properties, and indeed physics too has a two-dimensional world (Geim & Novoselov, 2007). Since then, the development of the physics and chemistry of single and multilayer 2D materials has grown dramatically and has witnessed an astonishing range of functionalities with possible technological applications.

Significance of Photocatalytic Properties

Photocatalysis which means the enhancement of a photoreaction through a photocatalyst, is an essential procedure for various environmental and energy uses. 2D materials have also been found to be excellent photocatalysts because of their highly large surface area and the ability to adjust band positions relative to the solar spectrum and efficient charge transport. For instance, graphene oxide and its derivatives have earlier on been shown to eliminate organic pollutants by the use of UV light (Zhang et al., 2015). Moreover, the use of TMDs akin to MoS also exhibits outstanding photocatalytic activity in water splitting and the abatement of contaminants thus qualifying them for efficiency and sustainability in environmental cleaning (Zhu et al., 2016).

Importance of Photovoltaic Properties

Another application that has received much attention is photovoltaics, the conversion of light into electrical electricity with 2D materials exhibiting significant potential in the field. High device mobility and the ability to control the bands for these 2-D-based materials prove valuable in photovoltaics. For instance, the band gap of TMDs depends on the number of layers and when a strain is applied, the efficiency of TMDs as light absorbers in PVs is significantly improved (Mak et al., 2010). By itself, graphene has a zero band gap and thus it is nearly always used to create heterojunctions to enhance the efficiency of photovoltaic applications (Gao et al., 2012).

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Challenges in 2D Materials for Photocatalysis and Photovoltaics

Nevertheless, some challenges should be solved to make the best 2D materials for photocatalytic and photovoltaic activities. As a result, the challenges arising when organizing synthesis at the molecular level include stability under operating conditions, scalability of synthesis, and compatibility with existing technologies. For example, although graphene-based photocatalysts possess high activity, the stability issue of photocatalysts in aqueous solution may be an issue (Zhu et al., 2018). Likewise, the performance of TMD-based photovoltaic devices can be reduced due to several factors including the lack of proper interface with electrodes and photodegradation under continuous illumination (Wang et al., 2018).

Objective

The purpose of this review is to provide an accurate account of the current understanding of photocatalytic and photovoltaic properties of 2DMs. The primary objectives are

1. To reveal the intrinsic properties of 2D materials that affect photocatalytic and photovoltaic activities.
2. To revisit the recent progress in the synthesis and characterization of 2D materials for the above-mentioned applications.
3. To highlight the current issues as well as potential opportunities of 2D materials on application in photocatalytic as well as photovoltaic systems.

As the scope of this review, this paper intends to describe systematically the photocatalytic and photovoltaic performances of 2D materials. This will include aspects such as new developments, breakthroughs and discoveries, how they work, issues affecting these fields together with their promising future. In this paper, the present literature on 2D materials is systematically reviewed to provide future research directions for enhancing the applicability of 2D materials in photocatalysis and photovoltaics.

Scope and Organization

As a result, the review consists of two major chapters only. The introduction offers a general understanding of the topic under discussion as well as stating its relevance before delving deep into the literature review section. When performing the literature review chapter, it is crucial to place the emphasis on the recent investigations sort them based on the types of material and look through the significance of the outcomes again. The structure outlined below is planned to offer a rational and sequential manner in which to dissect the photocatalytic and photovoltaic properties of 2D materials.

New Development of Photocatalysis

This has led to breakthroughs in photocatalytic systems based on 2D material, which now focus on the enhancement of the efficiency and stability of the systems. For instance, the example of the synthesis of new photocatalysts based on hybrid materials based on 2D materials and nanostructures was shown as a potential approach to the improvement of photocatalytic activity (Li et al., 2020). In addition, the techniques of synthesizing materials such as chemical vapor deposition and liquid-phase exfoliation helped in enhancing the control of the

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peculiar characteristics of the material, which in this case gave benefits in performance for photocatalytic applications (Liu et al., 2021).

New trends in photovoltaic system

In the photovoltaic area, research project updates that the usage of 2D material for solar cells is progressing. There has been evidence that TMDs when buried in the heterojunction and tandem solar cells perform better than the usual materials the main evidence being Ryu et al., 2020. Also, the advancement of 2D materials and particularly, the ability to understand the processing of 2D materials and the fabrication of photovoltaic devices using these materials has demonstrated better performance and stability of these devices (Zhang et al., 2021).

Future Directions

Subsequently, potential future work on 2-dimensional materials in photocatalytic and photovoltaic applications will focus on considerations of material degradation, as well as integration into the system. The novel material, hybrid systems, and fabrication techniques that have been incorporated into the improvement of the material design are anticipated to play a central role in the advancement of these technologies (Chen et al., 2022). This program has been receiving contributions from chemistry, physics, and engineering disciplines which will continue to improve the findings.

Literature Review

Overview of Photocatalytic Properties of 2D Materials

Photocatalysis can be related to the photocatalytic process whereby a photocatalyst is used to enhance the photoreaction in processes like degradation of environmental pollutants and generation of energy. Besides, the photocatalytic performance also established that 2D materials possess a high surface area as well as unusual electronic characteristics. Photocatalytic degradation has for instance been studied using Graphene oxide for example in the degradation of organic pollutants. In a similar study, Zhang et al. (2015) concluded that graphene oxide contributes to the photodegradation of methylene blue and as such could be used as water purification material.

Transition Metal Dichalcogenides (TMDs) in Photocatalysis

TMDs such as MoS2_22 and WS2_22 are potential photocatalytic materials resulting from their layered structure and tunable band gaps. In this respect, Zhu et al., (2016) found that MoS 2 _22 has high efficiency of carrying out water-splitting reactions because it has photocatalytic activity under visible light and can separate charges. Somewhat similar to WS2_11, WS2_22 shows the capability to generate photocatalytic hydrogen, which means it is suitable for use in the renewable energy industry (Liu et al., 2018).

Graphene-Based Photocatalysts

Graphene as well as graphene oxide and reduced graphene oxide, is also a potential photocatalyst. The photocatalytic activity of the re-doped graphene oxide has been found to be higher than that of the raw material graphene oxide due to enhanced electrical conductivity and surface area, Kumar et al., 2017.

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Furthermore, for higher photocatalytic efficiency, the graphene–metal nanoparticle composites have been introduced (Wang et al., 2019).

Photovoltaic Properties of 2D Materials

2D material photovoltaic is determined by the process of converting light to electricity. Graphene possesses the disadvantage of zero band gap that can nevertheless be used as a base for forming heterojunctions with other materials which enhance the properties of photovoltaic cells. Electronic application of graphene Gao et al. showed that the incorporation of graphene as electrode material in the fabrication of organic photovoltaic cells can greatly improve its performance.

TMDs in Photovoltaic Devices

Other TMDs such as MoS2_22 and WS2_22 have also shown the potential to be used in photovoltaic devices because they possess direct band gaps and exhibit high carrier mobility. The first principles calculations which were presented by Mak et al. (2010) also revealed the direct band gap and strong light absorption of monolayer MoS2_22 suggesting its potential use in photodetectors and solar cell applications. Moreover, the latest works on TMD-based solar cells also aim to optimize its efficiency through various approaches such as design engineering of the device structure (Ryu et al., 2020).

Hybrid and Composite Materials

The incorporation of 2D materials with other types of nanomaterials has often led to photocatalytic activities as well as photovoltaic performances being boosted. For example, the incorporation of graphene with TMDs has been studied to enhance the photocatalytic capability and efficiency of the Photovoltaic system as reported by Li et al., 2020. These composite systems are preferred since they incorporate favorable characteristics of the components and thus they possess high photocatalytic activity and photovoltaic conversion efficiency.

Challenges in the area of Photocatalysis and Photovoltaics

However, there are a few drawbacks which are proving to be challenging if the 2D material has to be put to real use. There are still questions including material stability, scalabilities of the synthesis as well as the integration into today's technologies that have been posed. For example, while TMDs display an excellent photocatalytic performance, their photostability often becomes an issue when the photocatalytic process is performed for a long time (Wang et al. 2018). Similarly, there are challenges affecting the efficiency of photovoltaic devices fabricated from 2D materials for instance; inadequate interface contact and degradation amongst others as highlighted in Zhang et al., 2021).

Future Directions and Research Opportunities

It can be expected that future research within the area of application of 2D materials for photocatalytic and photovoltaic processes will address these issues. In particular, research on topics like new material design 2D and improved fabrication technology will be important. In the same vein, interdisciplinary work that addresses chemical, physical and engineering methodologies will remain

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relevant in the furtherance of this field (Chen et al., 2022).

Key Findings
All in all, 2D materials have great promise to boost the capabilities of photocatalytic and photovoltaic technologies. Some of the recent studies have focused on aspects such as the unique characteristics of graphene, MoS2_22 and WS2_22 and its use in the environment and energy sector. However, challenges presumably to be faced when it comes to the stability of materials and reliability of the devices will be critical to the actualization of these benefits.

Methodology
Literature Search Strategy
To gather information used to prepare the final review of the photocatalytic and photovoltaic properties of 2D materials, a literature search was performed. The following databases were utilized: Hence, sources like Scopus, Web of Science, Google Scholar and IEEE Xplore can be considered as the most appropriate ones. This was achieved by using certain terms including "photocatalytic properties of 2D materials," "photovoltaic properties of 2D materials," "2D materials in photocatalysis," and "2D materials in photovoltaics." The articles that were sourced were specifically from peer-reviewed journals that are indexed from the period between 2010 and 2024 containing the most recent innovations.

Inclusion and Exclusion Criteria
Articles were included if they met the following criteria:
1. Consequently, a subset of these fields is concerned with the photocatalytic or photovoltaic behavior of 2D materials.
2. Published in peer-reviewed journals.
3. In the case of an application of the article in the field of photocatalysis or photovoltaics, provide experimental or theoretical data on 2D materials that can be used for these purposes.

Data Extraction and Analysis
Data extraction involved the following steps:
1. Identification of Key Properties: The properties crucial for photocatalysis and photovoltaics were defined and grouped: band gap, charge mobility and surface area.
2. Data Extraction: In this research, experimental conditions, materials synthesis and performance data were obtained from the chosen articles.
3. Comparative Analysis: The photocatalytic activity of different 2D materials was compared according to the degradation rates, quantum yields and photovoltaic properties such as the power conversion efficiency and the fill factor.

Synthesis and Interpretation
The synthesized data generated were grouped in tables and charts to show trends and patterns. The obtained materials were sorted according to the given performance indicators as well as fields of usage. A comparison was also conducted among the different subcategories of 2D materials including graphene, TMDs, and other layered materials regarding photocatalytic and

photovoltaic applications. The theoretical predictions and other experimental results were compared to reveal the fundamental factors that influence the characteristics of 2D materials.

Limitations

Exceptions and drawbacks identified in the review include variation of the experimental conditions, differences in the approach to measurements, and insufficient data on the long-term stability of some 2D materials. There are some important considerations, which should be taken into consideration regarding the generalizability of the findings.

Results and Discussion

Overview of 2D Materials in Photocatalysis

Graphene and transition metal dichalcogenides including MoS2, WS2 and TiS2 belong to the category of 2D materials which have a high potential in photocatalytic reactions. Graphene-containing electrodes because they are offer a large surface area and good electronic conduction to degrade organic pollutants under the visible light irradiation. For example, Wu et al. (2021) designed a visible-light-driven graphene oxide-based photocatalyst capable to decompose over 90% methylene blue dye within 60 min (Wu et al., 2021).

As a result, TMDs possessing direct bandgap and high absorption coefficients including MoS2_22 exhibit high photocatalytic activity. For MoS2_22 nanoflakes, the photocatalytic hydrogen evolution rate was recorded to be 10 as stated by Zhang et al. (2022). Regarding the photocatalytic activity they claimed the conversion efficiency of CO2 as 5 µmol·h−1^{-1}−1 when using the visible light (Zhang et al., 2022). They have such characteristics that suggest their future capability of sustainable hydrogen generation.

Solar Characteristics of Two-Dimensional Materials

In photovoltaic applications, 2D materials including perovskites, graphene and transition metal dichalcogenides have been considered. Organometal halide perovskite-based 2D materials have demonstrated high PCEs. Li et al. (2023) achieved a PCE of up to 23 % as mentioned earlier in the present paper as well. A 5% efficiency level in perovskite/graphene hybrid solar cells is achieved, which is even higher than many traditional silicon-based cells (Li et al., 2023).

Transition metal dichalcogenides equally have good photovoltaic performances. For example, MoS2_22 has been employed in the synthesis of flexible photodetectors with multisensory, high responsivity, and fast response to signals. The sensitivity of MoS2_22 photodetectors was found to be 4 according to the work of Xu et al. (2022). Among them, the most significant laser output power was measured to be 2 A/W at the wavelength of 650 nm (Xu et al., 2022).

Relative Performances and Reality's Mechanism

The comparative analysis shows that although graphene possesses superior electronic properties and high surface area which is favourable for photocatalysis, TMDs usually exhibit considerably higher photocatalytic activity as a result of their appropriate band gaps and improved light capture. Likewise, TMDs and perovskites have the highest absorption coefficients and scalable band gap therefore, they are leading in photovoltaic applications.

The theoretical analysis reveals that the enhancement of photocatalytic activity of 2D materials depends on processes like charge carrier dynamics, surface characteristics and light-materials interaction. For example, MoS2_22 has a direct band edge excited attribute, and charge separation and transfer rates which enable faster formation and separation of electron-hole pairs (Zhang et al., 2022).

Future Directions

Further studies should be dedicated to enhancement of stabilities and the commercial potentiality of 2D materials. The incorporation of 2D materials with other semiconductors and/or metals may improve the performance of the integrated device to a larger extent. However, long-term stability, and the synthesis of these materials at lower costs for large-scale applications, long-term stability studies and cost-effective synthesis methods are necessary to enable the commercialization of these materials in photocatalytic and photovoltaic areas.

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