

# 2D Semiconductor Nanostructures for Solar-Driven Photocatalysis: Unveiling Challenges and Prospects in Air Purification, Sustainable Energy Harvesting, and Water Treatment

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The use of solar light to accelerate chemical processes (photocatalysis) has the potential to alleviate the pollution and energy crises. Thanks to their large surface area, unusual electronic structure, and abundance of low-coordinate surface atoms, 2D semiconductors have shown enormous promise in photocatalytic applications. The synthesis, photoexcitation processes, design, and development of 2D semiconductor photocatalysts are thoroughly examined in this perspective, as well as their possible applications in air purification, solar energy conversion, organic synthesis, carbon capture and storage, and water treatment. This work highlights ongoing research efforts focused on improving the selectivity and efficiency of photocatalytic applications based on 2D semiconductors by means of hybrid systems, heterostructures, doping, and computational methodologies, together with open challenges. Finally, the integration of 2D semiconductor photocatalysts into indoor and outdoor environments is discussed, thereby facilitating the purification of air and water and generating clean energy, which assists in the pursuit of sustainable development objectives.

## 1. Introduction

One possible solution to the problems of energy shortage and pollution is photocatalysis, which uses sunlight to accelerate chemical processes.<sup>[1–7]</sup> Since the pioneering discovery of the photocatalytic water splitting capacity of a TiO<sub>2</sub> electrode in 1972,<sup>[8]</sup> the scientific community has widely explored the potential of light for both sustainable energy generation and tackling environmental challenges.<sup>[9]</sup>

Semiconductors have always been crucial in photocatalysis,<sup>[5]</sup> due to the presence of a band gap. Currently, with the energy needs growing and environmental pressures escalating,<sup>[10]</sup> there is a pressing need to improve the efficiency and adaptability of photocatalytic materials. 2D semiconductors are suitable candidates for such aims.<sup>[11–23]</sup> Specifically, 2D semiconductors, characterized

by their large surface area, abundant low-coordinate surface atoms, and unique electronic configurations, have shown immense promise for redefining the boundaries of photocatalytic performance.<sup>[11–21]</sup> Their thinness ensures shorter electron and hole migration paths,<sup>[24]</sup> whereas their abundant number of surface defects offer more active sites for the reactions.<sup>[25]</sup> Moreover, their electronic properties can be fine-tuned using various strategies (exfoliation,<sup>[26]</sup> strain,<sup>[27]</sup> or doping),<sup>[28]</sup> paving the way for tailoring photocatalytic solutions for diverse applications. In processes ranging from water splitting<sup>[20,23,29,30]</sup> and CO<sub>2</sub> reduction<sup>[16,31,32]</sup> to N<sub>2</sub> fixation,<sup>[33,34]</sup> 2D semiconductors are poised to drive advances in photocatalysis.

This Perspective explores the compelling area of 2D semiconductor photocatalysts to provide a comprehensive overview of recent experimental and theoretical findings in the field and provide an outlook for 2D photocatalysts for environmental sustainability.

### 1.1. Photoexcitations in 2D Semiconductors

Understanding the photoexcitation process plays a crucial role in assessing the performance of materials in photocatalysis.<sup>[35]</sup>

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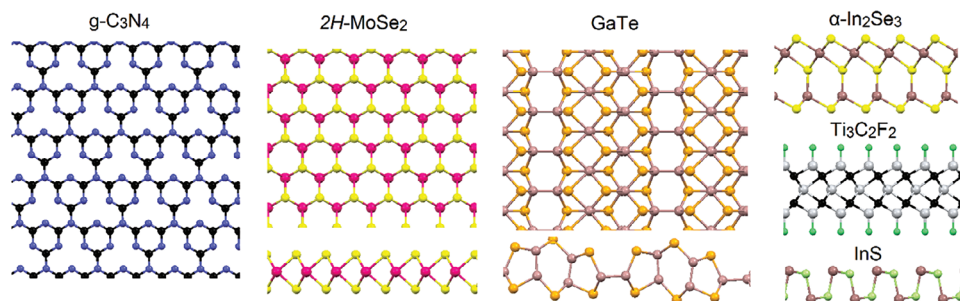
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**Figure 1.** Atomic structures of the most representative configurations of 2D systems discussed in the text.

Focusing on bulk semiconductors, the process of photoexcitation involves photon absorption and the generation of electron-hole pairs, which can either recombine or drive chemical reactions. The absorption of photons and the generation of electron-hole pairs can occur either on the surface or in deeper areas of bulk semiconductors. In the latter case, migration of the electrons to the surface corresponds to possible recombination between electrons and holes and scattering of photoelectrons on various defects of the lattice. In contrast, atomically thin 2D semiconductors (several representative examples are shown in **Figure 1**) provide new pathways. In the case of strong electron-hole interactions, owing to the pronounced Coulomb forces at play, charge carriers are closer than those in bulk materials, enabling the generation of excitons or bound pairs of electrons and holes. The energy landscape and behavior of these excitons set them apart from regular carriers.

In the process of photocatalysis shown in **Figure 2**, excitons play an ambivalent role.<sup>[36]</sup> Although their presence can impede the separation of charge carriers, thereby potentially diminishing the photocatalytic activity, under certain conditions, they may facilitate multi-electron transfer reactions.

The large surface areas of 2D semiconductors, coupled with their atomic thicknesses, also have significant implications for light absorption and carrier dynamics. These materials can absorb a substantial fraction of incident light, leading to high electron-hole pair generation rates. Moreover, the reduced di-

imensionality ensures that these carriers travel shorter distances to reach the surface, minimizing recombination losses. The combination of high carrier generation rates and reduced recombination pathways can significantly enhance the photocatalytic efficiency of 2D materials.

Furthermore, the electronic structures of 2D semiconductors are highly tunable. The band structure of these materials can be modulated by introducing defects (usually perforations),<sup>[37,38]</sup> doping with heteroatoms,<sup>[39]</sup> or creating heterostructures.<sup>[40]</sup> Such modifications can influence the light absorption spectrum, carrier lifetime, and reactivity of 2D semiconductors, allowing tailored photocatalytic solutions for specific applications.<sup>[41]</sup>

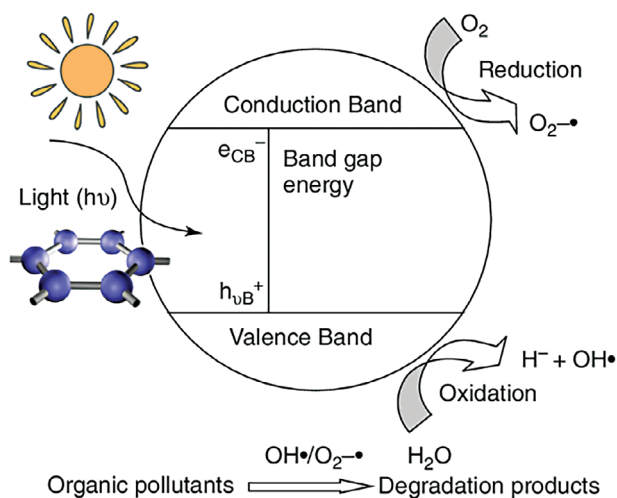
In addition to these intrinsic properties, external factors such as the surrounding environment,<sup>[36]</sup> interaction with substrates or co-catalysts,<sup>[42]</sup> and applied external fields<sup>[3]</sup> can further influence the photoexcitation processes in 2D semiconductors. For instance, the presence of a dielectric environment can screen Coulomb interactions and alter exciton properties of excitons.<sup>[43]</sup> Similarly, interactions with substrates can introduce charge transfer dynamics, influencing the reactivity of photogenerated carriers.<sup>[44]</sup>

## 2. 2D Photocatalyst Design and Development

The absence of a bandgap in graphene has led researchers to investigate alternative 2D photocatalytic materials. In particular, photocatalysis with transition metal dichalcogenides (TMDs),<sup>[45–48]</sup> metal oxides,<sup>[49–51]</sup> layered double hydroxides (LDHs),<sup>[52–56]</sup> hexagonal boron nitride (h-BN),<sup>[57–59]</sup> graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>),<sup>[60–63]</sup> MXenes,<sup>[64–66]</sup> and black phosphorus<sup>[67–69]</sup> has been reported for many reactions, such as water splitting,<sup>[70]</sup> CO<sub>2</sub> reduction,<sup>[71]</sup> N<sub>2</sub> fixation,<sup>[72]</sup> organic synthesis,<sup>[73]</sup> and pollutant removal.<sup>[74,75]</sup>

The synthesis of 2D materials, including 2D semiconductors, can be achieved via top-down or bottom-up approaches.<sup>[76]</sup> In top-down methods, bulk crystals are exfoliated to produce atomically thin layers.<sup>[77]</sup> In contrast, hydro/solvothermal synthesis, surfactant-assisted self-assembly, template-based approaches, interfacial synthesis, and chemical vapor deposition have been used to assemble atoms or molecules into 2D structures using a bottom-up strategy.<sup>[78]</sup>

Despite advances in 2D photocatalytic nanomaterial fabrication, the reaction rates for key activities, such as water splitting and CO<sub>2</sub> reduction, remain unsatisfactory for practical applications.<sup>[79]</sup> For technological transfer to the chemical sector,



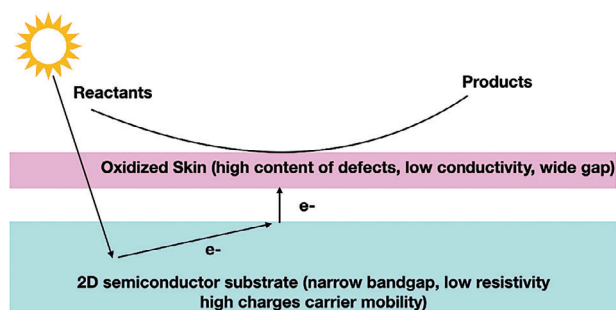
**Figure 2.** Schematic of photocatalysis using 2D semiconductor.

2D photocatalysts must have reaction rates at least 100 times higher than the present standard.<sup>[24]</sup>

## 2.1. Theoretical Modeling

The traditional iterative approach to synthesize catalysts and photocatalysts, which involves extensive screening and subsequent modifications, is gradually being complemented by computational methodologies. These computational strategies, guided by parameters such as efficiency, selectivity, and cost, exploit advanced simulations, and are widely available at reasonable cost computer clusters to screen potential catalytic materials.<sup>[80]</sup> Density functional theory (DFT)-based first-principles calculations have become the instrument of choice for exploring material properties and understanding catalytic mechanisms at various scales.<sup>[81]</sup> An advantage of DFT calculations is the minimal data from experiments required for starting the simulation of structures. In contrast to semi-empirical methods, only the chemical structure of the simulated materials is essential for starting calculations.<sup>[82]</sup> Other non-technical parameters for the simulations were derived from the quantum mechanical calculations of the atoms. The initial crystal structure (obtained in experiments or proposed by researchers) was used to optimize the atomic positions and lattice parameters and to determine the most energetically favorable structure of the considered compounds. Thus, the catalytic properties of hypothetical materials can be evaluated using DFT-based simulations. Note that standard DFT-based calculations consider either strong (covalent, ionic, or metallic) or weak (hydrogen or van der Waals) chemical bonds.<sup>[83,84]</sup> Standard first-principles calculations consist of determining the most energetically favorable atomic structure of the materials with the following calculation of the physical properties, such as the width of the bandgap.<sup>[84,85]</sup> Current computational frameworks include distinct approaches to simulating defects (intrinsic, such as vacancies, and extrinsic, such as impurities).<sup>[86,87]</sup> In recent years, an approach for simulating the interfaces between 2D materials and substrates has been extensively developed. The reciprocal influence of the formation of the interface on the electronic structure of the substrate and cover can be evaluated numerically.<sup>[88]</sup>

DFT-based calculations are also feasible for simulating chemical reactions. For this purpose, simulations of the atomic structures and total energies of the reactants and products were carried out. The enthalpy of the reactions is calculated as the difference between the sum of the total energies of the products and the reactants. Simulations of transition states are also possible; however, this type of calculation is much more computationally expensive. In recent decades, calculations of the pathways of various reactions, such as hydrogen and oxygen evolution reactions in different media (acidic and alkaline), have been developed for metal-based catalysts and successfully used to screen the catalytic properties of 2D materials.<sup>[81,89]</sup> Based on the calculation results, one can conclude which reaction and in which media the studied material is most suitable. Another recent improvement in the area of DFT-based modeling of catalytically active 2D materials is the development of an approach to simulate the chemical stability of the systems under consideration. For this purpose, adsorption and subsequent decomposition of oxygen or water



**Figure 3.** A scheme of formation of surface heterostructure due to oxidation of utmost layers.

molecules are modelled.<sup>[90]</sup> Theoretical calculations can also be used to predict the effect of surface oxidation on catalytic,<sup>[91]</sup> sensing,<sup>[92]</sup> and optical properties.<sup>[2]</sup> Based on the simulation results, the effect of surfaces oxidation on various physical properties and catalytic performance (**Figure 3**) can be simulated.

## 2.2. Heterostructures and Hybrid Systems in 2D Photocatalysis

Heterostructures of 2D semiconductors (vertical or lateral<sup>[93]</sup>) may adjust their electronic characteristics and provide new functions that the individual layers cannot.

Vertical heterostructures align the bands by stacking 2D materials.<sup>[94,95]</sup> Photoinduced electron-hole pairs are spatially separated by this band alignment, minimizing recombination and increasing the charge carrier mobility. For example, interfacing graphene with transition metal dichalcogenides (TMDs) has been demonstrated to boost charge separation and transfer, subsequently enhancing photocatalytic hydrogen evolution reactions.<sup>[96,97]</sup> The oxidation of the surface can also lead to the formation of semiconductor-oxide heterojunction, as shown in **Figure 3**.

In contrast, lateral heterostructures refer to an adjacent assembly of diverse 2D materials, creating a junction that boasts distinctive electronic characteristics. Such structures can introduce p-n junctions, which can be exploited for directional charge transfer, further enhancing the efficiency of the photocatalytic reactions.<sup>[98]</sup>

Blending 2D materials with nanostructures or molecular species may boost the photocatalytic activity. The excitation of the localized surface plasmon resonance (LSPR) by light irradiation may concentrate and enhance the electromagnetic field at 2D semiconductors with plasmonic nanostructures,<sup>[99]</sup> optimizing light absorption and hot electron generation.

Hybrid systems using 2D semiconductors and molecular catalysts<sup>[100–102]</sup> are also intriguing because they combine the high catalytic activity related to light absorption in 2D semiconductors and charge separation. This synergy may increase the rate and selectivity of the photocatalytic reaction.

## 2.3. Self-Assembled Heterostructures formed by Native Oxides formed on the Surface of 2D Semiconductors

Recent works demonstrate experimentally and theoretically the formation of the oxide skin of a few nanometers on the surface

of various layered materials. These materials include metal dichalcogenides such as  $\text{SnSe}_2$ ,<sup>[103]</sup> monochalcogenides ( $\text{GaTe}$ ,  $\text{InSe}$ ,  $\text{GaSe}$ ,  $\text{GeSe}$ ,  $\text{InS}$ ),<sup>[1,2,104]</sup> and trichalcogenides ( $\text{In}_2\text{Se}_3$ ).<sup>[105]</sup> Experiments<sup>[2,103–105]</sup> demonstrate the presence of the surface oxide-like phase with a thickness of a few nanometers. Thus, surface oxidation can be described as a self-limited process. Theoretical simulations also prove the favorability of oxidation and predict outstanding catalytic and sensing properties of thin oxide layers supported by 2D semiconductors. Experiments validate these theoretical predictions for selected materials with oxidized surfaces. A possible mechanism of the catalytic efficiency of oxidized layers is the combination of chemical activity of the oxides doped by subsurface substrates with outstanding electrical properties of subsurface 2D semiconductors. Another peculiarity of oxidized layers is the larger width of the bandgap. Therefore, oxidized layers are transparent to sunlight and, hence, do not affect the photo-activity of 2D semiconductive substrate. Photo-electrons generated in the substrate migrate to the oxidized surface where they participate in various chemical reactions, as shown in Figure 3.

## 2.4. Air Purification with 2D Semiconductors

The severity of air pollution in metropolitan areas is increasing; therefore, innovative solutions are essential.<sup>[106]</sup> Particulate matter, nitrogen oxides, and airborne pollutants contribute to environmental deterioration and health problems. Conventional approaches to degrade these contaminants are frequently characterized by high energy use and very limited efficacy. Conversely, photocatalysis using 2D semiconductors is environmentally friendly and effective.

Reactive oxygen species (ROS), including hydroxyl radicals, are produced when electron-hole pairs are generated in oxidative environments during photocatalytic processes. These radicals possess significant oxidizing capabilities and can degrade various airborne pollutants into harmless compounds, including carbon dioxide and water. The abundant number of active sites in 2D semiconductors, enabled by their high surface-to-volume ratio, facilitates the adsorption and subsequent breakdown of contaminants.<sup>[107]</sup>

The incorporation of 2D semiconductor photocatalysts into the infrastructure of urban landscapes represents a paradigm shift. If facades or windows can be covered with 2D semiconductors (see the visionary representation in Figure 4) to filter air invisibly and continually, when exposed to sunlight or artificial light, the contaminants adsorbed to these surfaces will decompose, resulting in improved air quality. This passive air cleaning approach, which does not require the use of external energy, is consistent with the objectives of sustainable urban development.

Uncommonly neglected indoor air quality is an additional area where these photocatalysts may have a substantial influence. Benzene from paints and formaldehyde from furniture are examples of indoor contaminants that may be effectively destroyed by 2D semiconductor-based purification devices.<sup>[108]</sup> Integrating these devices into HVAC (Heat, Ventilation, Air Conditioning) units or running independently as air purifiers may protect inhabitants from respiratory ailments and other health dangers



**Figure 4.** Conceptual visualization intended to illustrate the potential application of 2D semiconductors in environmental purification processes when integrated into the structures of urban buildings. It must be noted that the representation of the hexagonal structure on the building facade is a highly magnified artistic interpretation, serving to convey the idea rather than the actual scale.

caused by indoor air pollution, thereby providing healthier indoor environments.

Future research could improve the selectivity and efficiency. Similarly, as synthesis processes scale up, incorporating 2D semiconductors into urban infrastructure and indoor purification systems will become more economically viable.

## 2.5. Carbon Capture and Storage using 2D Semiconductor Photocatalysis

Atmospheric  $\text{CO}_2$  levels are crucial in monitoring climate change. Therefore, global warming necessitates novel carbon capture and storage (CCS) methods.<sup>[109]</sup>

2D semiconductors can efficiently trap  $\text{CO}_2$  and safely store or convert it.<sup>[31,110]</sup> Sunlight can be used to catalyze  $\text{CO}_2$  reduction to produce hydrocarbons or other valuable chemicals.<sup>[111]</sup> The ability of 2D semiconductors to absorb a broad spectrum of light, combined with their efficient charge separation and transport properties, facilitates the activation and reduction of  $\text{CO}_2$  molecules.<sup>[112,113]</sup> Moreover, the tunable band structures of 2D semiconductors can be suitably exploited to match the redox potentials of  $\text{CO}_2$  reduction reactions,<sup>[114]</sup> ensuring the efficient and selective conversion of  $\text{CO}_2$  to the desired products (see Figure 5 for a sketch).

Beyond the direct reduction of  $\text{CO}_2$ , 2D semiconductors also offer potential for the capture and storage of carbon.<sup>[110]</sup> Their large surface areas and tunable surface chemistry can be harnessed to adsorb  $\text{CO}_2$  from flue gases or ambient air. Once captured,  $\text{CO}_2$  can either be converted using photocatalysis or stored in geological formations, ensuring long-term sequestration.<sup>[115]</sup>

However, selectivity for  $\text{CO}_2$  reduction reactions is a critical concern. Given the myriad of possible products from methane and ethylene to alcohols and carbonates, ensuring the selective production of a desired compound is crucial. Research efforts have focused on tailoring the surface properties of 2D materials,<sup>[116]</sup> introducing co-catalysts,<sup>[117]</sup> or modulating the reaction environment to achieve the desired selectivity.<sup>[118]</sup>



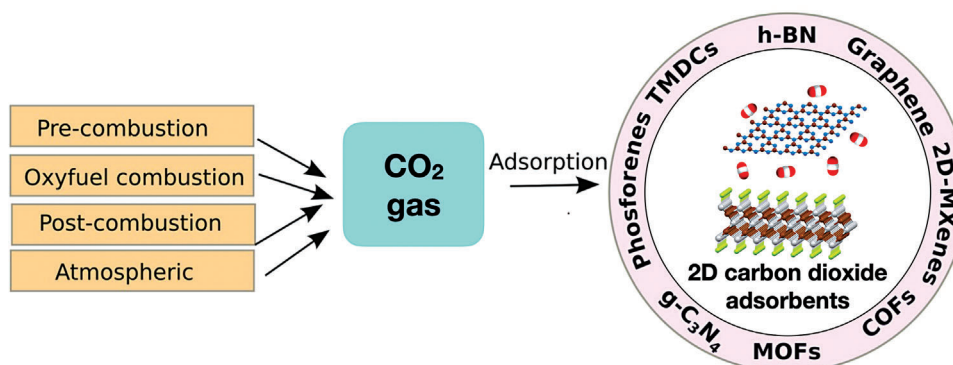


Figure 5. Carbon capture with 2D materials.

### 2.6. New Pathways for Organic Synthesis with Photocatalysis with 2D Semiconductors

Organic synthesis, which produces many compounds required for pharmaceuticals and agrochemicals, is regulated by dangerous reagents, high temperatures, and pressures.<sup>[119]</sup> 2D semiconductors-based photocatalysis<sup>[120]</sup> may enable lower-temperature processes while boosting selectivity and efficiency. As a matter of fact, redox-capable electron-hole pairs created in the photoexcitation process might help create or break chemical connections in organic compounds.<sup>[73]</sup>

2D photocatalysts excel in terms of functional group conversion and bond formation: oxidation, reduction, and halogenation can be performed more selectively and efficiently.<sup>[121]</sup>

Avoiding harmful chemicals and high temperatures and pressures has an evident positive environmental impact, as well as economic advantages arising from energy and resource savings. Selectivity also increases yields, minimizing waste and costs related to purification.

### 3. 2D Semiconductors in Photocatalysis for Water Purification

Remarkably, photocatalysis with 2D semiconductors also provides an innovative solution for water purification, overcoming the traditional limits of state-of-the-art methods (such as reverse osmosis<sup>[122,123]</sup>) for removing trace contaminants.

On the other hand, 2D semiconductor-powered photocatalysis degrades several pollutants by producing ROS, including hydroxyl radicals,<sup>[124]</sup> by exploiting the abundant number of active sites and large surface area of 2D semiconductor photocatalysts.

Photocatalytic disinfection powered by 2D semiconductors can also effectively inactivate pathogenic microbes,<sup>[125]</sup> such as viruses and bacteria, which cause most waterborne diseases,<sup>[126]</sup> thereby ensuring safe drinking water.<sup>[127]</sup> The reactive species generated during photocatalysis can damage the cellular structures of microorganisms,<sup>[65]</sup> rendering them harmless.

However, there is little evidence of the stability and recyclability of 2D materials in aquatic environments. Despite the outstanding photocatalytic characteristics of 2D materials, they are susceptible to degradation or loss of effectiveness when subjected to multiple cycles. Various research initiatives are currently

in progress to tackle this difficulty by implementing surface changes, protective coatings, and hybrid material designs.<sup>[128–130]</sup>

One such obstacle pertains to the possible discharge of nanomaterials into treated water (Figure 6). To avoid secondary contamination, nanomaterials must be efficiently separated and recovered after purification.

#### 3.1. From Lab to Market: Assessing the Scalability of 2D Semiconductor Technologies

In the assessment of the scalability of 2D semiconductors-based technologies, it is crucial to replicate the unique properties of these materials also in adjusted synthesis methods adequate to meet industrial demands, transitioning from small-scale lab syntheses to large-scale production. Scale-up requires a reassessment of production methods, material flow, and quality control

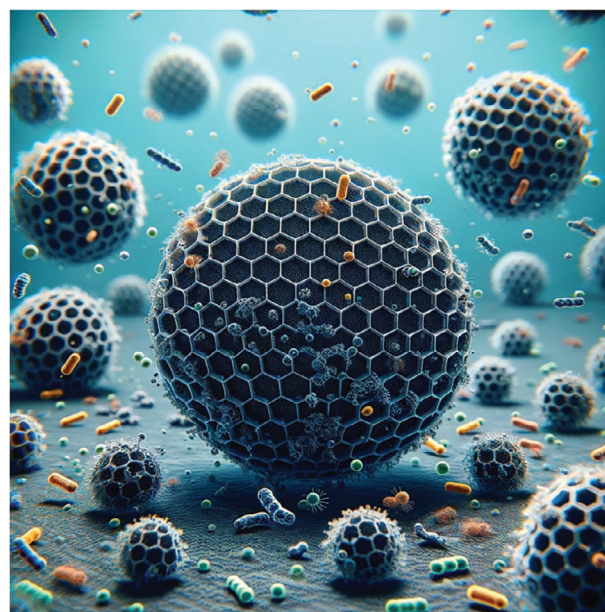


Figure 6. 2D materials-enabled filters for water purification. It must be noted that the representation of the hexagonal structure on the sponge is a highly magnified artistic interpretation, serving to convey the idea rather than the actual scale.

to maintain the essential properties of 2D semiconductors for photocatalytic purposes, such as defect density and surface area. The discussion on scalability should include the development of continuous production processes like roll-to-roll manufacturing. This could help integrate 2D semiconductors into current manufacturing lines, lowering the entry barrier in different markets.

The economic feasibility of 2D semiconductor technologies depends on their production cost, material durability, and performance effectiveness. The cost per unit area of semiconductor material is a critical factor that impacts the utilization of these technologies in environmental and energy applications. It is crucial to take into account not only the costs of raw materials and energy needed for synthesis but also the operational durability of these materials in real-world applications. A comprehensive cost analysis should compare the initial investment and operational costs with the benefits derived from the improved efficiency and performance of these materials in photocatalytic processes.

### 3.2. Conclusion and Outlook

Herein, we have discussed the potential of 2D semiconductors in photocatalysis, synthesis, photoexcitation processes, design, and development of 2D semiconductor photocatalysts, as well as their prospective applications in solar energy conversion, water treatment, and air purification. Nevertheless, insufficient reaction rates for CO<sub>2</sub> reduction and water splitting pose a challenge in enhancing selectivity and efficiency. Our focus is on the critical need for economically feasible approaches to incorporate these technologies into the municipal infrastructure and indoor purification systems.

In addition, 2D photocatalysis has a significant environmental impact on water purification and green energy generation.

The promise of 2D photocatalysis must be fully realized, despite the obstacles posed by its rapid development. The operational stability of the 2D materials is critical. Although these materials possess notable photocatalytic efficiency, their effectiveness diminishes with time, particularly when exposed to adverse conditions. This degradation is attributed to photocorrosion, accumulation of chemical intermediates, and structural damage.

Another concern is the recombination of electron-hole pairs created by light. Despite the shorter migration paths of these carriers in 2D materials, recombination continues to impede the effectiveness of photocatalysis. Thus, the design of heterostructures, doping, and surface modification may be beneficial.

Scalability of 2D photocatalysts is a concern. Although laboratory-scale synthesis processes are well established, industrialization is challenging. To encourage the use of 2D photocatalysts in practical applications, it is necessary to address their uniformity, large-scale availability with standard quality enabling reproducible results, and cost effectiveness.

Despite these challenges, 2D photocatalysis has many advantages, with novel possibilities enabled by the recent progress in science and technology. For example, the efficiency and selectivity of 2D semiconductor photocatalysts can be optimized by high-throughput computational screening of thousands of 2D semiconductors. Moreover, the combination of 2D semiconductors with plasmonic nanostructures and/or molecular catalysts could lead to further performance improvements.

Definitely, one can envision that photocatalysis with 2D semiconductors could become a leading tool for environmental remediation and sustainability in a few years.

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### Conflict of Interest

The authors declare no conflict of interest.

### Keywords

2D semiconductors, air purification, photocatalysis, surface science, water treatment

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