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# Future Challenges of Photocatalytic Water Splitting: Sustainability

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## *Abstract*

*Photocatalytic water splitting has emerged as a promising technology for sustainable hydrogen production through the direct utilization of solar energy. This process mimics natural photosynthesis, using semiconductor materials to absorb light and drive the decomposition of water into hydrogen and oxygen. The method provides a sustainable and eco-friendly solution to the global energy challenge by enabling the reduction of carbon emissions. Among various solar-to-chemical energy conversion approaches, photocatalytic water splitting to generate hydrogen stands out as a particularly promising option. This light-driven process is regarded as an ideal renewable technology, capable of yielding high energy output without reliance on fossil fuels. In photocatalytic water splitting, water undergoes a redox reaction facilitated by photo-generated electrons and holes, resulting in the production of hydrogen. This review outlines the fundamental mechanisms of photocatalysts used for hydrogen evolution from aqueous media and discusses recent strategies for developing photocatalysts responsive to visible light. Recent advances have focused on engineering band structures, heterojunction formation, and surface modification to enhance charge separation efficiency and visible-light absorption. The incorporation of co-catalysts, defect engineering, and nanostructuring techniques has significantly improved photocatalytic activity and stability. Moreover, computational modeling and in-situ characterization methods have provided deeper insights into charge carrier dynamics and reaction pathways. Despite these advancements, challenges such as low quantum efficiency, photocorrosion, and scalability remain critical barriers to commercialization. Continued research integrating materials innovation, reaction kinetics, and reactor design optimization is essential to achieve efficient, cost-effective, and sustainable hydrogen production through photocatalytic water splitting.*

**Keywords:** Photocatalytic water splitting; Hydrogen evolution; Semiconductor photocatalysts; Solar energy conversion; Visible-light activation

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## INTRODUCTION

The growing global demand for sustainable and environmentally friendly energy alternatives has driven significant research into renewable technologies that can serve as substitutes for fossil fuels and help combat environmental degradation. Among the available renewable energy sources, hydrogen has emerged as a leading candidate due to its high energy content and clean combustion, which yields only water as a byproduct. However, conventional hydrogen production methods, such as steam methane reforming, are still heavily reliant on fossil fuels and contribute substantial amounts of carbon dioxide to the atmosphere. The continuous rise in global population and improvements in living standards have substantially increased worldwide energy consumption. A large share of this energy is still derived from fossil fuels, particularly in the industrial and transportation sectors. This not only accelerates the depletion of finite carbon-based resources but also leads to massive emissions of greenhouse gases like carbon dioxide. Therefore, the shift toward renewable energy systems is essential to mitigate the adverse effects of fossil fuel consumption, such as global warming, energy insecurity, and market volatility.

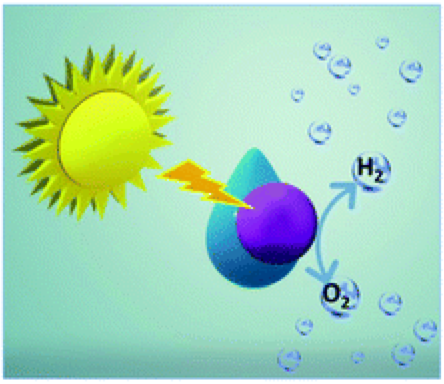

**Figure 1.** Photocatalytic water splitting.

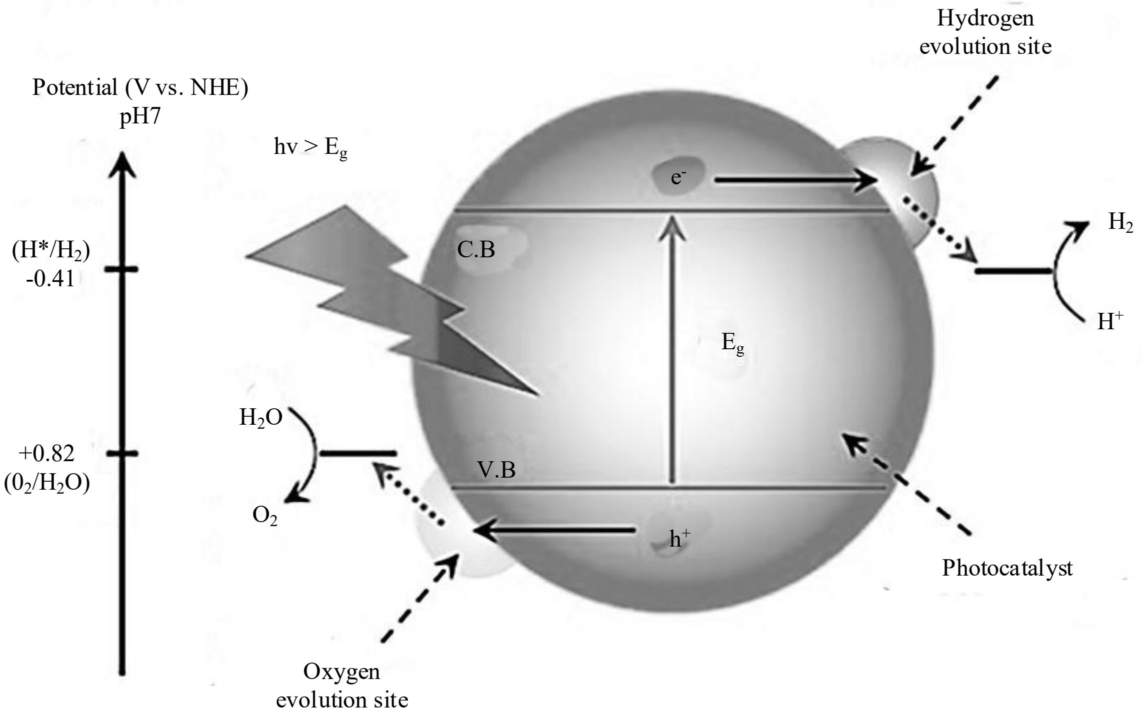

**Figure 2.** Photocatalysis using semiconductor water splitting.

Among various emerging technologies, photocatalytic water splitting (Figure 1) has gained prominence as a promising approach for hydrogen production. The breakthrough in this field came in 1972 when Fujishima and Honda first demonstrated the photo-assisted decomposition of water into hydrogen and oxygen using titanium dioxide ($TiO_2$). This discovery opened the door to the practical use of solar energy in driving chemical reactions. Since then, extensive research has been devoted to advancing fields such as photocatalysis and solar energy conversion.

In recent years, the strategic importance of hydrogen as a clean energy vector has been re-emphasized due to the pressing need to address global energy demands and the environmental impacts associated with conventional fuels. Photocatalytic overall water splitting—which involves generating both hydrogen and oxygen from water using sunlight—has attracted considerable attention as it offers a zero-emission route for renewable fuel production. Currently, two main strategies dominate successful photocatalytic systems: one involves the use of a single visible-light-responsive photocatalyst capable of providing sufficient redox potential to drive the complete water-splitting reaction.[1-5]

Effective production of hydrogen requires an efficacious interaction among light, catalysts as well as reactants. Photocatalysis begins with radiation of light consisting of energy more than or same as the band separation pertaining to a photo catalyst having features of a semiconductor, disconnecting vacant conduction band (CB) from occupied valence band (VB). Thus, the electrons generated under light irradiation participate in reduction while the holes take part in oxidation (Figure2).

Solar energy is renewable, free as well as unlimited due to which it is capable of producing heat or electricity without too much investment on maintenance or the necessity of costly parts. The utilization of energy in one year could be furnished by just a few minutes of exposure of the earth to solar irradiation. Successful overall water splitting via two step photo excitation by visible light[6-15] using several combinations of photo catalysts and electron relays has been reported.

The above results indicate that $Cr_2O_3$ modification is a highly useful technique for improving $H_2$ evolution activity in overall water splitting. Another co-catalyst for photo catalytic overall water splitting, Ni core/NiO shell nanoparticles, has been applied to many heterogeneous photocatalytic systems. It has several advantages, including the possibility of using various noble metals. Among the noble metals and metal oxides examined as nanoparticulate cores, Rh was the most effective at enhancing activity (Figure 3).[6-8]

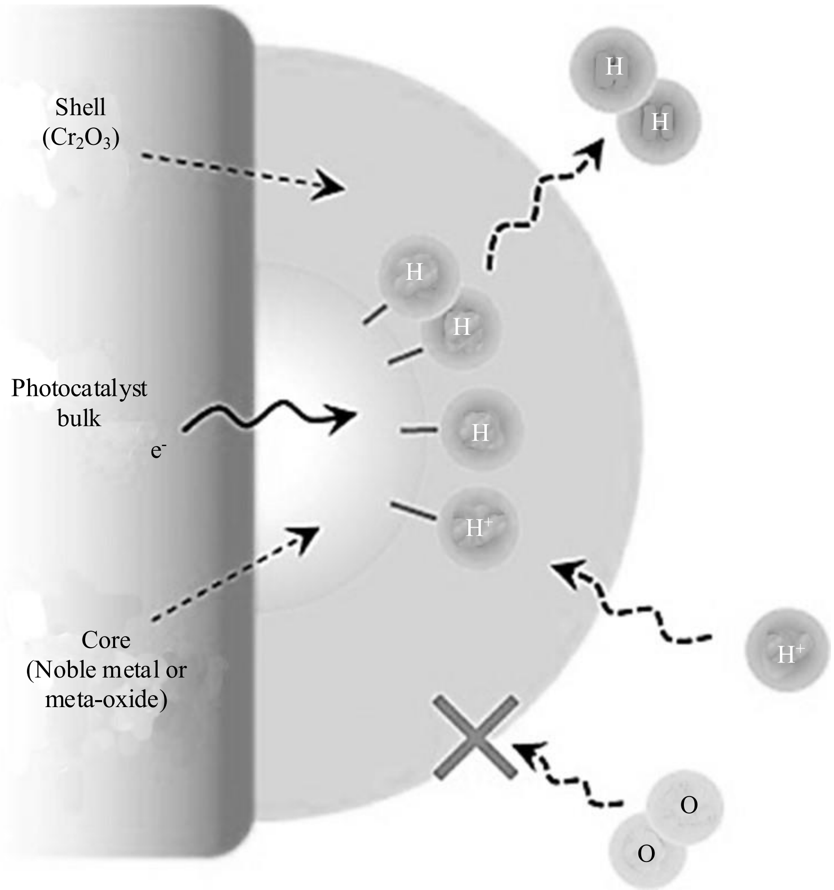

**Figure 3.** Photocatalysis of water splitting using catalyst

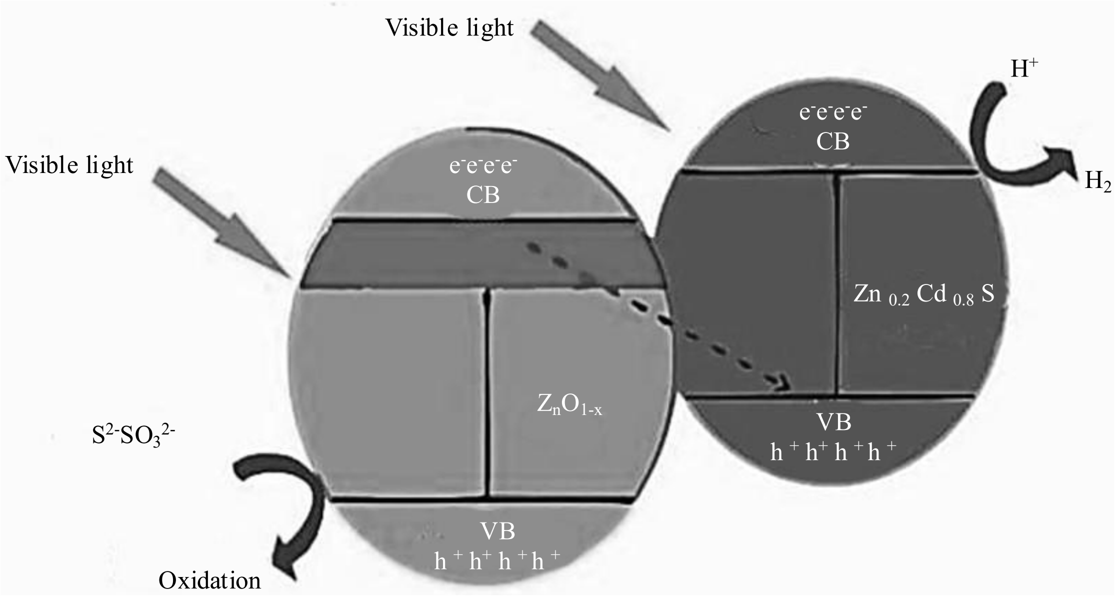

**Figure 4.** Photocatalysis of water splitting using catalyst

Future Prospects for Photocatalytic Water Splitting: As described above, in the search for visible-light- responsive photocatalysts, significant effort has been devoted to the development of active sites on photocatalysts and elucidating reaction mechanisms, leading to significant progress in the field of heterogeneous photocatalysis for water splitting. For efficient photocatalysis, the energy level of the acceptor must be lower than that of the conduction band in the semiconductor, ensuring favorable electron transfer. From a thermodynamic perspective, hydrogen evolution involves the hydrogenation of intermediate species, wherein photo-generated electrons reduce protons ($H^+$) at the active sites, leading to the formation of molecular hydrogen.

Titanium dioxide ($TiO_2$) is widely studied for water splitting due to its suitable band edge positions: the upper edge of its valence band is more positive than the $O_2/H_2O$ redox potential, while the lower edge of the conduction band is more negative than the $H^+/H_2$ redox potential. This alignment makes it theoretically ideal for overall water splitting. However, $TiO_2$ has a relatively large band gap of 3.2 eV, restricting its photoresponse primarily to the ultraviolet region, which constitutes only a small fraction of the solar spectrum.

To enhance its utility under visible light irradiation, $TiO_2$ must be modified. Approaches include doping with metal or non-metal elements, forming heterojunctions with other semiconductors, or employing structural modifications that enable band gap narrowing. These strategies aim to extend the material's light absorption into the visible range and thus improve its overall photocatalytic performance for hydrogen generation (see Figure 4).

A very advantageous fuel is hydrogen as it is available in adequate quantity from different renewable sources (biomass or water), it has huge energy yield, it is eco-friendly and possesses capability of high storage. Therefore, hydrogen is considered as a perfect and benign substitute as an energy source for fossil fuels.

## Material Sustainability and Resource Scarcity[9-10]

One of the major challenges in advancing photocatalytic water splitting lies in the sustainability of the materials used in photocatalyst development. Many high-performance photocatalysts rely on rare or expensive elements such as platinum, ruthenium, or iridium, which are not only scarce but also environmentally and economically unsustainable for large-scale applications. The global supply chain for such critical raw materials is limited, making the long-term availability and affordability of these components a serious concern. Moreover, the mining and processing of these elements can have significant environmental impacts, contradicting the green objectives of hydrogen production technologies. To address this, there is a growing need to develop earth-abundant, low-cost, and non-toxic alternatives that can match or exceed the efficiency of noble-metal-based systems. This includes exploring transition metal oxides, sulfides, carbon-based materials, and metal-free photocatalysts. Ensuring material sustainability will be essential not only for reducing environmental impact but also for enabling the scalable and equitable deployment of photocatalytic water splitting technologies globally.

## Water Resource Considerations and Contaminant Tolerance[11-13]

While photocatalytic water splitting offers a promising route to sustainable hydrogen production, the nature and quality of the water feedstock present significant challenges that must be addressed for practical deployment. Laboratory-scale demonstrations of water splitting typically use high-purity deionized or distilled water, often mixed with sacrificial agents to enhance photocatalytic activity. However, such ideal conditions are neither economically viable nor scalable for large-scale applications, especially in regions facing water scarcity or lacking access to purified water sources.

Given that freshwater resources are limited and already under stress from agriculture, industry, and population growth, it is critical to explore the use of non-traditional water sources, such as seawater, brackish water, wastewater, or rainwater, for photocatalytic hydrogen production. However, these sources often contain a variety of contaminants, salts, organic matter, and microorganisms, which can interfere with photocatalytic reactions, degrade catalyst surfaces, and lead to system inefficiencies or even catalyst poisoning.

For instance, chloride ions in seawater can participate in side reactions that generate reactive chlorine species, leading to the corrosion of photocatalyst materials and undesired byproducts. Similarly, organic pollutants in wastewater may compete with water molecules for active sites, thereby reducing hydrogen yield. Scaling, fouling, and biofilm formation on photocatalyst surfaces are additional concerns in non-purified water environments, often requiring pre-treatment steps that introduce additional energy and cost burdens.[14-15]

## CONCLUSION

Photocatalytic water splitting represents a groundbreaking approach for sustainable hydrogen production using abundant solar energy and water, offering a clean and renewable alternative to fossil fuel based hydrogen generation. However, despite these advances, the technology still faces major obstacles that hinder large scale application. The low solar to hydrogen conversion efficiency, poor stability of photocatalysts under real conditions and high material and fabrication costs remain critical challenges. Achieving efficient charge separation and low cost photocatalysts are essential for the future of this technology.For practical applications, photocatalysts must exhibit high photocatalytic activity and very stable photocatalytic performance. In the meantime, they can be easily attained and reused. The mechanism of water splitting and simulation model for hydrogen production need to be further investigated for hydrogen utilization. These areas create many opportunities and challenges for both in the basic and applied research field. With the development of science and technology as well as the untiring effort of the scientists from all over the world, the efficiency of photocatalytic water splitting will be further improved. And if this large scale hydrogen production from photocatalysts is successfully achieved, the world would benefit from the Hydrogen Economy.

In conclusion, while photocatalytic water splitting is still in its developmental phase, it holds immense potential as a sustainable, zero-emission energy technology. With continued interdisciplinary research and technological innovation, photocatalytic hydrogen production could become a key component of the global transition toward a clean and carbon-free energy future.

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