Learn from Photosynthesis: A Summary of Photocatalysis Mechanisms and Applications

Size Chen[1,a,*]

[1]Aquinas International Academy,3200 E Guasti Rd, Suite, Ontario, CA 91761, USA
a. 2899912044@qq.com
**corresponding author*

Abstract: Amid the surge in global energy demand and worsening environmental pollution, the development and utilization of renewable energy have become a research focus. Photosynthesis, as an efficient natural energy conversion process, has inspired the development of photocatalytic water splitting technology. This technology converts solar energy into chemical energy, playing a significant role in hydrogen production and renewable energy fields. This study delves into the materials and photoconversion mechanisms related to photocatalytic water splitting and explores its potential and challenges in environmental purification and industrial hydrogen production. This work provides a reference for further research and application of photocatalytic water splitting technology.

Keywords: photosynthesis, photocatalysis, water splitting, Z-scheme mechanism, industrial application

1. Introduction

Photosynthesis is a critical chemical reaction on Earth, providing energy for life globally. Investigating its mechanism not only enhances crop yields but also guides the development of optoelectronic devices, such as photovoltaics and photocatalysis. The light reaction stage of photosynthesis occurs on the thylakoid membrane in chloroplasts, where photosystem II (PSII) serves as the core component. The manganese (Mn) cluster in PSII plays a pivotal role in water splitting, oxidizing water molecules through redox reactions to release oxygen. During this process, the Mn cluster undergoes sequential oxidation, releasing electrons that are transferred via electron carriers to plastoquinone (PQ), forming a proton gradient that drives ATP synthesis. These reactions not only provide energy but also supply oxygen for the biosphere. In photosynthesis, the Z-scheme electron transport chain describes the sequential transfer of electrons through two photosystems during the light reaction stage (as shown in Figure 1). Each step in this chain has a distinct redox potential, ensuring the orderly transfer of electrons, which drives the production of ATP and NADPH [1]. The potential differences from PSII to PQ, from PQ to cytochrome b6f, and from PSI to $NADP^+$ collectively ensure the flow of electrons from high-energy states to low-energy states. This flow simultaneously drives the formation of the proton gradient, which provides energy for ATP synthesis.

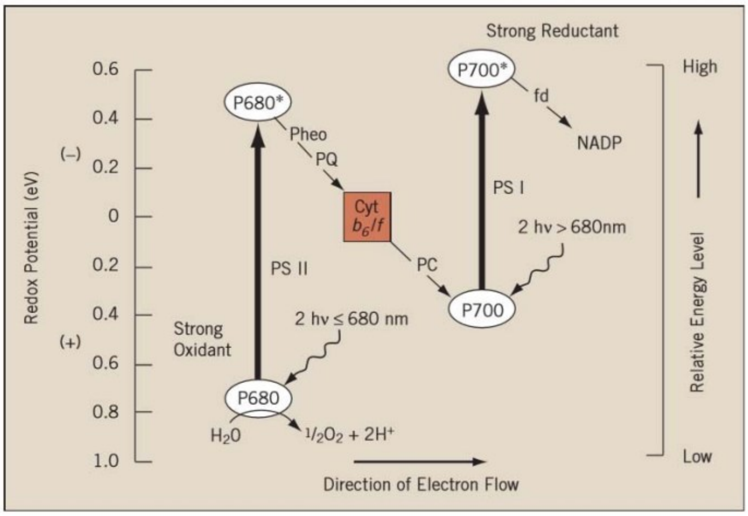

Figure 1: Schematic diagram of the Z-Scheme electron transport chain in photosynthesis

Photocatalysis technology mimics the reaction mechanism of photosynthesis by utilizing light energy to drive chemical reactions. Under illumination, photocatalysts generate electron-hole pairs, which initiate or accelerate chemical reactions. This process achieves efficient solar energy conversion and promotes the development of environmentally friendly chemical processes. The surface properties and band structure of photocatalysts directly influence light absorption, charge separation and transfer, and reaction efficiency. To enhance the performance of semiconductor photocatalysts, researchers have employed various strategies, such as metal doping, dimensional regulation, heterostructure construction, and cocatalyst loading. These strategies have improved photocatalytic performance, paving the way for applications in environmental protection, energy conversion, and other fields [2].

Titanium dioxide (TiO_2) is a common photocatalytic material, characterized by low cost, high photocatalytic activity, and non-toxicity. It is widely used in water treatment and air purification. Its photocatalytic activity [3] depends on the quantity of electrons and holes, and broadening its light absorption range is an effective way to enhance activity [4]. TiO_2 can excite electrons to transition from the valence band to the conduction band, generating electron-hole pairs that participate in water reduction and oxidation reactions. However, TiO_2 faces challenges in photocatalytic water splitting, including recombination of photogenerated electron-hole pairs, low utilization of ultraviolet light, and catalyst stability. These remain hot topics in the field of photocatalysis research.

2. Optimization Strategies for TiO_2 Photocatalytic Systems

Dye sensitization is a method to extend the light absorption range of TiO_2. By combining organic dyes with TiO_2, visible light can be effectively utilized to drive the water-splitting reaction. The basic principle of dye sensitization is that when dye molecules absorb visible light, electrons transition from the excited state to the conduction band and are injected into the conduction band of TiO_2, initiating water decomposition. This approach not only enhances the photocatalytic efficiency of TiO_2 but also enables its application across a broader spectrum range. However, the stability of dye molecules and their binding efficiency with TiO_2 remain aspects requiring further optimization [5].

Loading noble metals, such as platinum (Pt), on the surface of TiO_2 is another common method to improve photocatalytic efficiency. Noble metals, with their high work function, can form Schottky barriers, effectively separating photogenerated electrons and holes while facilitating hydrogen production. Noble metals can capture photogenerated electrons, reducing the probability of electron-hole recombination and thereby increasing water-splitting efficiency. Additionally, noble metal loading enhances the stability of the catalyst, extending its service life.

Apart from noble metal modification and dye sensitization, other modification techniques, such as element doping and heterojunction formation, are widely used to improve the photocatalytic performance of TiO_2. For instance, doping with metallic or non-metallic elements can adjust the bandgap structure of TiO_2, enhancing its ability to absorb visible light. Furthermore, heterojunction structures, through the synergistic effects of different materials, can effectively separate photogenerated carriers, reduce electron-hole recombination, and increase photocatalytic efficiency. Non-metal doping influences the energy band structure and energy level distribution of semiconductor materials, promoting the migration of photogenerated electrons to active sites and enhancing light absorption. Nitrogen atoms, for example, replace oxygen atoms in the TiO_2 lattice through the formation of Ti–N bonds [6], weakening orbital confinement on electrons and allowing faster electron and hole migration to the crystal surface for reactions [7].

3. Other Photocatalytic Materials

In addition to TiO_2, materials such as zinc oxide (ZnO) and bismuth vanadate ($BiVO_4$) have also received extensive attention in water-splitting research. ZnO is characterized by being non-toxic, inexpensive, easy to prepare, and having high catalytic activity, making it significant in the field of photoelectrochemical water splitting. Although ZnO shares similar photocatalytic properties with TiO_2, its conduction band position is higher, giving it stronger electron reduction capabilities. Under visible light, ZnO can absorb photons and generate electron-hole pairs, which participate in redox reactions, enabling pollutant degradation or water splitting. However, ZnO is less stable than TiO_2 in aqueous solutions and is prone to photo-corrosion. $BiVO_4$, as an economical and non-toxic semiconductor material, has a lower bandgap, strong visible light responsiveness, and high chemical stability. Under simulated sunlight, $BiVO_4$ exhibits excellent photoelectric conversion efficiency, with a theoretical photocurrent density of up to 7.5 mA cm^{-2} [8]. However, it faces challenges such as surface charge recombination, poor charge transport, and sluggish water oxidation kinetics, resulting in actual performance far below its theoretical value. To address these issues, researchers have developed a series of modification techniques to optimize $BiVO_4$ photoanodes, including element doping, morphology and facet regulation, heterojunction construction, and surface modification [9]. Nevertheless, due to its low conduction band position and insufficient electron reduction capability, $BiVO_4$ needs to be combined with other materials to improve water-splitting efficiency. The combination of ZnO and $BiVO_4$ can form a heterojunction structure, where the interfacial electric field and band structure alignment enable effective separation and transfer of photogenerated electrons and holes, enhancing photocatalytic performance. Further optimization of the $ZnO/BiVO_4$ heterojunction structure and performance can be achieved through techniques such as crystal facet engineering and defect regulation.

4. Current Status and Prospects of Water Splitting Applications

Photocatalysis technology dates back to 1972, when it was first discovered by Japanese scientist Akira Fujishima. Since 1999, with breakthroughs in nanotechnology, photocatalysis has become synonymous with environmental protection in developed countries. After years of research and development, Japan has achieved significant maturity in the technology and application of photocatalytic products. Photocatalysis technology is widely used in air purification, such as air purifiers and photocatalytic coatings. By applying photocatalysts to exterior and interior building surfaces, harmful substances like formaldehyde and benzene in the air can be decomposed, purifying indoor and outdoor air. For instance, some carriages of Japan's Shinkansen trains are equipped with

DOI: 10.54254/2755-2721/129/2025.20944

photocatalytic air purification systems, which effectively improve air quality inside the carriages. Moreover, photocatalysis has achieved remarkable results in water purification. Using titanium dioxide (TiO_2) photocatalysis technology, organic pollutants in water can be degraded. Researchers at Chiba University in Japan have developed TiO_2 photocatalytic film-coated beads, which enable the efficient recovery and reuse of powdered TiO_2, further improving the efficiency of water purification. Photocatalysis also holds vast potential for solar hydrogen production. By converting solar energy into hydrogen energy, efficient storage and utilization of solar energy can be achieved. In recent years, Japanese researchers have made significant advancements in hydrogen production through photocatalytic water splitting. For example, Professor Kazunari Domen's team at the University of Tokyo successfully increased the quantum efficiency of strontium titanate ($SrTiO_3$) photocatalysts to over 96%. Photocatalysis technology is also widely applied in self-cleaning materials, antibacterial materials, and agricultural preservation. For example, building materials such as tiles and glass with photocatalytic properties can effectively reduce the adhesion of bacteria and dirt, keeping surfaces clean. In agriculture, photocatalysis can decompose ethylene gas, which accelerates the ripening and aging of fruits and vegetables, thereby extending their shelf life.

The applications of water-splitting technology are highly diverse, extending beyond the energy sector to environmental protection and industrial production. For instance, in environmental protection, water-splitting technology demonstrates great potential by decomposing organic pollutants, heavy metal ions, and antibiotics. In industrial production, the hydrogen generated through water splitting can serve as green energy for fuel cell vehicles, industrial ammonia synthesis, and more. Additionally, photocatalysis can decompose toxic substances in water, achieving water purification and recycling. With continuous technological advancements, the cost of photocatalytic materials has been gradually decreasing, and the efficiency of water splitting is steadily improving. Large-scale commercial applications are expected in the future. For example, some countries and regions have already begun developing hydrogen production industry chains based on water splitting, from the development of catalyst materials to hydrogen storage and transportation. Breakthroughs in various stages are accelerating the rapid development of the entire industry. As a green and sustainable technology, photocatalysis shows tremendous potential in energy conversion and environmental management.

5. Conclusion

The development of photocatalytic water-splitting technology has progressed from foundational theoretical research to innovations in experimental techniques. This paper begins with the mechanisms of photosynthesis and explores the principles and applications of photocatalysis. Despite significant advancements, photocatalysis still faces challenges related to materials, cost, and efficiency. Looking ahead, research in this field is expected to deepen, characterized by diversification, the integration of theory and experiments, and expanded applications. Experimental research will provide valuable data and validation for theoretical studies, driving continual breakthroughs in photocatalytic water-splitting technology. Interdisciplinary integration is also a crucial trend in the development of photocatalysis technology. This field spans multiple disciplines, including physics, chemistry, and materials science, and its research and applications require cross-disciplinary collaboration. By drawing on theories and methods from other disciplines, photocatalysis can achieve further innovation and development. For instance, integrating physics can help elucidate the physical mechanisms of photocatalytic reactions and improve efficiency, while combining with chemical engineering can optimize reaction processes and enable industrial-scale production. As technology continues to mature, photocatalytic water-splitting technology will find broader applications in areas such as solar energy utilization, wastewater treatment, and air purification. This

DOI: 10.54254/2755-2721/129/2025.20944

will provide new momentum for advancements in these fields, contributing to environmental protection and the process of sustainable development.

References

[1] Yilong Wang. (2010). *Photosynthetic water consumption characteristics and influencing factors of major tree species in two typical forest stands in the semi-arid region of the Loess Plateau (Doctoral dissertation). Graduate School of the Chinese Academy of Sciences (Research Center for Soil and Water Conservation and Ecological Environment, Ministry of Education), Beijing, China.*

[2] *University of Science and Technology of China. (2021). Surface site-sensitive interfacial charge transfer and photocatalytic reaction efficiency revealed. USTC News. Retrieved from https://www.ustc.edu.cn/news.*

[3] *Gelle, A., & Moores, A. (2017). Water splitting catalyzed by titanium dioxide decorated with plasmonic nanoparticles. Pure and Applied Chemistry, 89(12), 1817–1827.*

[4] *Yongzhen Liu, Jiabing Chen, Sheng Zhan, Kui Xiong, Rui Zhang, & Xiaojun Lu. (2024). Research progress of black titanium dioxide photocatalysts. Journal of Wuhan Institute of Technology, 1, 1–20.*

[5] *Science Times. (2013). Microscopic mechanisms of surface photocatalytic reactions of titanium dioxide clarified. USTC News. Retrieved from https://www.ustc.edu.cn/news.*

[6] *Petala, A., Tsikritzis, D., Kollia, M., et al. (2014). Synthesis and characterization of N-doped* TiO_2 *photocatalysts with tunable response to solar radiation. Applied Surface Science, 305, 281–291.*

[7] *Asahi, R., Morikawa, T., Ohwaki, T., et al. (2001). Visible-light photocatalysis in nitrogen-doped titanium oxides. Science, 293(5528), 269–271. https://doi.org/10.1126/science.1058876.*

[8] *Kim, J. H., & Lee, J. S. (2019). Elaborately modified* $BiVO_4$ *photoanodes for solar water splitting. Advanced Materials, 31(18), 1806938.*

[9] *Smith, J., & Chen, X. (2019). Rational design and construction of cocatalysts for semiconductor-based photo-electrochemical oxygen evolution: A comprehensive review. Advanced Science, 6(18), 1802160.*