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Exploring nanoparticle-based semiconductor materials for sustainable hydrogen production: A short review

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ABSTRACT

Amid the urgent demand for eco-friendly and renewable energy solutions, hydrogen emerges as a compelling substitute for traditional fossil fuels. This review aims to guide researchers and policymakers by critically assessing semiconductor-based photocatalysts for sustainable hydrogen production. The methodology involved a systematic examination of approximately 85 publications, focusing on photophysical properties, photocatalytic efficiency, and stability. The novelty of this work lies in its integration of quantitative performance indicators with comparative evaluation, offering both numerical benchmarks and contextual insights. Among the materials studied, titanium dioxide (TiO_2) demonstrates the highest efficiency, achieving hydrogen generation rates up to 6715 μmol/g/h under UV light, while cadmium sulfide (CdS) delivers 500 μmol/g/h under visible light. This comparison illustrates TiO_2's stability but UV-only activation versus CdS's broader solar utilization but photocorrosion challenges. Other materials, such as ZnO (1200 μmol/g/h), Cu_2O (530 μmol/g/h), and $BiVO_4$ (1060 μmol/g/h), further highlight the trade-offs between efficiency, stability, and environmental impact. Beyond performance metrics, the environmental and economic benefits of semiconductor-based photocatalysts are discussed, underscoring their contributions to sustainable energy frameworks. The article also examines obstacles linked to scaling these materials, including cost, stability, and infrastructure requirements. Possible applications include hydrogen fuel cells for transportation, electricity generation, and industrial feedstocks such as steel and chemicals. By integrating numerical comparisons, methodological clarity, and application relevance, this review identifies the most advantageous materials and outlines future research trajectories for eco-friendly hydrogen production.

Keyword: sustainable energy, photocatalysis, hydrogen production, semiconductor materials, energy efficiency.

INTRODUCTION

Due to increasing population growth and globalization, global energy demand has risen significantly, elevating the lifestyle of human civilization [86-87]. Among various forms of energy, electrical energy and transportation energy are in particularly high demand because of their essential roles in modern society [1,2]. Electricity is indispensable for powering homes, industries, and digital infrastructure, which are the backbones of economic growth and technological innovation. Similarly, transportation energy plays a critical role in enabling mobility, connecting global markets, fueling commerce, and supporting urbanization. To meet these growing demands, the world has heavily relied on fossil fuels [3,4]. The world continues to depend heavily on coal, diesel, petrol, and methane. These energy sources have historically been the foundation of industrialization due to their availability, energy density, and established infrastructure [88,89]. However, excessive reliance on non-renewable energy sources has resulted in major ecological issues such as greenhouse gas emissions, air contamination, and global warming [5,6]. The International Energy Agency reported that global energy-related CO_2 emissions reached 37.4 gigatonnes in 2023, marking one of the highest levels in history. The Hydrogen Council further projects that hydrogen could contribute up to 18 percent of global energy needs by 2050, generating 2.5 trillion dollars in revenue and creating 30 million jobs worldwide [7,8]. These figures underscore hydrogen's strategic importance in the global energy transition.

Renewable and eco-friendly energy options, including solar, wind, hydro, and hydrogen, together with advancements in energy-saving technologies, play a vital role in overcoming these challenges. While solar, wind, and hydro energy are promising alternatives, they face limitations such as dependency on climatic conditions and energy storage challenges. These factors hinder their ability to provide consistent and reliable energy supply. In this context, hydrogen has gained prominence as a potential solution [9,10].

Hydrogen stands out owing to its adaptability and substantial energy retention capacity. It can be generated using renewable energy through water electrolysis, stored for long periods, and utilized when needed. It offers a clean and efficient energy solution, especially when used in fuel cells or combined with advanced technologies for transportation, electricity generation, and industrial applications [11,12]. Unlike fossil fuels, hydrogen combustion produces only water vapor, making it an attractive option for reducing greenhouse gas emissions. Global initiatives are actively exploring its potential for large-scale deployment [13,14].

The International Energy Agency projects that hydrogen may fulfill as much as 18 percent of worldwide energy needs by 2050, playing a key role in reducing carbon emissions across multiple industries. Based on insights from the Hydrogen Council, the worldwide hydrogen industry has the potential to yield 2.5 trillion dollars in earnings and provide employment to 30 million individuals by 2050 [15,16]. Moreover, hydrogen holds significant potential for reducing carbon emissions in sectors like transportation, heavy manufacturing, and electricity production. An example includes vehicles powered by hydrogen fuel cells, which release no tailpipe emissions, and hydrogen's application as a feedstock in industries like steel and chemicals helps in lowering their carbon footprint [17,18]. Despite these advancements, challenges remain regarding hydrogen's production methods [19,20].

Currently, the majority of hydrogen generation relies on processes like methane steam reforming and biomass decomposition, classified as blue hydrogen. While hydrogen is frequently regarded as a clean fuel, this is not completely precise. The production of blue hydrogen relies on natural gas, coal, and methane, which are fossil-based energy sources, making it not fully clean or green [21,22]. However, innovative technologies are reshaping this narrative. Progress in modern hydrogen generation methods has significantly enhanced its promise as an eco-friendly energy medium [23,24]. Electrolysis, a promising method that involves separating water into its elemental components using electrical power, is gaining attention. Driven by eco-friendly energy inputs like solar and wind systems, electrolysis produces green hydrogen with negligible ecological harm, setting the stage for authentically sustainable hydrogen alternatives [25,26].

Various renewable energy sources are being utilized for water splitting, among which solar energy stands out as an optimal choice due to its abundant availability and cost-effectiveness in many regions. Solar-driven electrolysis harnesses sunlight to produce electricity, which is then used to split water molecules efficiently. This method considerably lowers greenhouse gas emissions and harmonizes effectively with the aim of establishing a genuinely sustainable hydrogen economy [27,28]. Notably, three different routes for water splitting using solar energy have been explored, namely photobiological, thermochemical, and photocatalytic. Of these, photocatalytic water splitting has drawn considerable attention for its numerous advantages. These include advanced heat management, negligible or zero CO_2 emissions, higher yields, reduced susceptibility to catalyst poisoning, compact reactor designs, low costs, and greater solar-to-hydrogen efficiency compared to other solar-based water splitting methods [29,30].

Photocatalysis was first demonstrated by Fujishima and Honda in 1972, who used TiO_2 electrodes to split water under UV light [31]. Since then, research has expanded to nanostructured semiconductors such as ZnO, CdS, Cu_2O, and $BiVO_4$, each offering unique advantages and challenges. While numerous studies have reported promising results, most focus on individual materials or specific modifications. The literature reveals a clear gap, as systematic comparative evaluations that integrate quantitative performance indicators, environmental implications, and scalability potential remain limited.

This review addresses that gap by synthesizing recent advances in semiconductor-based photocatalysts for hydrogen production. It provides a comparative evaluation of TiO_2, ZnO, CdS, Cu_2O, and $BiVO_4$, highlighting their efficiencies, limitations, and environmental impacts. By integrating numerical benchmarks with contextual insights, the article aims to guide researchers and policymakers toward effective and eco-friendly strategies for sustainable hydrogen production. The Figure 1 illustrates the flow for selection of sustainable hydrogen production technique.

ASSESSMENT OF PHOTOCATALYSIS FOR WATER DECOMPOSITION

Photocatalysis originated from the basic concept of an electrochemical cell [32,33]. This cell was developed to decompose water into its hydrogen and oxygen components using a titanium dioxide (TiO_2) electrode and a platinum black electrode, as depicted in Figure 2. On the surface of the TiO_2 electrode, oxygen evolution occurs through water oxidation when irradiated with UV light or another light source. Simultaneously, hydrogen evolution occurs across the platinum black electrode through hydrogen reduction. This electrochemical principle later evolved into a photocatalytic system, which employs semiconductor powders or particles as catalysts and replaces UV light irradiation with sunlight [34,35].

Mechanism of hydrogen production by semiconductor

In a photocatalytic system, the semiconductor serves as a catalyst, incorporating both an energy conduction layer and a valence energy layer. When the semiconductor is exposed to sunlight or another illumination source, it enters a photo-excited state, where electrons within the valence layer absorb energy and migrate to the conduction layer, leaving behind positively charged vacancies. The effectiveness of this photo-excited state relies on the material's capacity for light absorption, shaped by its intrinsic characteristics and the frequency of the light source [36,37].

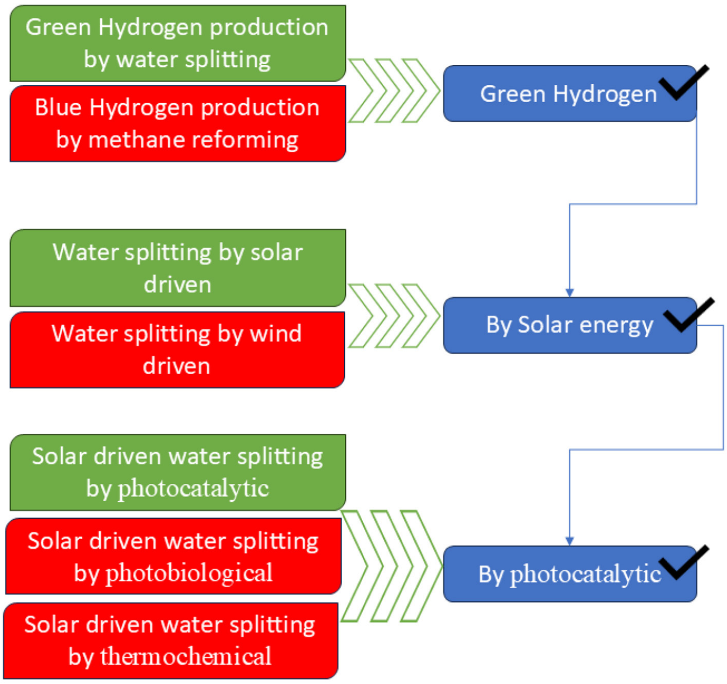

Figure 1. The chosen pathway for hydrogen production via photocatalysis

In the photo-excited state, the energized electrons within the conduction layer and the positively charged vacancies in the valence layer drive essential reactions. Energized electrons within the conduction layer engage in reduction reactions, such as transforming hydrogen ions into molecular hydrogen, whereas positively charged vacancies in the valence layer facilitate oxidation reactions, like splitting water to release oxygen [38,39]. This simultaneous process of reduction and oxidation is supported by suitable oxidizing and reducing agents to optimize the reaction dynamics. Advancements in photocatalysis include tailoring semiconductor materials to enhance light absorption, for instance, through doping with metals or other modifications, making the process more efficient under sunlight [39,40]. A schematic representation of this process is described in Figure 3.

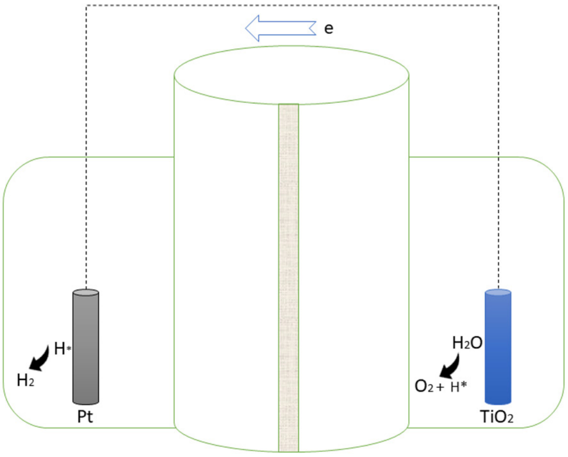

Figure 2. The basic principle of electro-chemical cell

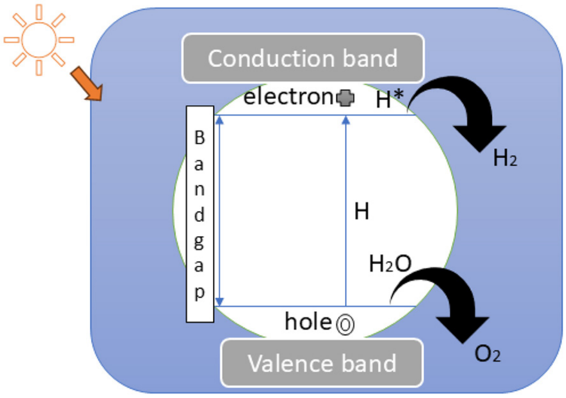

Figure 3. The fundamental mechanism of semiconductor-based water splitting

SEMICONDUCTOR BASED PHOTOCATALYTIC HYDROGEN PRODUCTION

TiO_2 as a photocatalytic

Among semiconductor compounds, TiO_2 ranks as a key focus in research on photocatalytic hydrogen generation, attributed to its robust stability, safe handling, and high oxidative potential. TiO_2 possesses an energy bandgap near 3.2 eV, enabling its activation under ultraviolet radiation. The conduction band of TiO_2 lies at approximately –0.5 eV vs. NHE, while the valence band is positioned near +2.7 eV, which provides sufficient driving force for water oxidation but limits visible-light absorption. The efficiency of its photocatalytic behavior greatly relies on the arrangement of its crystals, with anatase and rutile being the primary structures studied [41,42]. TiO_2 demonstrates remarkable photophysical characteristics, such as superior electron movement and an enhanced capacity to form electron-hole pairs when exposed to light. Nevertheless, the merging of generated charge carriers, specifically electrons and holes, can hinder the overall effectiveness of its photocatalytic performance. Researchers have employed numerous approaches to improve the performance of TiO_2 in photocatalysis, including the incorporation of transition metals, the formation of heterojunctions with alternative semiconductors, and altering surfaces using co-catalysts. Such adjustments focus on broadening the spectrum of light absorption, enhancing charge separation, and boosting the rate of hydrogen generation [43,44].

The hydrogen generation of TiO_2-based photocatalysts varies widely depending on the specific modifications and experimental conditions. For instance, introducing noble metals such as platinum (Pt) into TiO_2 has demonstrated a substantial improvement in its photocatalytic efficiency. Studies have reported hydrogen production rates of up to 200 μmol/g/h for Pt-doped TiO_2 under UV light illumination [45,46]. Additionally, the creation of TiO_2-based heterojunctions with other semiconductors, such as graphene oxide, has further improved hydrogen production efficiency, as shown in Figure 4. TiO_2 is widely available and economical, positioning it as a compelling choice for extensive hydrogen generation. Its non-toxic nature and stability further enhance its positive environmental impact. However, the requirement for UV light to activate TiO_2 presents a challenge, given that ultraviolet radiation constitutes only a limited portion of the solar spectrum. Research

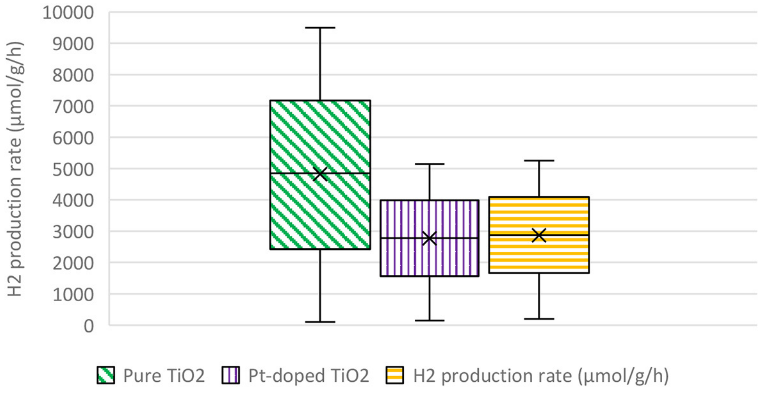

Figure 4. Hydrogen production rate for TiO_2

aimed at creating TiO_2-based photocatalysts responsive to visible light is actively progressing and shows potential for improving the material's real-world usability [47,48].

ZnO as a photocatalytic

ZnO is another widely researched semiconductor material for photocatalytic hydrogen production, known for its excellent electrical and optical properties. ZnO features an energy bandgap near 3.37 eV along with a notable exciton binding energy of 60 meV, both of which enhance its stability and potent photocatalytic efficiency under ultraviolet illumination [49,50]. The conduction band of ZnO lies close to –0.3 eV vs. NHE, while the valence band is near +3.0 eV, providing strong oxidative potential but restricting visible-light absorption. ZnO demonstrates high electron movement and effective separation of charge carriers, establishing it as a strong contender for use in photocatalysis. However, as with TiO_2, the merging of charge carriers can reduce its overall effectiveness. Approaches such as introducing transition metals, forming heterostructures, and modifying surfaces with co-catalysts have been adopted to broaden the spectrum of light absorption and optimize charge separation [51,52]. For instance, incorporating noble elements like silver (Ag) into ZnO has demonstrated notable improvements in efficiency. Research findings indicate that Ag-doped ZnO can achieve hydrogen generation efficiencies reaching 150 μmol/g/h under UV radiation [53,54]. Additionally, ZnO-based heterojunctions with semiconductors such as $g\text{-}C_3N_4$ have further improved hydrogen production efficiency, as shown in Figure 5.

ZnO is widely available and economically viable, establishing it as a practical choice for extensive hydrogen generation. Its non-toxic characteristics and stability further enhance its environmentally friendly attributes. However, the reliance on ultraviolet radiation for ZnO activation presents a drawback, since UV light constitutes only a limited segment of the solar spectrum. Current research focuses on creating ZnO photocatalysts that respond to visible light, showing

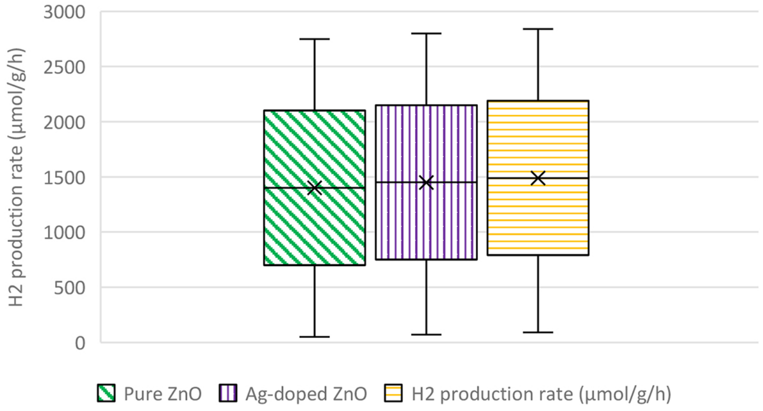

Figure 5. Hydrogen production rate for ZnO

significant potential for improving the material's practical usage [55,56].

Cadmium sulfide as a photocatalytic

Cadmium sulfide (CdS) is a prominent semiconductor in hydrogen generation through photocatalysis, especially appreciated for its capacity to capture visible light. CdS possesses a direct energy bandgap near 2.4 eV, enabling efficient harnessing of a broad range of the solar spectrum [57,58]. Its conduction band lies at approximately –1.0 eV vs. NHE, while the valence band is near +1.4 eV, making it suitable for hydrogen evolution under visible light. CdS showcases outstanding photophysical characteristics, such as superior absorption and efficient charge separation. However, photocorrosion under illumination significantly reduces its stability. To address this, methods including co-catalyst integration, surface passivation, and composite structures have been adopted [59,60].

Pt/CdS systems have achieved hydrogen generation efficiencies of up to 500 μmol/g/h under visible light [61]. CdS-based heterojunctions with TiO_2 and ZnO further improve charge separation and stability, as shown in Figure 6. Despite cadmium's toxicity, CdS remains a favored choice due to its strong visible-light response and scalability [62].

Copper oxide as a photocatalytic

Copper oxide (Cu_2O) is an emerging semiconductor material known for its visible-light absorption and excellent photocatalytic properties. Cu_2O features an energy bandgap close to 2.0 eV, with a conduction band near –0.7 eV vs. NHE and a valence band around +1.3 eV, enabling efficient absorption of a considerable portion of the solar spectrum [63,64]. Cu_2O demonstrates effective charge carrier movement and strong light absorption. However, electron-hole recombination and photocorrosion remain challenges. Strategies such as surface passivation and co-catalyst addition have been utilized to enhance durability [65].

Hydrogen generation rates of Cu_2O-based photocatalysts vary depending on modifications. Cu_2O/ZnO heterojunctions have achieved rates up to 300 μmol/g/h under visible light illumination [65], as shown in Figure 7. The Cu_2O is widely available and economically feasible, establishing itself as a promising choice for photocatalytic uses. Its capacity to harness visible light and the potential for low-cost production contribute to its environmental and economic benefits [66].

Bismuth vanadate as a photocatalytic

Bismuth vanadate ($BiVO_4$) stands out for its visible-light absorption and robust stability. $BiVO_4$ has an energy bandgap near 2.4 eV, with a conduction band at approximately +0.3 eV vs. NHE and a valence band near +2.7 eV, which allows water oxidation but limits hydrogen evolution directly [67,68]. $BiVO_4$ demonstrates strong light capture and effective charge separation, though recombination remains an issue. Techniques such as co-catalyst integration and heterojunction formation have been used to improve efficiency [69,70].

Hydrogen generation rates of $BiVO_4$-based photocatalysts vary with modifications. $BiVO_4$/WO_3 heterojunctions have achieved rates up to 400 μmol/g/h under visible light illumination [67,69], as shown in Figure 8. $BiVO_4$'s scalability and non-toxic nature position it as a sustainable choice for photocatalysis [71,72].

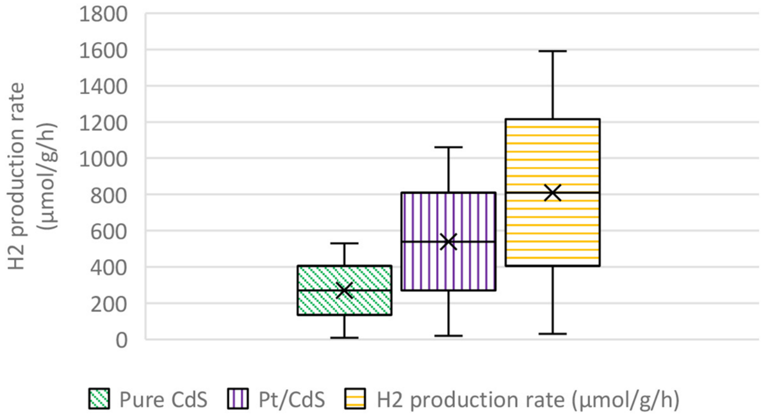

Figure 6. Hydrogen production rate for CdS

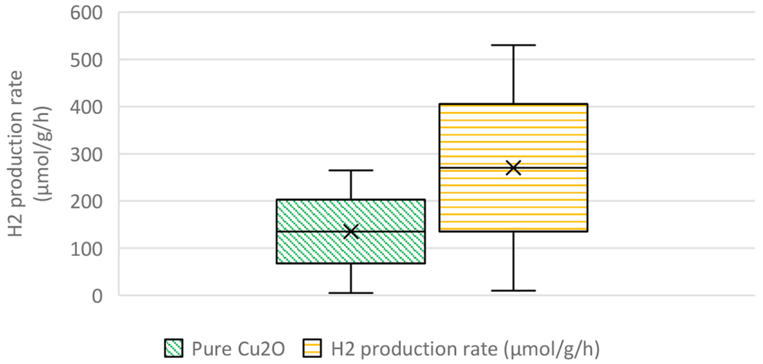

Figure 7. Hydrogen production rate for Cu_2O

Table 1 summarizes the key quantitative parameters of the semiconductor photocatalysts discussed above, including their band gaps, band edge positions, and confirmed hydrogen production rates.

Among these, TiO_2 exhibits the highest reported hydrogen production rate when modified with noble metals, while CdS and Cu_2O offer strong visible-light response but face stability challenges. ZnO and $BiVO_4$ remain attractive for their environmental safety and scalability, though their efficiencies are moderate compared to TiO_2 and CdS.

Environmental impact of contaminants

Apart from efficiency, it is important to assess the environmental implications of semiconductor photocatalysts. The presence of contaminants derived from photocatalyst composition, by-products, or other sources can play important roles in sustainability as well as environmental friendliness. Cadmium, in CdS-based photocatalysts, is one contaminant that has serious implications because of photocorrosion, which causes Cd^{2+} ion leakage into aqueous systems, resulting in toxicity. Cu_2O, which can be degraded by light, causes soluble copper ions, which are sources of secondary pollution. Even noble metals, which include Pt and Ag, used as dopants or co-catalysts, have the possibility of leaching into the reaction medium, which causes concerns about long-term accumulation in the environment. Moreover, sacrificial agents, which are typically used to increase charge separation, have by-products that act as sources of pollution, making the reaction less environmentally friendly. These agents include sulfide, sulfite, methanol, or ethanol [78,79].

To address the challenges posed by the use of photocatalysts, several methods have been suggested. For instance, surface passivation and the use of protective layers may help reduce photocorrosion. Additionally, the use of a heterojunction structure may help improve the stability of the charge carriers and reduce the problem of leaching. On the other hand, the reuse of spent photocatalysts may help address the challenges. However, in terms of sustainability, the most preferred photocatalysts

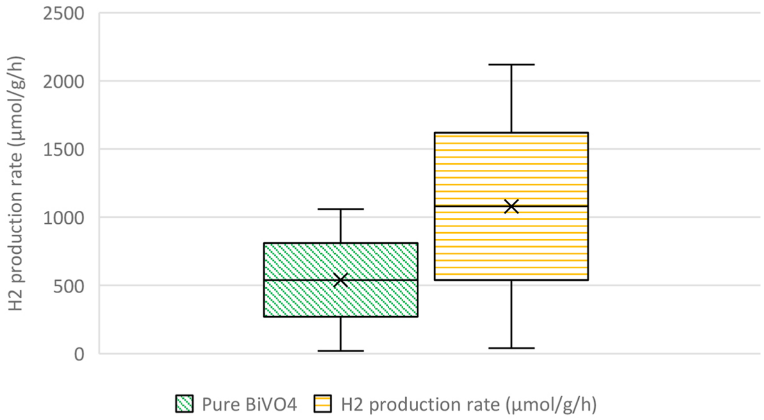

Figure 8. Hydrogen production rate for BiVO4

Table 1. Comparative summary of semiconductor photocatalysts for hydrogen production

Source & Year	Material	Band gap (eV)	CB / VB position (vs. NHE)	Reported H_2 production rate (µmol/g/h)
Rafique et al. (2023) [73]	TiO_2	~3.2 eV	CB: –0.5 eV, VB: +2.7 eV	Up to 23,500 µmol/g/h for Ag-doped TiO_2
Rizky at al. (2025) [74]	ZnO	~3.37 eV	CB: –0.3 eV, VB: +3.0 eV	~150 µmol/g/h for Ag-doped ZnO
Su et al. (2023) [75]	CdS	~2.4 eV	CB: –1.0 eV, VB: +1.4 eV	~500 µmol/g/h for Pt/CdS under visible light
Wang et al. (2025) [76]	Cu_2O	~2.0 eV	CB: –0.7 eV, VB: +1.3 eV	~511 µmol/g/h for Cu_2O/CuO composites
Sun et al. (2025) [77]	$BiVO_4$	~2.4 eV	CB: +0.3 eV, VB: +2.7 eV	~400 µmol/g/h for $BiVO_4$/WO_3 heterojunction

should be non-toxic and stable [80,81]. Some of the most preferred photocatalysts include TiO_2, ZnO, and $BiVO_4$.

Kinetic analysis of photocatalytic hydrogen production

The kinetics of photocatalytic hydrogen evolution provide critical insight into the efficiency and mechanism of semiconductor photocatalysts. Reaction rates are typically evaluated in terms of rate constants (k), which describe the speed of hydrogen generation under given illumination and catalyst conditions. Higher rate constants indicate more efficient charge separation and faster surface redox reactions. For example, noble-metal-modified TiO_2 and CdS systems often exhibit enhanced rate constants due to improved electron transfer pathways and reduced recombination [82,83].

Another key parameter is the apparent quantum yield (AQY), defined as the ratio of the number of reacted electrons to the number of incident photons. AQY values directly reflect the photon-to-hydrogen conversion efficiency. Reported AQY values vary widely depending on the material and modification strategy: Ag-doped TiO_2 has demonstrated AQY values approaching 19% under UV irradiation, while CdS-based systems under visible light typically achieve AQY values in the range of 10–15%. These metrics highlight the importance of both band structure alignment and surface engineering in optimizing photocatalytic performance [84,85].

Overall, kinetic analysis through rate constants and AQY provides a quantitative framework for comparing different photocatalysts. It underscores that while TiO_2 offers stability and high AQY under UV light, visible-light-responsive materials such as CdS and Cu_2O require stabilization strategies to maintain competitive kinetics.

COMPARATIVE ASSESSMENT

TiO_2 demonstrates remarkable efficiency, achieving hydrogen generation levels as high as 6715 µmol/g/h under UV irradiation with Ag modification. Its advantages lie in its stability, non-toxicity, extensive research backing, and cost-effectiveness, although it is limited to UV light absorption [73]. ZnO achieves hydrogen generation rates as high as 1200 µmol/g/h under UV light and is valued for its efficient electron movement, widespread availability, affordability, and durability. Like TiO_2, it is restricted to UV light absorption [74]. Cadmium sulfide (CdS), with hydrogen generation levels reaching 500 µmol/g/h under visible light with Pt co-catalyst, excels in capturing visible light efficiently and showcases remarkable photocatalytic performance. However, it faces significant challenges, including photocorrosion and environmental concerns due to cadmium [75]. Copper(I) Oxide (Cu_2O) attains hydrogen generation levels as high as 530 µmol/g/h when modified with ZnO heterojunctions, prized for its efficient visible-light capture and affordability. It is hindered by electron-hole recombination and photocorrosion [76]. Lastly, Bismuth Vanadate ($BiVO_4$) has a hydrogen generation level as high as 1060 µmol/g/h under visible light with WO_3 coupling, with advantages such as visible-light absorption, non-toxicity, and stability, though it suffers from limited photocatalytic efficiency due to electron-hole recombination [77]. The detailed comparison was exposed in Table 2.

As shown in Table 2 and Figure 9, TiO_2 exhibits the highest hydrogen production rate

Table 2. The summary of the semiconductor-based materials comparison for hydrogen production rate

Source & Year	Material	Maximum hydrogen production rate (µmol/g/h)	Percentage of maximum hydrogen production	Key advantages	Key challenges	Experimental conditions
Rafique et al. (2023) [73]	TiO_2	6715	100%	Stable, non-toxic, cost-effective, widely studied	Limited to UV absorption	UV irradiation, Ag-doped
Rizky at al. (2025) [74]	ZnO	1200	17.87%	High electron mobility, abundant, low-cost, durable	Restricted to UV absorption	UV irradiation, Ag-doped
Su et al. (2023) [75]	CdS	500	7.45%	Visible-light absorption, high efficienc	Photocorrosion, cadmium toxicity	Visible light, Pt co-catalyst
Wang et al. (2025) [76]	Cu_2O	530	7.89%	Visible-light absorption, low cost	Electron-hole recombination, photocorrosion	Visible light, ZnO heterojunction
Sun et al. (2025) [77]	$BiVO_4$	1060	15.78%	Visible-light absorption, non-toxic, stable	Limited efficiency due to electron-hole recombination	Visible light, WO_3 coupling

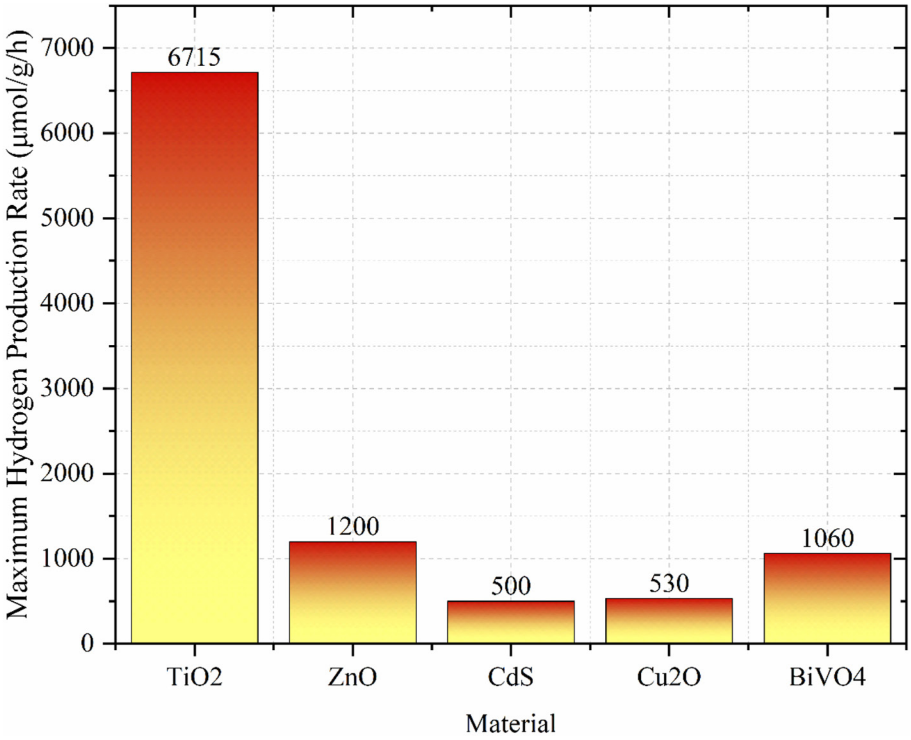

Figure 9. Comparative hydrogen production rates of semiconductor photocatalysts under reported experimental conditions

under UV irradiation, reflecting its stability and extensive optimization. ZnO follows with moderate yields but shares TiO_2's limitation of UV-only activity. CdS and Cu_2O demonstrate visible-light activity, yet their performance is constrained by photocorrosion and recombination, alongside environmental concerns in the case of CdS. $BiVO_4$ offers a balance of visible-light absorption, non-toxicity, and stability, though its efficiency remains moderate compared to TiO_2.

Overall, the comparative evaluation underscores the trade-off between high efficiency (TiO_2) and sustainability ($BiVO_4$, ZnO), while highlighting the need for stabilization strategies in CdS and Cu_2O systems.

CONCLUSIONS

Each semiconductor material has its own unique advantages and challenges when it comes to photocatalytic hydrogen production. Here's an evaluative comparison to determine the most advantageous material

- Titanium dioxide is stable, non-toxic, and widely studied. It possesses excellent photophysical properties and strong oxidative power, making it cost-effective. Nevertheless, its absorption is restricted to ultraviolet light, accounting for only a minor portion of the solar spectrum, necessitating adjustments to improve its functionality. It is best for applications where stability and non-toxicity are crucial and where UV light can be effectively utilized.
- Zinc oxide boasts high electron mobility and charge carrier separation. It is abundant, low-cost, and similar in stability to TiO_2. However, it also suffers from limited UV light absorption and requires modifications to enhance performance. ZnO is best for cost-sensitive applications needing stable materials, particularly in environments with high UV light exposure.
- Cadmium sulfide absorbs visible light, allowing for broader utilization of the solar spectrum, and demonstrates high photocatalytic efficiency. However, it faces challenges such as photocorrosion and environmental concerns due to cadmium toxicity, requiring modifications for stability. CdS is best for applications requiring high efficiency and visible light absorption, with careful handling and environmental management.
- Copper(I) oxide offers visible light absorption, excellent photocatalytic properties, and low cost. However, it is plagued by issues with electron-hole recombination and photocorrosion, requiring surface passivation and co-catalyst incorporation. Cu2O is best for low-cost applications utilizing visible light, with ongoing improvements in stability.
- Bismuth vanadate excels in visible light absorption, good stability, and non-toxicity. However, it has limited photocatalytic efficiency due to electron-hole recombination and requires enhancements like co-catalyst loading and heterojunctions. $BiVO_4$ is best for environmentally friendly applications needing visible light absorption and stable materials.

Considering both efficiency and practicality:

- Optimal for ultraviolet light absorption: TiO_2 recognized for its exceptional hydrogen generation capacity of 6715 µmol/g/h, alongside its stability, eco-friendly nature, and affordability.
- Best for visible light absorption: CdS due to its high efficiency under visible light, although it comes with challenges of photocorrosion and environmental concerns.

Despite providing a comprehensive comparative evaluation, this study has limitations. Reported hydrogen generation rates are derived from diverse experimental setups, which may not be directly comparable due to variations in light intensity, reactor design, and co-catalyst loading. Long-term stability data remain limited, particularly for materials prone to photocorrosion such as CdS and Cu_2O. Furthermore, while environmental impacts were discussed qualitatively, quantitative life-cycle assessments were beyond the scope of this work. Future research should focus on developing photocatalysts that combine high efficiency with environmental safety, such as heterojunctions involving non-toxic oxides (TiO_2, ZnO, $BiVO_4$). Advanced surface engineering and protective coatings can mitigate photocorrosion in CdS and Cu_2O, while coupling with co-catalysts may enhance charge separation. Expanding kinetic studies, including rate constant determination and apparent quantum yield measurements under standardized conditions, will provide deeper mechanistic insights. Additionally, integrating photocatalytic hydrogen production with renewable energy systems and scaling up reactor designs will be critical for practical deployment.

This study contributes theoretically by consolidating quantitative performance metrics (band gaps, hydrogen production rates, AQY values) into a unified comparative framework. It highlights the interplay between band structure alignment, charge-carrier dynamics, and environmental sustainability, offering a mechanistic basis for material selection. The inclusion of environmental analysis and kinetic parameters extends the theoretical scope beyond efficiency, emphasizing the importance of stability and ecological impact in photocatalyst design.

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