

# Design of Semiconductor-Based Photocatalysts for CO<sub>2</sub> Reduction and Green Hydrogen Production to Advance Environmental Sustainability

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**Abstract:** The global energy crisis and climate change constitute immense challenges, largely due to rising CO<sub>2</sub> emissions and dependence on fossil fuels. Transitioning to low-carbon, renewable technologies is crucial for the long-term security of energy and achieving climate goals. Thus, photocatalytic CO<sub>2</sub> reduction and production of hydrogen (H<sub>2</sub>) have emerged as solutions, providing dual advantages of mitigating greenhouse gases (GHG) and generating sustainable solar fuels. Semiconductor-based photocatalysts are vital, facilitating light-driven redox reactions that convert carbon dioxide into useful chemicals and split water to produce hydrogen. Various material classes emerge from recent advances, with traditional oxides such as ZnO and TiO<sub>2</sub> and advanced systems such as graphitic carbon nitride, perovskites, and metal-organic frameworks, including emerging nanostructures ranging from single-atom catalysts to quantum dots, among others. Design strategies, namely heterostructure formation, band gap engineering, and co-catalyst integration, have improved charge separation, light harvesting, and product selectivity. Evidence from literature also demonstrates significant progress in the enhancement of photocatalytic activity and stability, as efficiencies approach practical thresholds in certain systems. Yet, some challenges remain, such as limited long-term durability, rapid charge recombination, barriers to large-scale implementation, and competing side reactions. Future perspectives also emphasize the importance of integrating artificial photosynthesis, machine learning-driven catalyst discovery, earth-abundant materials, and techno-economic & life-cycle analyses to ensure industrial and environmental viability. Semiconductor-based photocatalysis generally presents a pathway for achieving carbon-neutral energy, as long as ongoing research strives to bridge the gap between laboratory practices and scalable applications in different industries.

**Keywords:** Semiconductor, Photocatalysts, CO<sub>2</sub> Reduction, Hydrogen Production, Photocatalysis, Environmental Sustainability.

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## I. INTRODUCTION

Global CO<sub>2</sub> emissions are the main cause of climate change. Greenhouse gases, especially CO<sub>2</sub>, are the primary reason for global warming (Yoro & Daramola, 2020). CO<sub>2</sub> emissions and temperature change have a linear relationship. Cumulative emissions create lasting impacts that persist for

centuries, even if emissions stop (Hope, 2020). This permanence highlights the urgency of immediate action across multiple sectors and industries. A large fraction of emitted CO<sub>2</sub> remains in the atmosphere even thousands of years later (Hammed, 2023). Recent research emphasizes the need for comprehensive mitigation across sectors and better technologies for carbon capture.

Jelley (2020) argued that the urgency to use renewable energy sources comes from the environmental dangers of fossil fuels. Transitioning to low-carbon alternatives is critical for meeting international climate goals, like the Paris Agreement's target of keeping temperature rise below 2 degrees Celsius (Shcherbyna et al., 2022). Carbon capture, utilization, and storage (CCUS) technologies help reduce emissions. They capture CO<sub>2</sub> from industrial processes and power generation for storage or conversion into value-added products, such as chemicals, fuels, and building materials (Verma et al., 2021). Currently, there are thirty-five (35) commercial CCUS facilities worldwide, with a total capacity of 45 million tons per year (Shcherbyna et al., 2022).

Tahir et al. (2020) defined photocatalysis as a technique with huge potential for environmental remediation via light-powered redox reactions in semiconductor materials. Heterogeneous photocatalysis refers to a sustainable strategy comprising semiconductor-fluid interfaces with energy light, providing applications in solar fuel production, water splitting, air purification, and pollutant degradation (Li et al., 2020). This typically begins when photons with at least approximate energy as the semiconductor's bandgap develop electron-hole pairs, which initiates surface redox reactions (Guo et al., 2019). These principles include kinetic and thermodynamic parts that determine photocatalytic performance, where energy transfer processes are directly related to breaking and forming procedures (Li et al., 2020). Meanwhile, critical factors impacting performance range from light response to quantum efficiency, interaction between photocatalyst and light surface properties, pH, doping, heterostructures, and photochemical stability (Garcia-Lopez & Palmisano, 2021). Environmental applications comprise pollutant degradation, water & air purification, disinfection, and detection of chemical oxygen demand (Liu et al., 2023).

Semiconductor-based photocatalysts harness solar energy for thermodynamic reactions. This provides a sustainable way to address climate change mitigation and renewable energy storage (Mishra et al., 2023). These materials convert CO<sub>2</sub> into valuable chemicals and produce hydrogen by splitting water. This process creates artificial photosynthetic systems. The dual functionality enables syngas production and supports biorefineries. In these systems, CO<sub>2</sub> acts as both an electron acceptor and a feedstock (Wang, Zhou, & Wang, 2023).

#### ➤ Aim and Objectives

The primary aim of this review is to critically examine the current state-of-the-art in semiconductor-based photocatalyst design for reducing CO<sub>2</sub> and producing hydrogen.

#### • The Objectives are:

- ✓ To analyze the processes of photocatalytic CO<sub>2</sub> reduction and H<sub>2</sub> production on semiconductor surfaces
- ✓ To evaluate the performance of different semiconductor materials for improved and efficient solar-to-fuel conversion

- ✓ To identify design strategies such as band gap engineering, surface modification, and heterostructure formation techniques
- ✓ To compare recent material development advancement and their impact on the selectivity and stability of products
- ✓ To assess current challenges limiting the implementation and scaling of photocatalytic systems
- ✓ To propose future research directions for developing economically viable photocatalytic technologies.

## II. FUNDAMENTALS OF SEMICONDUCTOR PHOTOCATALYSIS

### ➤ Photocatalytic Mechanisms

Despite the widely agreed definition of semiconductor photocatalysis capturing complex processes involving the generation of electron-hole pairs generated by light absorption, which must supersede recombination to reach the chemical reaction's surface, one challenge remains, which is achieving effective charge carrier usage due to low quantum yields as a result of conflicting processes (Zhang et al., 2016). Through the initial carrier generation, to-the-surface migration, and surface redox reactions, each step must be optimized for effective performance. Goodarzi et al. (2023) observed that enhancement strategies such as conductivity improvement via graphitic materials, morphology control to reduce migration distances, cocatalyst application for surface reactions, and heterojunction construction for separating charge can be applicable, while band structure engineering, reaction condition optimization, and defect engineering are essential for improving performance in environmental remediation and energy production applications.

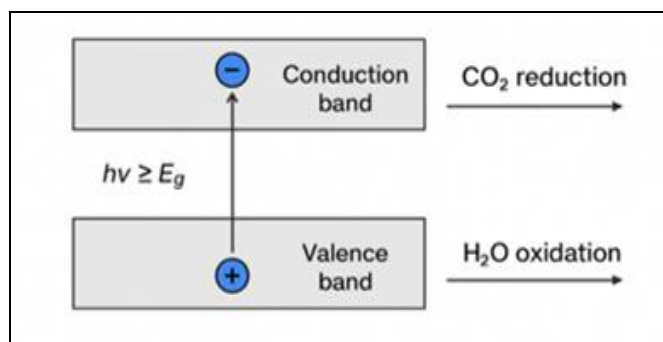


Fig 1 Mechanisms of Photocatalysis

Electrons are moved from the valence band (VB) to the conduction band (CB) with the absorption of energy  $h\nu \geq E_g$ , which consequently creates electron-hole pairs ( $e^-/h^+$ ). Regarding the reduction of carbon dioxide and production of hydrogen, the conduction band minimum must be more negative than CO<sub>2</sub> reduction potentials (CO<sub>2</sub>/CO: -0.53 V, CO<sub>2</sub>/CH<sub>4</sub>: -0.24 V vs. NHE). Likewise, the valence band maximum must be more positive than the H<sub>2</sub>O oxidation potential (+1.23 V vs. NHE). There are multiple strategies through which band gap engineering enables optimisation, some of which include substitutional doping with metals or non-metals to shift band positions or create intermediate states; quantum size effects in nanostructures, and compositional tuning in solid solutions (Cd<sub>x</sub>Zn<sub>1-x</sub>S) to ensure

continuous band gap adjustment (Orizu et al., 2023). Charge separation is facilitated through proper band alignment in heterojunctions, via band structures in Z-scheme configurations or Type II systems, which is in the form of natural photosynthesis.

Likewise, charge separation and transport are essential bottlenecks, where carriers recombine in nanoseconds without intervention. Therefore, strategies to enhance separation range from morphological control using nanostructured architectures to co-catalyst loading for selective charge extraction, heterojunction formation for built-in electric fields, and crystal facet engineering to uncover high-energy surfaces (Wang et al., 2025). Surface reactions determine product efficiency and selectivity, where reduction of carbon dioxide follows pathways producing  $\text{CH}_4$ , CO, or  $\text{CH}_3\text{OH}$  via surface-bound complexes and intermediate radical species. Production of hydrogen, on the other hand, takes place through the hydrogen evolution reaction (HER), which is often limited by proton adsorption methods (Ferriday, Middleton, & Kolhe, 2021). Active sites such as oxygen vacancies, acid/base sites, and undercoordinated metal centers oversee reactant activation and product formation processes, and the synergy between charge dynamics, light absorption, and surface chemistry determines solar-to-fuel conversion efficiency (Lv et al., 2025).

#### ➤ Key Performance Parameters

Semiconductor photocatalysis performance is fostered by different parameters that determine practical viability and efficiency. Sahu et al. (2024) wrote that quantum efficiency (QE) is a fundamental limitation, where defective n-type semiconductor particles (approximately 100nm) exhibit  $\text{QE} < 5\%$  in visible light and thus reach only about 10% in slurry systems, which implies just 1.4% solar-to-hydrogen (STH) efficiency. One of the limitations of the QE is the bulk recombination processes hindering charge separation before carriers get to surface catalysts (Wang et al., 2025). Catalyst loading, light intensity, pH, temperature, dissolved oxygen concentration, and crystalline structure influence mass transfer effects and reaction kinetics. Also, surface charge and subsurface electric fields in the space charge region affect catalyst selectivity and activity. According to Chen, Ren, & Yuan (2023), the electrochemical nature of surface reactions facilitates quantitative description via Faradaic efficiencies and charge collection yields while low quantum yield is the major barrier to commercialization.

The primary challenges of semiconductor photocatalysis for solar-to-fuel conversion face different key performance limitations and parameters, including kinetic mismatches between catalytic surface reactions and charge carrier photogeneration, and electronic recombination phenomena within materials as a result of inefficient extraction of photogenerated charges (Stephan et al., 2025). This conversion, however, depends on five major processes, namely light absorption, charge recombination, charge separation, charge migration, and surface redox reactions. These processes and their operational parameters affecting the performance of solar-to-fuel include light capture ability,

reactant nature, operating mode, phases, and photoreactor geometry (Chung et al., 2025).

### III. SEMICONDUCTOR MATERIALS FOR PHOTOCATALYTIC APPLICATIONS

#### ➤ Traditional Metal Oxide Semiconductors

Traditional metal oxide semiconductors, especially  $\text{TiO}_2$  and  $\text{ZnO}$ , are photocatalysts benchmark owing to their non-toxicity, chemical stability, and band-edge alignment (Ramchiary, 2020). Although studies have shown other important metal oxides such as  $\text{CdS}$ ,  $\text{CuO}$ , and  $\text{WO}_3$ , which have been studied for their photocatalytic properties (Karthikeyan et al., 2020), the materials typically generate electron-hole pairs due to irradiation and produce reactive species such as superoxide anions and hydroxyl radicals, which degrade organic pollutants into  $\text{CO}_2$  and  $\text{H}_2$ .

Based on their ability to absorb light and drive redox reactions, including strong oxidative potential, low cost, chemical stability, and non-toxicity, traditional metal oxides such as titanium dioxide ( $\text{TiO}_2$ ) show a wide band gap, which makes it very active under ultraviolet light. This constitutes just a small fraction of solar energy, while the UV-dependence is a limitation on its overall efficiency for solar-powered processes (Vemula & Raavi, 2022).

Zinc oxide ( $\text{ZnO}$ ) is another widely studied oxide with a huge band gap and photocatalytic performance, providing high-cost effectiveness and electron mobility, while suffering from lower long-term stability in aqueous environments and photocorrosion (Weng et al., 2019). Others, such as tungsten trioxide ( $\text{WO}_3$ ), have a narrower band gap and can absorb visible light while maintaining chemical stability under acidic conditions. However, it exhibits limited activity for generating hydrogen and shows weak reduction power (Quan, Gao, & Wang, 2020).

#### ➤ Advanced Semiconductor Systems

Advanced semiconductor systems have expanded the capacity of photocatalysis beyond traditional oxides by allowing for broader absorption of light, tunable properties, and improved charge transport (Sundaram et al., 2024). Perovskite-based oxides such as lanthanum ferrite ( $\text{LaFeO}_3$ ) and bismuth vanadate ( $\text{BiVO}_4$ ) have attracted attention as a result of their narrow band gaps and strong visible-light activity (Nkwachukwu & Arotiba, 2021). In particular,  $\text{BiVO}_4$  demonstrates efficient oxygen evolution, although it suffers from recombination losses and short hole diffusion lengths, which are usually mitigated by surface co-catalysts and heterojunction construction (Xie, 2020).

In addition, layered materials, especially graphitic carbon nitride ( $\text{g-C}_3\text{N}_4$ ), provides a metal-free, chemically stable photocatalyst with visible light response. However, the efficiency is limited by rapid e-hole recombination, which prompts modification via heterostructures with graphene or  $\text{MoS}_2$ , which enhances charge separation with its abundant edge sites and 2-dimensional structure (Dias, 2019; Qin, 2025). Graphene-based composites, on the other hand,

improve conductivity while facilitating interfacial electron transfer to boost the overall activity.

In addition, porous crystalline photocatalysts such as metal-organic frameworks (MOFs) combine functional organic linkers, high surface area, and tunable band structures, which serve as platforms and photocatalysts for hybrid systems with semiconductors to enable pollutant degradation and visible-light harvesting (Porcu, Secci, & Ricci, 2022). Although MOFs experience stability concerns under irradiation, they are designable and versatile photocatalysts for environmental and solar-driven energy applications.

#### ➤ Emerging Materials and Nanostructures

Photocatalysis is being reshaped by emerging nanostructures and semiconductor materials, which help in overcoming limitations of conventional systems (Xu et al., 2019). Quantum dots (QDs) have tunable band gaps through quantum confinement, and demonstrate optical properties and wide light absorption based on their sizes. This makes them efficient in solar-to-chemical energy conversion (Garcia de Arquer et al., 2021). In addition, Ag, Au, and notable plasmonic nanoparticles enhance visible-light activity by localised surface plasmon resonance (LSPR), which generates hot electrons and amplifies electromagnetic fields for improved charge separation (Zhao et al., 2021).

Two-dimensional (2D) materials such as metal dichalcogenides and black phosphorus provide large surface-to-volume ratios and speedy charge transport (Cheng et al., 2020). These materials enable efficient transfer of charge when integrated into van der Waals heterostructures, while expanding spectral response and enhancing catalytic selectivity. In addition, single-atom catalysts (SACs) in semiconductors enable maximisation of atomic efficiency, enhances redox reactions via electronic interactions, and offer well-defined active sites. These nanostructures are a transformative dimension to the design of efficient photocatalysts (Singh et al., 2021).

## IV. DESIGN STRATEGIES FOR ENHANCED PERFORMANCE

### ➤ Band Gap Engineering

Band gap engineering is a core strategy in semiconductor photocatalysis for reducing CO<sub>2</sub> and generating H<sub>2</sub>. Many traditional oxides, such as ZnO and TiO<sub>2</sub>, have wide band gaps for absorbing only UV light; hence, the need for applying doping to extend absorption into the visible range (Ayyub & Rao, 2020). Through metal doping with Fe, Cu, and Mn, the band gap gets localized states, which helps to improve charge separation, although excessive doping can be used as recombination centers.

On the other hand, non-metal doping with N, S, and C transforms the valence band via p-orbital hybridization, which helps to lower band gap energy while enhancing visible light response (Hussain et al., 2022). The formation of solid solution, such as exists in mixed oxides (BiVO<sub>4</sub>-WO<sub>3</sub> or TiO<sub>2</sub>-ZrO<sub>2</sub>), allows for compositional band edges tuning, which helps in balancing solar absorption and redox potentials (Rajamanickam, Kanmani, & Ramachandran, 2022). In addition, defect engineering, especially the introduction of oxygen vacancies, offers shallow trap states for improved carrier mobility and adsorption and activation of CO<sub>2</sub>. However, precision is required to avoid recombination pathways that may be detrimental (Zhong, Sun, & Xu, 2025). These approaches collectively optimise the use of charge and light harvesting in the conversion of solar to fuel energy.

### ➤ Heterostructure Design

Heterostructure design can also be used to improve the efficiency of photocatalysis by promoting the separation of directional charge (Chen et al., 2021). For efficient electron-hole separation, type II heterojunctions, which are formed between semiconductors characterised by staggered band alignments, are applied, although this often affects redox potential (Balapure, Dutta, & Ganesan, 2024). Therefore, the Z-scheme heterojunctions are introduced to overcome this, which mimic photosynthesis through retention of strong redox capability and improving charge transfer as in g-C<sub>3</sub>N<sub>4</sub> or TiO<sub>2</sub>, or RGO systems (Behera, Kar, & Srivastava, 2022).

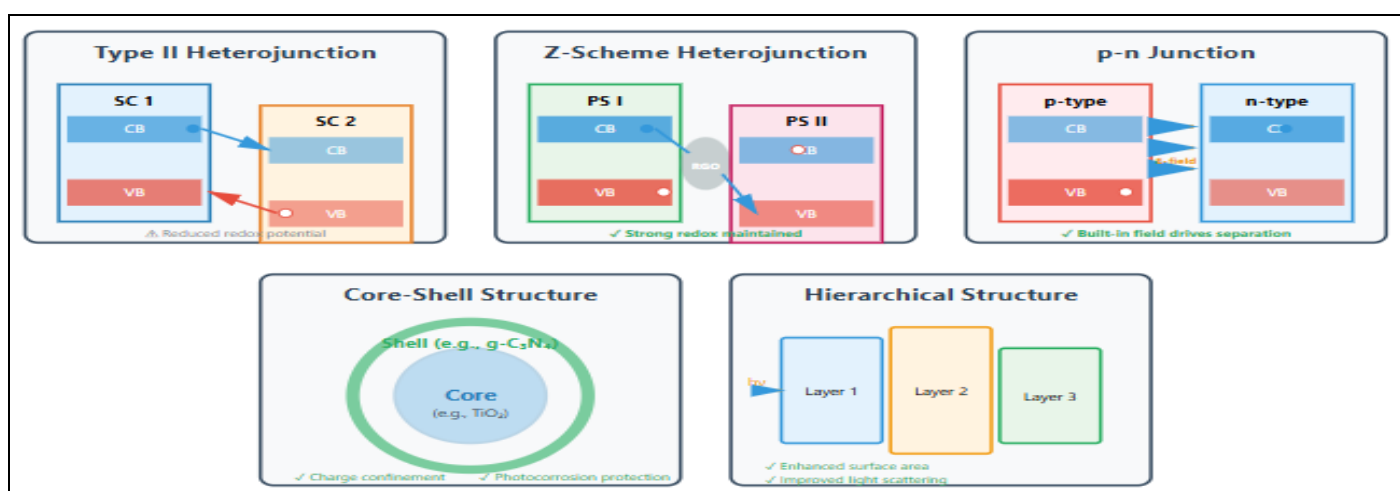


Fig 2 Comparison of Heterostructure Architectures for Improved Charge Separation



P-n junction photocatalysts depend on built-in electric fields to propel the separation of charge while improving stability. Hierarchical and core-shell structures provide synergistic benefits by confining charges and suppressing photocorrosion, and increasing surface area, and improving light scattering (Liu, 2023). Through these engineered architectures, photocatalytic efficiency is bound to improve alongside durability under solar irradiation. Hence, strategic heterostructure design is critical for advancing water-splitting and CO<sub>2</sub> photoreduction technologies.

#### ➤ *Co-Catalysts and Surface Modification*

Co-catalyst integration and surface modification are essential in accelerating the transfer of charge and selecting the tuning reaction. Well-established metals such as Ag, Au, and Pt act as electron sinks, minimising recombination while promoting hydrogen evolution kinetics (Kumar et al., 2024). Gold (Au) and Silver (Ag) introduce plasmonic effects, where light absorption is extended into the near-infrared and visible range. The scarcity and high cost of these metals, however, have allowed for increased interest in earth-abundant alternatives, including Cu-, Co-, and Ni-based co-catalysts, providing promising performance for reducing CO<sub>2</sub> and producing H<sub>2</sub> at lower cost, despite its reduced stability (Gelle et al., 2019). CO<sub>2</sub> adsorption can also be improved through surface functionalization with anchoring molecular catalysts or organic linkers, while also helping to control product selectivity and lower activation barriers (Song et al., 2023). Integrating relevant co-catalysts with semiconductor photocatalysts is a major strategy for selective, efficient, and scalable solar fuel generation.

### V. APPLICATIONS AND RECENT ADVANCES

#### ➤ *CO<sub>2</sub> Photoreduction*

Photocatalytic reduction of CO<sub>2</sub> provides a sustainable pathway to produce value-added chemicals, including CH<sub>4</sub>, CH<sub>3</sub>OH, HCOOH, and CO (Bhatia, Dharaskar, & Unnarkat, 2021). The semiconductor's band structure, number of electrons in the reduction process, and surface catalytic sites govern the product selectivity (Zhou, Luo, & Guo, 2022). For example, HCOOH and CO are favored in bi-electron pathways, while CH<sub>3</sub>OH and CH<sub>4</sub> require more complex transfers of many electrons. Generally, the mechanism involves adsorption of CO<sub>2</sub>, activating through reduction or bending to intermediates (HCOO and CO<sub>2</sub>) and proton-coupled electron transfer. Recent breakthroughs range from atomically dispersed Cu on TiO<sub>2</sub> for the selective formation of CH<sub>4</sub>, MOF-based composites getting more CO selectivity under visible light, and bi-based semiconductors with oxygen vacancies (Kong & Chen, 2024). However, despite these advances, competing hydrogen evolution, low conversion efficiencies, and other challenges persist. Nevertheless, recent materials have shown quantum efficiencies approaching practical levels, which implies the potential of catalyst design for selective conversion of CO<sub>2</sub> to fuel (Hasani et al., 2019).

#### ➤ *Photocatalytic Hydrogen Production*

The generation of hydrogen via photocatalysis proceeds through reforming reactions or water splitting. Although

thermodynamically demanding, water splitting offers a clean route to achieve this, while requiring efficient charge separation and necessary redox potentials (Rafique et al., 2020). Meanwhile, recombination is suppressed by using different systems, which adopt sacrificial agents such as triethanolamine and methanol, which also help in improving rates of hydrogen evolution (Kumaravel et al., 2019). Experts, however, argue that this reduces scalability. In general, water splitting is achieved in systems like Rh-doped SrTiO<sub>3</sub> or GaN:ZnO solid solutions, which is the ultimate goal. Also, according to recent works, emphasis is on the integration of CO<sub>2</sub> reduction and production of H<sub>2</sub> to generate syngas (CO + H<sub>2</sub>), which is a versatile fuel and chemicals precursor (Varvoutis et al., 2022). In addition, strategies including tandem photocatalytic systems and dual-reactor setups help in coupling the reactions under solar irradiation. With advances in nanostructured catalysts, such as plasmonic-semiconductor hybrids and single-atom co-catalysts, H<sub>2</sub> evolution activity will be significantly improved. Scalability and stability, however, remain major challenges, which shows that low-cost and durable photocatalysts are needed to achieve practical conversion of solar energy to hydrogen (Puertolas et al., 2022).

### VI. CHALLENGES AND FUTURE PERSPECTIVES

#### ➤ *Current Limitations*

Despite advancements, photocatalytic reduction of CO<sub>2</sub> and production of hydrogen (H<sub>2</sub>) are constrained by many limitations. On the one hand, solar-to-fuel conversion efficiencies are below practical requirements (<2-3%), as a result of rapid charge recombination, limited catalytic activity, and insufficient light absorption (Liu et al., 2022). On another hand, catalyst stability is critical, as many materials undergo surface poisoning, photocorrosion, and structural degradation during a lengthened operation (Li et al., 2022). Selectivity in CO<sub>2</sub> reduction is problematic because competitive hydrogen evolution usually dominates, resulting in low product yields (Saha, Amanullah, & Dey, 2022). Finally, scale-up from laboratory practical to pilot plants faces engineering and economic barriers such as low quantum efficiency under natural sunlight, reactor design complexity, and high material costs, which collectively hinder effective industrial deployment of photocatalytic systems, and emphasize the need for more scalable technologies and robust materials (Mani et al., 2025).

#### ➤ *Future Directions*

Future efforts in this research should focus on the development of photosynthesis systems that imitate biological pathways, which enable efficient multi-electron CO<sub>2</sub> and water transformations. Integrating with renewable electricity through hybrid or photoelectrochemical systems can enhance efficiency and offer tunable reaction control (Niu et al., 2020). High-throughput computational screening and machine learning will accelerate catalyst discovery by predicting optimal compositions, surface modifications, and heterostructures (Benavides-Hernandez & Dumeignil, 2024). In addition, life-cycle assessment (LCA) and techno-economic analysis (TEA) are required for guiding research toward environmentally sustainable and economically viable

solutions (Zimmermann et al., 2020; Hammed et al., 2025). It is also critical to emphasize earth-abundant, recyclable, and stable photocatalysts to minimise dependence on scarce metals. Through the combination of advanced materials, systems-level evaluation, and innovative reactor engineering, future research can bridge the gap between large-scale implementation and laboratory feasibility, which paves the way for practical solar fuel production.

## VII. CONCLUSIONS

Semiconductor-based photocatalysts hold huge promises for sustainable CO<sub>2</sub> reduction and hydrogen production, although their practical application is limited by stability, scalability, and efficiency challenges. Design principles such as heterostructure formation, band gap engineering, and surface modification have improved photocatalyst performance, while emerging materials, including layered structures, perovskites, and single-atom catalysts, provide new opportunities. In recent developments, light utilization and selectivity are evidenced, although there is still a need to overcome fundamental bottlenecks in long-term stability and charge separation.

Thus, an integrated approach that combines advanced material design, techno-economic evaluations, and artificial photosynthesis concepts is required to address the challenges. Carbon-neutral fuels and a sustainable energy future are achievable with semiconductor photocatalysis transforming sustained innovation and research.

### ➤ Authors' Contribution

- Osasere A. Uwumwose – Conceived the research idea, supervised the study design, and coordinated manuscript integration.
- Victor Hammed – Developed the environmental sustainability framework and contributed to the abstract, introduction, and conclusion.
- Esther T. Omoyiwola – Managed manuscript organization, literature review, and correspondence throughout the submission process.
- Terfa J. Igba – Analyzed material synthesis and catalytic mechanisms and contributed to sections on metal oxides and surface modification.
- Nwankwo U. Dickson – Compiled data, validated technical details, and contributed to sections on CO<sub>2</sub> photoreduction and hydrogen production.

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