INSIGHTS-JOURNAL OF
LIFE AND SOCIAL SCIENCES

INSIGHTS-JLSS
Insights-Journal of Life and Social Sciences

DEVELOPMENT OF PHOTO-CATALYTIC MATERIALS FOR WATER SPLITTING- A TECHNICAL REPORT

Original Article

Amirab Nazir[1], Muhammad Ummad Abbasi[2], Ali Raza[3], Atfa Ashraf[4], Muhammad Asif[5], Dawood Ali[6], Muniba Riaz[7]*

[1]Student, University of Agriculture, Faisalabad, Pakistan.
[2]Department of Applied Chemistry and Chemical Technology, University of Karachi, Karachi, Pakistan.
[3]Riphah International University, Faisalabad, Pakistan.
[4]Lecturer, Department of Chemistry, Government Associate College (W), Narang Mandi, Pakistan.
[5]M.Phil Scholar, Department of Chemistry, University of Agriculture, Faisalabad, Pakistan.
[6]Forman Christian College University, Lahore, Pakistan.
[7]Lecturer, Department of Chemistry, Superior Group of Colleges, Raiwind, Pakistan.

Corresponding Author: Muniba Riaz, Lecturer, Department of Chemistry, Superior Group of Colleges, Raiwind, Pakistan, Munibamayo997@gmail.com

Conflict of Interest: None

Grant Support & Financial Support: None

Acknowledgment: The authors acknowledge the valuable insights and contributions from colleagues in the field of sustainable energy research.

ABSTRACT

Background: Photocatalytic water splitting has emerged as a promising pathway for sustainable hydrogen production, addressing global energy demands and environmental concerns. By harnessing solar energy to split water into hydrogen and oxygen, photocatalytic technologies offer a carbon-neutral alternative to fossil fuels. Recent advances in material science have led to the development of high-efficiency photocatalysts capable of improving solar-to-hydrogen conversion rates. This study provides an in-depth analysis of the latest trends in photocatalyst design, fabrication, and application, with a focus on real-world scalability.

Objective: To evaluate and synthesize recent developments in photocatalytic materials and their practical applications in water splitting for renewable hydrogen production.

Methods: This technical review compiles and analyzes peer-reviewed research from the past five years on the synthesis and modification of photocatalysts including semiconductor-based, heterostructured, and plasmonic materials. Characterization techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), and UV-Vis spectroscopy were critically examined. Key strategies including surface modification, cocatalyst integration, and bandgap engineering were reviewed for their impact on photocatalytic efficiency. The operational performance of photoelectrochemical cells and photocatalytic reactors was also analyzed.

Results: Recent studies demonstrated enhanced hydrogen evolution rates up to 61.5 mmol h^{-1} g^{-1} using dual cocatalyst systems on TiO_2. Apparent quantum yields have reached 42.5% under visible light, while solar-to-hydrogen (STH) efficiencies of up to 1.1% have been recorded using Al-doped $SrTiO_3$ with Rh/Cr_2O_3. Long-term durability studies showed 80% activity retention over 1300 hours. Modified $BiVO_4$ and GaN:ZnO photocatalysts demonstrated efficient charge separation and visible light absorption.

Conclusion: Advances in photocatalyst materials and system integration are steadily improving the feasibility of photocatalytic water splitting for green hydrogen production. Future research should focus on cost-effective scaling and integration with renewable energy sources.

Keywords: Bandgap Engineering, Cocatalyst Integration, Hydrogen Production, Photocatalysis, Semiconductors, Solar-to-Hydrogen Efficiency, Water Splitting.

INTRODUCTION

The global urgency to transition toward cleaner and sustainable energy sources has brought renewed attention to hydrogen energy, especially as fuel cell technologies gain momentum due to their minimal environmental footprint. Hydrogen, with its high energy content and emission-free combustion, represents a promising alternative to fossil fuels. However, industrial hydrogen production still largely relies on the steam reforming of hydrocarbons such as methane, a process that emits significant amounts of greenhouse gases and undermines its environmental benefits (1). For hydrogen to be a truly green energy carrier, it must be generated through water splitting using renewable energy sources, thus eliminating reliance on carbon-intensive feedstocks. Water splitting, the chemical decomposition of water into oxygen and hydrogen, stands out as one of the most promising pathways to clean hydrogen production. The challenge, however, lies in achieving this process efficiently and economically (2,3). Among various strategies, photocatalytic water splitting has garnered significant scientific interest, as it utilizes solar energy to drive the reaction. The concept is not new—dating back to the groundbreaking work on the Honda–Fujishima effect, where titanium dioxide (TiO_2) was employed as a photoanode to split water under ultraviolet light exposure (4). This discovery opened up a multidisciplinary field encompassing catalysis, electrochemistry, photochemistry, and materials science. Despite considerable efforts, only a limited number of photocatalysts have been found to split water into hydrogen and oxygen in stoichiometric proportions with practical efficiency (5,6).

To date, metal oxides remain the primary class of materials capable of demonstrating appreciable photocatalytic activity under experimental conditions. Even so, the majority suffer from limitations such as low quantum efficiency, poor visible light absorption, and rapid charge carrier recombination, all of which hinder their practical application (7). In response to these challenges, a wave of new photocatalytic materials has emerged, incorporating innovative design strategies such as heterojunction formation, doping, and nanostructuring to improve performance metrics (8). These advancements have positioned the field on the cusp of transformative breakthroughs, yet the path to widespread adoption remains encumbered by both material and mechanistic constraints. Given this backdrop, the present study aims to explore and evaluate emerging photocatalysts capable of efficient and sustainable water splitting, with the overarching goal of contributing to environmentally benign hydrogen production technologies.

Fundamentals of photocatalytic water splitting

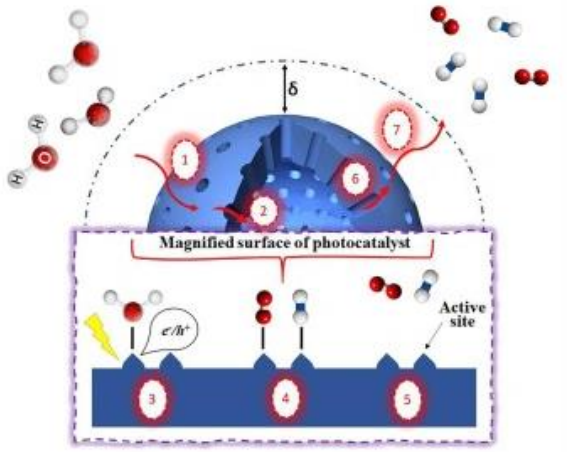
Photocatalytic overall water splitting (POWS) is a thermodynamically uphill process ($\Delta G > 0$), requiring an external energy input to cleave H_2O into hydrogen and oxygen gases. Light energy, especially from the solar spectrum, serves as the external input in heterogeneous photocatalysis. Photocatalytic reactions commence when a semiconductor absorbs photons with energy equal to or greater than its band gap, triggering the generation of charge carriers. For optimal performance, the semiconductor's conduction band (CB) and valence band (VB) must align appropriately with the redox potentials of H_2/H^+ (0 V) and O_2/H_2O (1.23 V), respectively. pH, band structure, and overpotentials for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) also impact efficacy (4,5). The inherent challenge of electron-hole recombination, occurring from femtoseconds to milliseconds, significantly curtails reaction efficiency and remains a central limitation.

Photochemistry of water splitting

Semiconductor photocatalysts, with defined band gaps (Eg), undergo photon-induced excitation leading to electron (e^-) transition to the CB and simultaneous creation of holes (h^+) in the VB. These photogenerated species migrate to the surface and initiate redox reactions with adsorbed water, producing H_2 and O_2. This multi-step process involves photon absorption, charge excitation, generation of e^-/h^+ pairs, and their surface reactions. However, rapid recombination remains a bottleneck. To be viable, materials must possess $Eg \geq 1.23$ eV and appropriate band edge straddling, excluding many semiconductors like CdSe and Fe_2O_3. Materials like ZrO_2, though promising, require high activation energy due to their wide band gap (6).

Surface phenomena of photocatalyst during water splitting

Photocatalytic water splitting involves several key stages, starting with diffusion of H_2O to the photocatalyst surface, internal transport through porous networks, adsorption, redox reactions, and finally desorption of H_2 and O_2 gases. Internal diffusion, particularly in nano-sized pores, is critical for maximizing access to active sites. Effective replenishment of water molecules and swift gas desorption are necessary to prevent reverse reactions and recombination. The kinetics of these surface interactions, coupled with material morphology, dictate overall system efficiency (7).



Fig, 1: Seven catalytic steps in heterogeneous photocatalytic water splitting

Thermodynamics of water splitting

The thermodynamic feasibility of POWS is tied to the band gap energy and the quasi-Fermi level differences between electrons and holes. The driving force for photoreaction (ΔG) must be sufficiently large to overcome the uphill energy requirements. As thermal energy alone cannot support this process (ΔH = 0), photon energy (hv > Eg) provides the necessary ΔG. Elevated temperatures improve reaction kinetics and H_2/O_2 desorption but also introduce complexities related to recombination dynamics and surface stability (7,8).

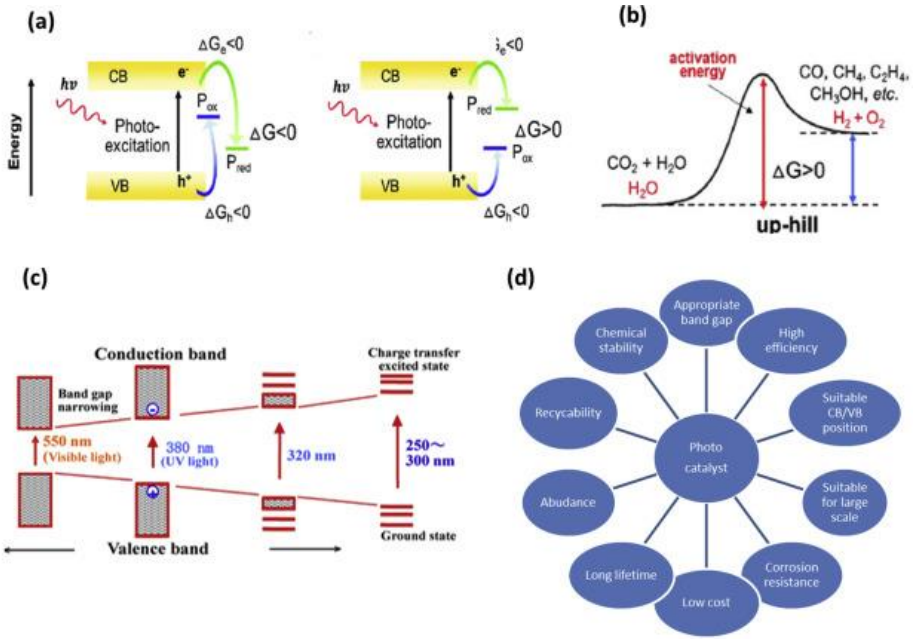


Fig. 2: (a): Electronic structure of semiconductor photocatalysts and Gibbs energy change in photocatalytic reactions; (b) water splitting as uphill reaction (c) Narrowing and expansion of band gap of semiconductor (d) water splitting as uphill reaction

Mechanism of photocatalytic overall water splitting

Efficient POWS requires materials that absorb visible light, align band positions with redox potentials, and possess strong charge separation and migration characteristics. To drive both HER and OER simultaneously, many systems incorporate co-catalysts or utilize Z-scheme mechanisms where multiple materials complement each other's band positions. Though some systems, such as Al-doped

$SrTiO_3$ with Rh/Cr_2O_3, have demonstrated stability and moderate solar-to-hydrogen (STH) efficiencies (up to 1.1%), most fail to reach the target 10% STH needed for commercial viability (8,9).

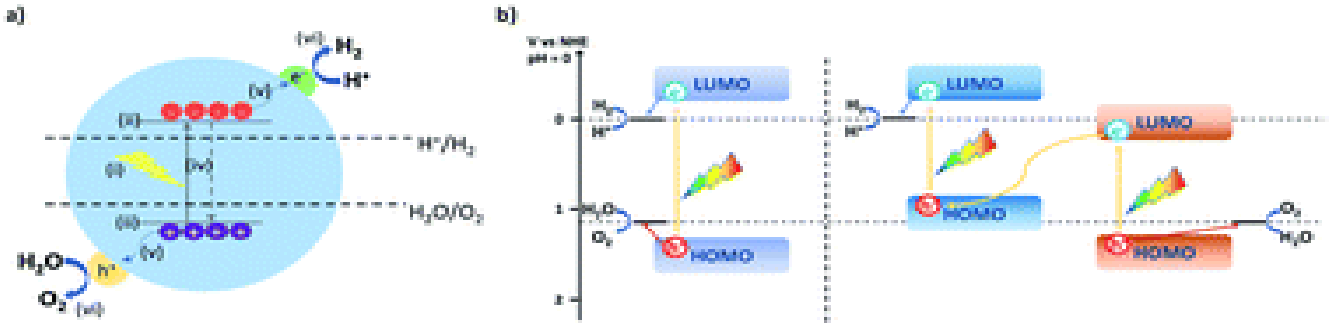


Fig.3: (a) Diagram showing the reactions during water splitting on a semiconductor photocatalyst; (b) working principle of single component photocatalysts (left) and photocatalyst Z-schemes (right) for overall water splitting

Constraints of photocatalytic water splitting

POWS research faces several challenges including: dependence on UV-responsive materials, lack of real-world scalability, seawater incompatibility, and high material/equipment costs. Laboratory conditions often fail to simulate environmental complexities, limiting external validity. Moreover, the energy input-output balance often remains unfavorable due to suboptimal conversion efficiencies and photocatalyst degradation (8,10).

PHOTOCATALYTIC REACTIONS

Types of reaction: Photocatalytic water splitting reactions are broadly classified into photochemical and photoelectrochemical categories.

Photochemical reactions

These involve a semiconductor suspended in an aqueous medium, where light initiates charge separation. The photogenerated electrons and holes react with water at the semiconductor-electrolyte interface. Band edge alignment and semiconductor stability in the electrolyte are essential to prevent degradation (11).

2.1.2. Photo-electrochemical reactions

In PEC systems, semiconductor electrodes directly exposed to light generate photocurrents. Here, oxidation and reduction occur at separate electrodes, providing better control over half-reactions. Semiconductors function as photoanodes or photocathodes depending on the desired reaction (5,12).

2.2. Reaction setup

Experimental setups include a reaction chamber, gas circulation pump, and analytical instruments such as gas chromatographs. Light sources vary depending on band gap requirements—UV for wide-gap semiconductors and xenon lamps for visible light response. Ensuring an air-free system is essential for accurate O_2 detection (12,13).

STRATEGIES FOR ENHANCED PHOTOCATALYTIC PERFORMANCE

3.1. Defect engineering in photocatalytics

Introducing defects like oxygen vacancies (Vo) modifies electronic structures and enhances light absorption. Methods include hydrogenation, plasma treatment, and anion doping. N-doped TiO_2, for instance, exhibits enhanced visible light activity due to narrowed band gap and altered electronic states (3,14).

3.2. Photocatalysis at elevated temperatures

Elevated temperatures accelerate reaction kinetics and increase H_2 evolution rates. Black TiO_2 treated under hydrogen shows extended light absorption up to 900 nm. Systems incorporating black phosphorus nanosheets have also demonstrated up to nine-fold performance improvements at 353K (7,15).

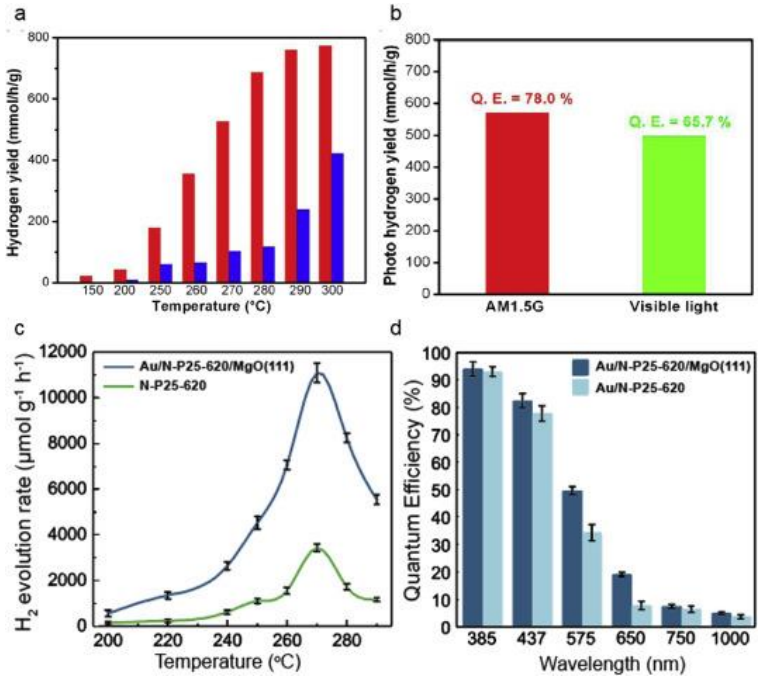


Fig. 4: (a)Temperature-enhanced from H_2O with a (30% methanol) without light illumination (b) apparent quantum efficiencies of visible light and AM 1.5 global sunlight over black Pt/TiO_2 catalyst at 280 °C(c) Photocatalytic activities of N–P25-620 and Au/N–P25-620 with at different temperatures; (d) QE of different wavelengths over Au/N–P25-620 with and without MgO (111) photocatalysts at 270 °C (QE, quantum efficiency)

3.3. Decoration with cocatalyst

Cocatalysts like Pt, Au, and Rh facilitate HER, while metal oxides (e.g., CoO, IrO_2) support OER. They reduce activation energies, enhance charge separation, and prevent recombination. Rh@Cr_2O_3 core-shell structures, for example, restrict back-reactions, maintaining high water-splitting rates (11,16).

3.4. Dual cocatalyst system for water splitting

Dual cocatalyst systems use distinct materials for HER and OER. Synergistic effects have been reported, such as Pt-RuO_2 on Zn_2GeO_4 showing over 2x enhanced activity compared to single-catalyst systems. Strategic placement of Pt–Au on TiO_2 facets further enhances photocatalytic yield (15,17).

4.1. CRITICAL POINTS TO REMEMBER

4.1.1 Evolution of H_2 and O_2 stoichiometry

Accurate stoichiometric generation of H_2 and O_2 (2:1) confirms true photocatalytic water splitting. Absence of O_2 may indicate sacrificial reactions or incomplete processes (18).

4.1.2 Time sequence

Gas evolution should increase linearly over time under constant illumination. Time-resolved measurements are crucial for reliability and repeatability.

4.1.3 Turnover number (TON)

TON quantifies catalyst efficiency. Low TON suggests stoichiometric side reactions or inactive catalytic cycles.

4.1.4 Quantum yield

Apparent quantum yield (AQY) offers a standardized performance metric. It is calculated from the ratio of reacted electrons to incident photons, yet remains lower than actual due to photon scattering.

4.1.5 Photoresponse

Material response to monochromatic light helps determine true band gap activity. Control experiments are necessary to eliminate mechanocatalytic interference.

4.2 Experimental setup

A gas-closed circulation system equipped with real-time analysis tools is preferred. For UV-responsive materials, high-pressure mercury lamps are used, while solar simulators are employed for visible-light-active systems (19).

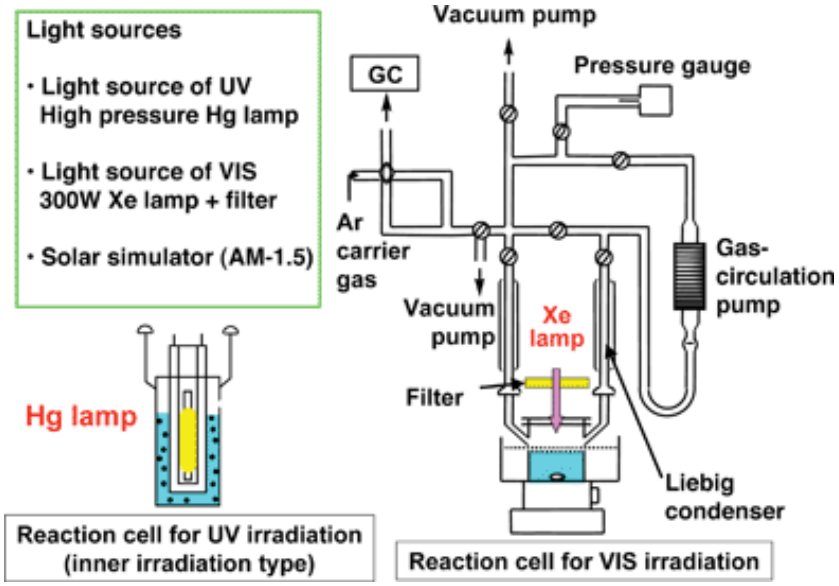


Fig. 5: An example of the experimental setup for photocatalytic

5. MATERIALS FOR PHOTOCATALYSIS

5.1. Exploring descriptions and material design

Ideal photocatalysts possess narrow yet sufficient band gaps, high surface area, and photostability. Co-catalysts and dopants fine-tune redox activity and spectral absorption.

5.2. Titanium dioxide

TiO_2 remains the most widely studied material. Despite its stability, its wide band gap restricts solar utilization. Doping with Br, Cl, C, and N has shown improved visible light absorption (20).

5.3. Metal oxides

Materials like $BiVO_4$, Fe_2O_3, and WO_3 offer better visible light response but often suffer from poor conductivity or recombination. Ternary systems show improved band edge alignment and current efficiency (21).

5.4. Metal sulphides

CdS and ZnS show promise under visible light but suffer from photodegradation. Incorporation of noble metals can enhance stability and HER rates (22).

5.5. Nitrides

Nitrides like GaN and ZnO exhibit better solar harvesting due to higher N 2p orbital energies. Though typically possessing wide band gaps, doped or alloyed nitrides remain under investigation for POWS (23).

6. Theoretical modeling approach for photocatalytic water splitting

Computational tools like density functional theory (DFT) and many-body perturbation theory (MBPT) have been critical in understanding band structures, surface energetics, and dopant effects. These models expedite material screening and guide experimental designs (24).

CONCLUSION

In conclusion, this study highlights the transformative potential of photocatalytic materials in advancing sustainable energy technologies, particularly through the efficient splitting of water into hydrogen and oxygen using solar energy. By focusing on semiconductors such as titanium dioxide, bismuth vanadate, and doped metal oxides, the research underscores their critical role in enabling clean, renewable hydrogen production. These materials not only align with global efforts to combat climate change and reduce dependency on fossil fuels but also offer broader applications in environmental remediation. As innovations in photocatalyst design and efficiency continue to emerge, their integration into real-world systems could mark a pivotal step toward a more sustainable and carbon-neutral energy future.

AUTHOR CONTRIBUTION

Author	Contribution
Amirab Nazir	Substantial Contribution to study design, analysis, acquisition of Data Manuscript Writing Has given Final Approval of the version to be published
Muhammad Ummad Abbasi	Substantial Contribution to study design, acquisition and interpretation of Data Critical Review and Manuscript Writing Has given Final Approval of the version to be published
Ali Raza	Substantial Contribution to acquisition and interpretation of Data Has given Final Approval of the version to be published
Atfa Ashraf	Contributed to Data Collection and Analysis Has given Final Approval of the version to be published
Muhammad Asif	Contributed to Data Collection and Analysis Has given Final Approval of the version to be published
Dawood Ali	Substantial Contribution to study design and Data Analysis Has given Final Approval of the version to be published
Muniba Riaz*	Contributed to study concept and Data collection Has given Final Approval of the version to be published

REFERENCES

1. Kravets VG, Grigorenko AN. Water and seawater splitting with MgB(2) plasmonic metal-based photocatalyst. Sci Rep. 2025;15(1):1224.
2. Askari N, Jamalzadeh M, Askari A, Liu N, Samali B, Sillanpaa M, et al. Unveiling the photocatalytic marvels: Recent advances in solar heterojunctions for environmental remediation and energy harvesting. J Environ Sci (China). 2025;148:283-97.

3. Wei Y, Wang R, Wang M, Hu L, Zhang X, Xu Y, et al. Research status and prospects of organic photocatalysts in algal inhibition and sterilization: a review. Environ Sci Pollut Res Int. 2024;31(4):5013-31.
4. Augustin A, Chuaicham C, Shanmugam M, Vellaichamy B, Rajendran S, Hoang TKA, et al. Recent development of organic-inorganic hybrid photocatalysts for biomass conversion into hydrogen production. Nanoscale Adv. 2022;4(12):2561-82.
5. Tao X, Zhao Y, Wang S, Li C, Li R. Recent advances and perspectives for solar-driven water splitting using particulate photocatalysts. Chem Soc Rev. 2022;51(9):3561-608.
6. Zhou H, Grigorenko AN, Kravets VG. Photocatalytic Seawater Splitting by Earth-Abundant Catalysts: Metal-Semiconductor Metamaterials Made of Plasmonic Magnesium Diboride and Transitional Metal Dichalcogenides. Chemistry. 2024;30(71):e202403050.
7. Li R, Chen H, Xiong J, Xu X, Cheng J, Liu X, et al. A Mini Review on Bismuth-Based Z-Scheme Photocatalysts. Materials (Basel). 2020;13(22).
8. Zhu X, Xiong J, Wang Z, Chen R, Cheng G, Wu Y. Metallic Copper-Containing Composite Photocatalysts: Fundamental, Materials Design, and Photoredox Applications. Small Methods. 2022;6(2):e2101001.
9. McQueen E, Bai Y, Sprick RS. Impact of Interfaces, and Nanostructure on the Performance of Conjugated Polymer Photocatalysts for Hydrogen Production from Water. Nanomaterials (Basel). 2022;12(23).
10. Sahoo P. Hydrogen-producing Photocatalyst at Sunscreen for Athletes in Preventing and Healing Muscle-nerve-skin Injuries. Curr Top Med Chem. 2023;23(4):249-56.
11. Prabhakar Vattikuti SV, Zeng J, Ramaraghavulu R, Shim J, Mauger A, Julien CM. High-Throughput Strategies for the Design, Discovery, and Analysis of Bismuth-Based Photocatalysts. Int J Mol Sci. 2022;24(1).
12. Ghosh R, Singh M, Chang LW, Lin HI, Chen YS, Muthu J, et al. Enhancing the Photoelectrochemical Hydrogen Evolution Reaction through Nanoscrolling of Two-Dimensional Material Heterojunctions. ACS Nano. 2022;16(4):5743-51.
13. Ray SK, Hur J. A critical review on modulation of NiMoO(4)-based materials for photocatalytic applications. J Environ Manage. 2021;278(Pt 1):111562.
14. Zhang J, Bifulco A, Amato P, Imparato C, Qi K. Copper indium sulfide quantum dots in photocatalysis. J Colloid Interface Sci. 2023;638:193-219.
15. Carminati SA, Rodríguez-Gutiérrez I, de Morais A, da Silva BL, Melo MA, Souza FL, et al. Challenges and prospects about the graphene role in the design of photoelectrodes for sunlight-driven water splitting. RSC Adv. 2021;11(24):14374-98.
16. Abbasi Asl H, Sabzehmeidani MM, Ghaedi M, Moradi Z. Bifunctional quaternary magnetic composite as efficient heterojunctions photocatalyst for simultaneous photocatalytic visible light degradation of dye and herbicide pollutants from water and bacterial disinfection. J Environ Manage. 2023;345:118656.
17. Porcu S, Secci F, Ricci PC. Advances in Hybrid Composites for Photocatalytic Applications: A Review. Molecules. 2022;27(20).
18. Sohail M, Imran S, Tariq M, et al. Recent progress in semiconductor photocatalysts for water splitting: fundamental insights and strategies. J Environ Chem Eng. 2024;12(2):110865.
19. Ng YH, Iwase A, Kudo A. Z-scheme water splitting under visible light: current status and future prospects. Phys Chem Chem Phys. 2021;23(4):1843–1864.
20. Tahir M, Amin NAS. Advances in visible light-responsive photocatalysts for hydrogen production. Renew Sustain Energy Rev. 2020; 132:110042.
21. Bai Y, Li X, Wang X, et al. Engineering efficient Z-scheme photocatalysts for solar water splitting. Nano Energy. 2021; 84:105922.
22. Li Y, Tsang SC. Visible-light-driven photocatalysis and advanced defect engineering. Chem Eng J. 2020; 389:124432.
23. Ahmed A, Khan MI, et al. First-principles computational modeling of photocatalysts: bridging the theory-experiment gap. J Mater Chem A. 2021;9(20):12290–12307.
24. Goodarzi M, Amini MM, et al. Evaluation protocols in photocatalytic water splitting. Mater Today Chem. 2023; 29:101269.

