A Conceptual Note on Photocatalytic Green Hydrogen Production Using g-C_3 N_4 -Based Systems

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Abstract—**With the growing demand for sustainable energy solutions, green hydrogen is increasingly recognized as a clean and sustainable energy carrier, offering significant potential in reducing carbon emissions and supporting global climate goals. However, the high cost of hydrogen production remains a major obstacle to large-scale adoption. This study presents a comprehensive techno-economic analysis of solar-driven photocatalytic hydrogen production using graphitic carbon nitride (g-C_3N_4)-based system with a focus on the South African energy landscape. The technical evaluation includes catalyst performance, solar-to-hydrogen conversion efficiency, and system scalability, while the economic assessment focuses on capital and operational costs, energy production, levelized cost of hydrogen (LCOH), and sensitivity to key parameters such as catalyst price and solar irradiance. the techno-economic estimate for photocatalytic hydrogen production is approximately $6.41 per kilogram of hydrogen, with a potential low-end cost ranging from $2 to $4/kg, assuming future technological improvements and access to low-cost renewable energy. On the other hand, high-end estimates can reach $10 to $15/kg, particularly for early-stage or small-scale systems. This is relatively high compared to conventional methods but shows promise for future cost reductions with technological improvements. Solar-powered hydrogen production systems demonstrate superior long-term sustainability and lower environmental impact compared to grid-powered alternatives. While conventional energy systems are more stable and less capital-intensive initially, they rely heavily on fossil fuels in many ways, contributing to greenhouse gas emissions and undermining environmental objectives. Results indicate that g-C_3N_4, due to its visible-light activity and low-cost synthesis holds promise for decentralized hydrogen production, though current efficiencies remain a limiting factor. These findings align with South Africa's Hydrogen Society Roadmap (HSRM) and the African Union's Agenda 2063 and contributes to the strategic development of cost-effective, solar-driven hydrogen technologies aligned with global decarbonisation targets under SDG 7 (Affordable and Clean Energy) and SDG 13 (Climate Action), SDG 9 (Industry, Innovation, and Infrastructure).**

Keywords— **g-C_3 N_4 (graphitic carbon nitride, Green hydrogen, Photocatalytic hydrogen production,), Solar energy, Techno-economic analysis About four key words or phrases in alphabetical order, separated by commas.**

I. INTRODUCTION

The energy crisis in South Africa and the implications it has on the energy markets reportedly has significant disruption in the economy and fossil fuels. Discussions of factors that contribute to such adverse effects such as: the increase in population, which has led to an energy demand, the use of fossil fuels, which has increased greenhouse gas emissions[1].

The demand for hydrogen is expected to significantly increase in the near future owing to the growing needs of refinery, chemical industries, as well as new applications such as synthetic fuel, bio-fuel production[2]

South Africa has been reported to be among the world's worst polluting countries due to its industrial activities continuing to rely on coal-power generation with a high carbon footprint[3]

South Africa has abundant renewable energy resources (wind, sun, and vast coastlines/sea), which can be utilized to meet its energy needs and reduce CO_2 emission[4]. This makes South Africa as a potential country in Africa to join others (European Union, Germany, Norway, Spain, China, Chile) to stimulate green hydrogen production.[3].

Hydrogen is a colorless gas, but depending on its environmental impact, energy source, and production method, it can be classified into different color codes [5] . Green hydrogen: Produced by water electrolysis using RE sources, which have no carbon emissions. Blue hydrogen: Produced by steam methane reforming. In this method, the generated CO_2 is captured and stored to prevent its release. Gray hydrogen: Produced by steam methane reforming CO_2 is released into the atmosphere Black/brown hydrogen: Produced by the gasification of coal or oil. CO_2 and other pollutants are emitted [6].. Hydrogen is expected to be a crucial energy carrier in future global energy systems. It can be used in several applications, from power fields, including the manufacturing industry, transportation, and power generation[7]

Despite the undeniable environmental benefit of using sustainable hydrogen for energy production, energy demand is inversely correlated with economic growth. Hydrogen is a clean energy carrier with potential to decarbonize multiple sectors [8]. Green hydrogen production via photocatalysis has emerged as a sustainable and environmentally friendly alternative to fossil fuel-based hydrogen generation. Two of the most extensively studied photocatalysts are titanium dioxide (TiO_2) and graphitic carbon nitride (g-C_3 N_4)[9]. TiO_2 is known for its chemical stability, non-toxicity, and wide availability, but its activity is limited to ultraviolet (UV) light due to its wide bandgap. In contrast, graphitic carbon nitride (g-C_3 N_4) stands out due to its visible-light activity, chemical stability, and tunable electronic properties [10]. Graphitic carbon nitride (g-C_3 N_4) is a metal-free polymeric semiconductor composed of carbon and nitrogen atoms

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arranged in a layered structure based on tri-s-triazine units. It has a moderate bandgap of ~2.7 eV, which allows it to absorb visible light up to ~460 nm. Its structure offers high thermal stability (up to 600°C in air), chemical inertness, and environmental friendliness, making it suitable for sustainable photocatalytic applications, making it attractive for scalable applications [11]

The material can be synthesized via thermal polymerization of nitrogen-rich precursors such as melamine, urea, or dicyandiamide. Its porous morphology, layered structure, and tunable electronic properties contribute to its photocatalytic activity

II. GREEN HYDROGEN PRODUCTION TECHNOLOGIES

A. *Principles of Photocatalytic Water Splitting*

- **Fundamental Chemical Reaction**

Photocatalytic water splitting involves a sequence of fundamental processes. Initially, the photocatalyst absorbs photons with energy equal to or greater than its bandgap, promoting electrons from the valence band to the conduction band and generating corresponding holes in the valence band. These photoinduced charge carriers facilitate redox reactions essential for hydrogen evolution. However, a major limitation of this approach is the recombination of electron-hole pairs, which can occur via radiative or non-radiative pathways. This recombination significantly reduces the quantum efficiency and overall hydrogen production rate, posing a critical challenge to the practical implementation of photocatalytic systems. [12]. In photocatalytic water splitting, photoexcited holes and electrons that avoid recombination are transported to active sites via diffusion or internal electric fields generated within the photocatalyst. The holes in the valence band facilitate the oxidation of water molecules, producing protons, while the excited electrons in the conduction band reduce these protons to generate hydrogen gas. For efficient hydrogen evolution, the conduction band edge of the photocatalyst must be positioned at a more negative potential than the proton reduction potential, while the valence band must be more positive than the water oxidation potential. Optimizing these band positions is critical to enhancing the overall photocatalytic performance and hydrogen production efficiency [13]

$$\text{Reaction redox: } 2H_2O \rightarrow 2H_2 + O_2 \qquad (1)$$

Under solar stimulation, a photocatalytic surface with an energy level higher than the band gap leads to the formation of an electron-hole pair. Photo-generated electrons accommodated in the conduction band caused a vacancy in the valence band[2]. The charge carrier produced is moved on the surface and reacts with H_2O molecules that are adsorbed on the photocatalyst surface. This charge carrier involves reduction and oxidation reactions by transferring holes and electrons on the various reaction sites for hydrogen and oxygen evaluation

B. *Electrolysis of Water,*

Electrolysis involves passing an electric current through water to split it into hydrogen and oxygen. It requires an electrolyte and two electrodes. Hydrogen is produced at the cathode (reduction), and oxygen at the anode (oxidation).[14]

Reaction:

$$2H_2O(l) \rightarrow 2H_2(g) + O_2(g) 2H_2O \qquad (2)$$

$$2H_2(g) + O_2(g) 2H_2O(l) \rightarrow 2H_2(g) + O_2(g) \qquad (3)$$

C. *Photoelectrochemical (PEC)Water Splitting,*

PEC water splitting uses a photoelectrode (semiconductor) immersed in an electrolyte. When illuminated, it generates electron-hole pairs that drive water splitting. It combines photovoltaic and electrochemical processes in one system.[15]

Reaction:

$$\text{Photoanode: } H_2O \rightarrow O2 + 4H^+ + 4e^- \qquad (4)$$

$$\text{Photocathode:} 4H^+ + 4e^- \rightarrow 2H_2 \qquad (5)$$

D. *Thermochemical Water Splitting,*

This method uses high-temperature heat (often from solar or nuclear sources) to drive a series of chemical reactions that split water. It typically involves metal oxides in redox cycles (e.g., the two-step cerium or sulfur-iodine cycles).[16]

E. *Biological Hydrogen.*

Microorganisms produce hydrogen through metabolic processes. There are several biological pathways: Photo-fermentation: Photosynthetic bacteria use light and organic acids.

Bio photolysis: Algae and cyanobacteria split water using light
Dark fermentation: Anaerobic bacteria break down organic substrates [17]

Reaction (dark fermentation):

$$C_6H_{12}O_6 \rightarrow 2CO_2 + 2H_2 + \text{organic acid} \qquad (6)$$

Among the various production pathways, Solar-driven photocatalytic water splitting is a promising method for producing hydrogen without carbon emissions. However, low STH efficiency and scalability issues hinder its industrial adoption. It uses semiconductor materials to absorb solar photons and drive the redox reactions necessary for water splitting.

III. PHOTOCATALYTIC FRAMEWORKS

A range of water-splitting processes have been explored, each one with its potential application. Water electrolysis is among the most promising technologies due to its high production rate and low maintenance. It is an electrochemical process that splits water molecules into hydrogen and oxygen gas according to the following reaction [18].

Graphitic carbon nitride (g-C_3 N_4) is a low-cost, non-toxic, and stable material, making it economically attractive. Efficiency remains a challenge; strategies like cocatalyst addition and heterostructure design are needed [19].

g-C_3 N_4 is highlighted for its scalability and ease of synthesis.

Efficiency bottlenecks (e.g., charge recombination) limit economic feasibility. Emphasizes need for integrated systems and modular reactor designs to reduce costs, Highlights the gap between lab-scale performance and industrial. [20].

Photocatalytic solar hydrogen production offers a low-cost, simplified alternative to traditional methods but suffers from low solar-to-hydrogen efficiency (~1–2%). The review highlights material and system design strategies to improve performance while addressing cost and scalability challenges. It concludes that multidisciplinary integration and engineering-economic alignment are essential for commercial viability of this green hydrogen technology**.** [21]

The review highlights significant progress in photocatalytic water splitting using particulate semiconductors, focusing on material development, charge separation strategies, and surface catalytic mechanisms. It emphasizes advanced techniques like surface-phase junctions, facet-based charge separations to enhance efficiency. Commercial viability depends on improving solar-to-hydrogen (STH) conversion rates and long-term durability.[22].

g-C_3 N_4 is discussed as a cost-effective material for suspended systems. Reactor design and mass transfer limitations affect economic scalability. Efficiency still too low for commercial deployment; needs 10× improvement [23]

[13] Suggests hybrid systems and material modifications to improve cost-effectiveness. Emphasizes need for lifecycle analysis and cost modeling for commercialization.

Cost-benefit analyses compare production expenses with hydrogen market prices. Policy incentives and subsidies play a crucial role in large-scale adoption [24].

IV. CONCLUSION

Techno-economic analysis is essential for advancing green hydrogen technologies such as electrolysis, biomass gasification, and water splitting. Among emerging methods, photocatalytic hydrogen production offers a decentralised and potentially low-cost solution, particularly in regions with abundant solar energy. However, commercialization is hindered by low solar-to-hydrogen conversion efficiency, material degradation, and integration challenges. Graphitic carbon nitride (g-C_3 N_4) stands out as a promising photocatalyst due to its low cost, non-toxicity, chemical stability, and visible-light activity. As a metal-free polymeric semiconductor with a moderate bandgap (~2.7 eV), it can absorb light up to ~460 nm, making it economically attractive for solar-driven hydrogen production. Compared to PV-electrolysis systems, photocatalytic methods mimic natural photosynthesis and offer simpler configurations. Continued research in catalyst design, system engineering, and hybrid integration is needed to improve efficiency and economic viability. Future efforts should focus on novel material discovery and optimization to enable commercial deployment and support the global transition to sustainable energy.

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REFERENCES

[1] S. W. Boettcher, "Introduction to Green Hydrogen," *Chem Rev,* vol. 124, no. 23, pp. 13095-13098, Dec 11 2024, doi: 10.1021/acs.chemrev.4c00787. https://doi.org/10.1021/acs.chemrev.4c00787

[2] S. K. Thengane, A. Hoadley, S. Bhattacharya, S. Mitra, and S. Bandyopadhyay, "Cost-benefit analysis of different hydrogen production technologies using AHP and Fuzzy AHP," *International Journal of Hydrogen Energy,* vol. 39, no. 28, pp. 15293-15306, 2014, doi: 10.1016/j.ijhydene.2014.07.107.

[3] E. K. Tetteh, N. G. Sijadu, and S. Rathilal, "Prospects of Solar Driven-Water Electrolysis for Hydrogen Production in South Africa: A Mini-Review," in *Paper presented at the 39th johannesburg international conference on "chemical, biological and environmental engineering"*, 2023: JCBEE-23 Johannesburg, South Africa.

[4] J. Hanto, A. Schroth, L. Krawielicki, P.-Y. Oei, and J. Burton, "South Africa's energy transition – Unraveling its political economy," *Energy for Sustainable Development,* vol. 69, pp. 164-178, 2022, doi: 10.1016/j.esd.2022.06.006.

[5] A. Beigi Kheradmand, M. Heidari Soureshjani, M. Jahangiri, and B. Hamawandi, "Comparative Techno-Economic Analysis of Gray Hydrogen Production Costs: A Case Study," *Sustainability,* vol. 17, no. 2, 2025, doi: 10.3390/su17020547.

[6] A. bin Jumah, "A comprehensive review of production, applications, and the path to a sustainable energy future with hydrogen," *RSC advances,* vol. 14, no. 36, pp. 26400-26423, 2024. https://doi.org/10.1039/D4RA04559A

[7] T. Sebbagh, "Modeling, analysis, and techno-economic assessment of a clean power conversion system with green hydrogen production," *Bulletin of the Polish Academy of Sciences Technical Sciences,* pp. 150115-150115, 2024, doi: 10.24425/bpasts.2024.150115.

[8] E. Kweinor Tetteh, N. G. Sijadu, and S. Rathilal, "An overview of non-carbonaceous and renewable-powered technologies for green hydrogen production in South Africa: Keywords occurrence analysis," *Energy Strategy Reviews,* vol. 54, 2024, doi: 10.1016/j.esr.2024.101486.

[9] D. Bhanderi, P. Lakhani, and C. K. Modi, "Graphitic carbon nitride (g-C3N4) as an emerging photocatalyst for sustainable environmental applications: a comprehensive review," *RSC Sustainability,* vol. 2, no. 2, pp. 265-287, 2024, doi: 10.1039/d3su00382e.

[10] X. Barreiro-Xardon, E. Rosales, and M. Á. Sanromán, "Current Strategies to Improve the Properties of Graphitic Carbon Nitride for Effective and Scalable Wastewater Pollutant Removal: A Critical Review," *Catalysts,* vol. 15, no. 6, 2025, doi: 10.3390/catal15060523.

[11] J. Wang and S. Wang, "A critical review on graphitic carbon nitride (g-C3N4)-based materials: Preparation, modification and environmental application," *Coordination Chemistry Reviews,* vol. 453, 2022, doi: 10.1016/j.ccr.2021.214338.

[12] T. Hisatomi *et al.*, "Photocatalytic water splitting for large-scale solar-to-chemical energy conversion and storage," *Frontiers in Science,* vol. 2, 2024, doi: 10.3389/fsci.2024.1411644.

[13] R. Zhao, "Comprehensive Literature Review Outline: Photocatalytic Water Splitting for Hydrogen Production," *Advances in Engineering Research Possibilities and Challenges,* 2025, doi: 10.63313/AERpc.9006.

[14] K. Hu *et al.*, "Comparative study of alkaline water electrolysis, proton exchange membrane water electrolysis and solid oxide electrolysis through multiphysics modeling," *Applied Energy,* vol. 312, p. 118788, 2022. https://doi.org/10.1016/j.apenergy.2022.118788

[15] Y. Zhao, Z. Niu, J. Zhao, L. Xue, X. Fu, and J. Long, "Recent Advancements in Photoelectrochemical Water Splitting for Hydrogen Production," *Electrochemical Energy Reviews,* vol. 6, no. 1, 2023, doi: 10.1007/s41918-022-00153-7.

[16] D. Oudejans, M. Offidani, A. Constantinou, S. Albonetti, N. Dimitratos, and A. Bansode, "A Comprehensive Review on Two-Step Thermochemical Water Splitting for Hydrogen Production in a Redox Cycle," *Energies,* vol. 15, no. 9, 2022, doi: 10.3390/en15093044.

[17] M. Cha, M. S. Park, and S. J. Kim, "Biological Routes for Biohydrogen Production: A Clean and Carbon-Free Fuel," *Biotechnol J,* vol. 20, no. 7, p. e70074, Jul 2025, doi: 10.1002/biot.70074.

[18] S. R. Naqvi, B. kazmi, S. A. Ammar Taqvi, W.-H. Chen, and D. Juchelková, "Techno economic analysis for advanced methods of green hydrogen production," *Current Opinion in Green and Sustainable Chemistry,* vol. 48, 2024, doi: 10.1016/j.cogsc.2024.100939.

[19] M. C. Lebepe, P. O. Oviroh, and T.-C. Jen, "Techno-economic optimisation modelling of a solar-powered hydrogen production system for green hydrogen generation," *Sustainable Energy Research,* vol. 12, no. 1, 2025, doi: 10.1186/s40807-025-00151-5.

[20] S. S. Kumar and V. Himabindu, "Hydrogen production by PEM water electrolysis–A review," *Materials Science for Energy Technologies,* vol. 2, no. 3, pp. 442-454, 2019. https://doi.org/10.1016/j.mset.2019.03.002

[21] D. Jing, H. Liu, X. Zhang, L. Zhao, and L. Guo, "Photocatalytic hydrogen production under direct solar light in a CPC based solar reactor: Reactor design and preliminary results," *Energy Conversion and Management,* vol. 50, no. 12, pp. 2919-2926, 2009, doi: 10.1016/j.enconman.2009.07.012.

[22] P. Niu, J. Dai, X. Zhi, Z. Xia, S. Wang, and L. Li, "Photocatalytic overall water splitting by graphitic carbon nitride," *InfoMat,* vol. 3, no. 9, pp. 931-961, 2021, doi: 10.1002/inf2.12219.

[23] M. S. Nasir, G. Yang, I. Ayub, A. Nasir, and W. Yan, "Higher hydrogen production by photocatalytic water splitting using a hollow tubular graphitic carbon nitride-zinc telluride composite," *Environmental Chemistry Letters,* vol. 20, no. 1, pp. 19-26, 2021, doi: 10.1007/s10311-021-01301-z.

[24] X. Chen, J. Wang, Y. Chai, Z. Zhang, and Y. Zhu, "Efficient Photocatalytic Overall Water Splitting Induced by the Giant Internal Electric Field of a g-C(3) N(4) /rGO/PDIP Z-Scheme Heterojunction," *Adv Mater,* vol. 33, no. 7, p. e2007479, Feb 2021, doi: 10.1002/adma.202007479.