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Research paper

Nanoengineered Catalysts for Efficient Hydrogen Production in Renewable Energy Systems

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Abstract

Hydrogen (H2) is gaining acceptance as a renewable energy source (RES) that may replace or supplement the current carbon-based power framework. Despite research in this domain frequently emphasizing the fundamental comprehension of catalytic mechanisms and showcasing their efficacy across various approaches, considerable effort remains necessary to create superior methods and sophisticated materials for extensive application. Nanoengineering methodologies at the nano or micron level are particularly compelling, as they facilitate the exploration of how activity fluctuates based on variables such as dimension, substance, framework, electronic properties, and support interactions. This understanding yields knowledge about structure–performance correlations in generating hydrogen, thereby optimizing efficiency and permitting systematic development of a Nanoengineering catalyst (NC) with targeted functions and preference for hydrogen generation. Traditional methods generate significant greenhouse gas (GHG) emissions owing to elevated manufacturing costs and restricted effectiveness. Water separation (WS) presents one of the most environmentally sustainable production methods when integrated with RES. Although expensive, it is afflicted by detrimental consequences that diminish efficiency. By elucidating physical properties and structural relationships, NC approaches profoundly influence green H2 production. Additional research is necessary for storage facilities for H2 that are robust for distant transportation networks with adequate refueling stations, while also improving the function of NC in RES-H2 generation frameworks.

Keywords: *Hydrogen; Renewable Energy Sources; Nanoengineering; Catalyst; Greenhouse Gas; Water Separation.*

1. Introduction

The power demand has increased markedly due to the increasing world economy, rapidly rising population, and fast industrialization. Carbon-based fuels, like petroleum, fossil fuels, and coal, are the predominant power sources. The supplies of petroleum and gas are limited, fossil-fueled in the near term, and irregularly dispersed across several locations. Current reserves will be insufficient to satisfy the projected energy needs. Furthermore, the utilization of energy from fossil fuels has highlighted the detrimental environmental impacts, including substantial GHG emissions, mostly CO2, and their significant contribution to climate change [1]. The United Nations Panel on Climate Change (UNPCC) seeks to attain a zero-carbon footprint by 2055 and recommends reducing the observed temperature increase to not over 2 ◦C since the age of industrialization to address the issue of global warming [8].
Mitigating GHG from human activities is essential to attaining this objective [15]. The clear ecological disadvantages and degenerative characteristics of petroleum and natural gas have necessitated research of alternate energy sources, notwithstanding their dominant role in worldwide energy availability. The proposed power source is expected to be adequately safe, easy to create and achieve, and suitably sustainable and eco-friendly to provide a consistent, continuous supply [3]. In the years to come, it will be able to replace petroleum and natural gas [10].
The periodic list starts with H2 as the initial atomic component. It is the most abundant component of space and the ninth most frequent in the Earth's outermost layer. H2 molecules are scarce in biological terms, and the environment has a low concentration of H2 [11].

Nonetheless, the majority of H2 atoms exist inside polymers. H2 cannot serve as a power transporter without synthetic production. Using H2 is considered a renewable and harmless power source since it generates water. Nonetheless, H2 manufacturing methods are not entirely environmentally sustainable [2]. The purity of H2 is contingent upon its raw materials, power inputs, and waste outputs over its whole cycle. Several methods and technologies may generate H2. These methods need raw materials and energy sources, including petroleum and gas, sustainable biomass, wind, and solar power [5].

Extracting H2 from RES is tremendously advantageous. Solar-based H2 generation systems exhibit reduced waste discharges compared to other techniques. Nonetheless, these methods forfeit their competitive edge when evaluating prices and efficiency. The worldwide demand for H2 is around 75 million metric tons (Mt) annually. Nevertheless, it is mostly generated from petroleum and gas [12]. In the past few years, steam reformation has emerged as the predominant H2 production method, accounting for over 50% of H2 output, following coal-fired combustion.

Most H2 is still sourced from petroleum and gas compared to RES. The use of biomass for H2 production has promise; however, it faces technical and economic challenges [7]. The electrolysis technology, which dissociates water to generate H2 gas, is always advancing [4]. Their advantages are more evident in small applications. Scholars regard WS as the most efficient approach for H2 production across all available techniques. However, this assertion needs further qualification. For instance, the efficiency of water splitting varies significantly depending on the method (thermochemical, electrochemical, or photoelectrochemical), catalyst type, and energy source. Recent comparative reviews (Elsapagh et al., 2024; Ayub et al., 2024) indicate that steam reforming remains more cost-effective ($1.20–1.50/kg H_2) than WS methods ($3–6/kg H_2), despite its carbon emissions. Photoelectrochemical WS has achieved solar-to-hydrogen (STH) efficiencies up to 15%, while thermochemical cycles remain below 5% under practical conditions. Thus, calling WS the most efficient requires contextual clarification—either based on sustainability, energy source, or H_2 purity. H2 may be generated by thermochemical WS processes (TWSPs), employing heat energy and waste materials for utilization [13] [6]. Hydro and thermo-biological transpiration may generate substantial quantities of H2 via decomposing biological waste; nevertheless, hazardous by-products like CO2 may adversely affect the surroundings. Nonetheless, the latter method is regarded as ecologically friendly due to the purity of the reaction procedure. The photoelectrochemical (PEC) technique has shown its capability to convert sunlight into chemical power via the separation of water. Diverse materials, including graphene carbons, metallic transitions, and cobalt-steel nanofilms, may be photosensitive electrodes for this technique [9].

The generation of H2 fuel from RES, such as aqueous and solar power, is called the NC separation of water. Using Nanomaterials (NM) as a photo-NC substance has substantiated this claim. This has resulted in an exponential rise in H2 generation relative to other compounds. A significant study regarding NC-based H2 synthesis has been undertaken lately. This discussion focuses on NC techniques within the H2 economy since it utilizes two distinct strategies: catalyst and non-catalyst ways. NM and blended catalyst components have been employed to develop NC for hydrogen production. This paper succinctly summarizes the main catalytic mechanisms for hydrogen synthesis. Consequently, NM may enhance the creation of biological hydrogen [14].

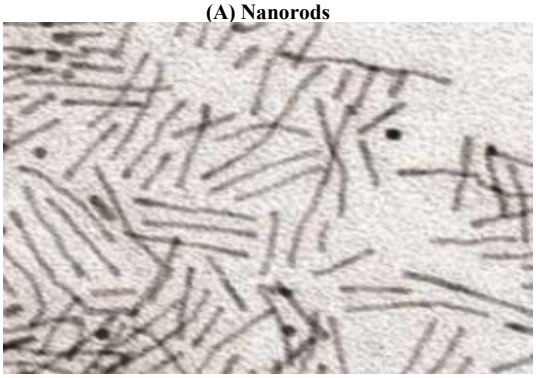
Current literature consistently highlights water separation (WS) as one of the most promising sustainable H_2 production methods when integrated with RES. However, the performance and cost-effectiveness vary across its subtypes. For instance, photoelectrochemical WS using nanostructured photoelectrodes has shown solar-to-hydrogen (STH) efficiencies up to 15% under lab conditions (Liu & Kuang, 2024 [12]; Elsapagh et al., 2024 [10]). Meanwhile, thermochemical cycles remain constrained by high operational temperatures and low conversion efficiencies.

The catalytic performance in H_2 evolution reactions (HER) is heavily dependent on factors such as surface energy, electronic structure, and active site availability—principles rooted in Sabatier's principle and further elaborated in classic catalysis literature (e.g., Boudart, 1991; Ertl, 1994).

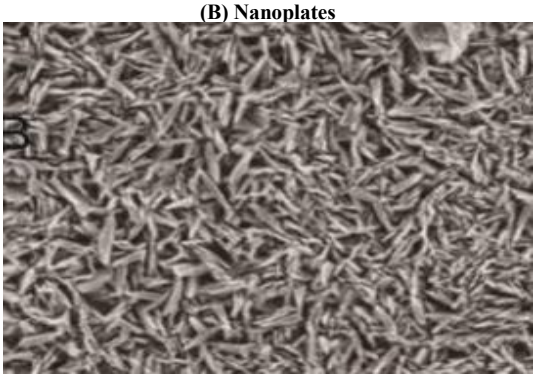
2. NC for H2 generation in RES

The emergence of many distinctive features of NM is attributed to their distinctions from bulk materials. The physical-chemical attributes of NM and designed NC, comprising dimensions, form, layout, equilibrium, and organization, enhance inherent surface qualities, including augmented total area, power, and surface defects, which directly influence their catalytic efficacy. In this regard, owing to the significant possibility for usage across various hydrogen production methodologies and the capacity to enhance or customize effectiveness, NM of diverse dimensions, shapes, formulations (e.g., Au, Ag, and Pt), and frameworks have been investigated for hydrogen production through various approaches, as illustrated in Fig. 1.

(A) Nanorods



(B) Nanoplates



(C) Nanosheets

(D) Nanocubes

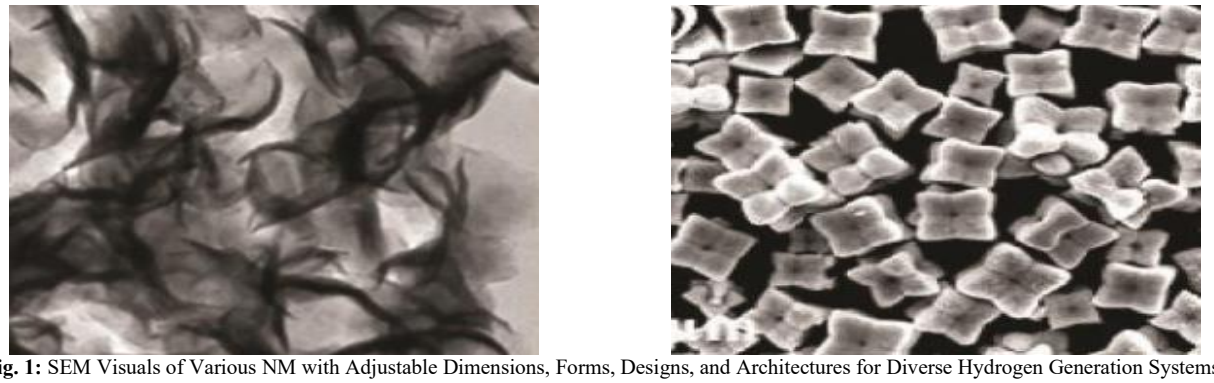


Fig. 1: SEM Visuals of Various NM with Adjustable Dimensions, Forms, Designs, and Architectures for Diverse Hydrogen Generation Systems.

Fig. 1 depicts the SEM visuals of various NM with adjustable dimensions, forms, designs, and architectures successfully documented for use in diverse hydrogen generation systems. In this scenario, reduced dimensions influence the distribution of elements on the uppermost surface of the nanomaterial, resulting in increased concentrations of elements at curves, rooftops, steps, and corners; moreover, it induces quantum entanglement effects. Therefore, one may manipulate the dimension of a material and its other attributes by meticulously regulating certain reaction parameters (e.g., temperature, duration, agitation), solvent, reducing substances, and stabilization agents. Nonetheless, it is essential to consider that the dimension is significant based on its use.

Plasmonic catalysis (PC) is at the forefront of photocatalysis (PCS) since it facilitates the swiftness and regulation of many chemical changes via targeted superficial plasmon resonance activation (SPRA). A magnetic field's cyclic electrical field aspect produces regional aggregate vibration of charged particles in the metal nanoparticles, enhancing their ability to perform. From a sustainability standpoint, the potential to harness solar energy and convert it into chemical power is a crucial aspect of PC and is much sought after in H2 economics. Consequently, metals like Au, Ag, and Pt exhibit regional SPRA in the optical and near-IR spectra and have garnered significant study attention in the past few years. The plasmonic effect is significantly influenced by the dimensions, form, and structure of the NM, which follows the leading techniques in PC.

Precisely engineered Au–Ag core–shell nanostructures have demonstrated significant promise in WS applications. Under optimized light conditions, an enhancement of up to 109.8% in catalytic efficiency was observed, outperforming traditional Pt-based catalysts by over 59.9% in certain cases (Elsapagh et al., 2024 [10]; Ayub et al., 2024). These findings align with earlier reports by Dalapati et al. (2020) [17], who used graphene-incorporated cupric oxide catalysts to enable efficient solar H_2 production through synergistic light absorption and charge separation.

To translate the benefits of nanocatalysts into scalable hydrogen production, it is essential to explore the underlying techniques of water separation where these materials are applied. The following section categorizes these techniques and examines how nanostructures optimize their performance.

2.1. Water separation (WS)

WS is receiving significant interest as the most viable technique for H2 generation among all current methods. This section elucidates WS and the methodologies used, along with evaluating their merits and demerits. Furthermore, WS's process of identifying appropriate substances to improve its effectiveness and H2 generation has been examined.

This section reviews key water separation (WS) techniques, with an emphasis on their integration with nanoengineered catalysts. Each method is evaluated in terms of hydrogen production efficiency, environmental impact, and the role of nanomaterials in enhancing system performance.

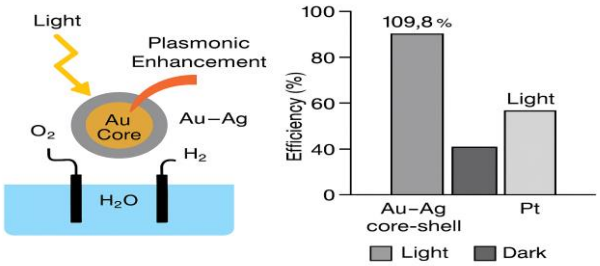


Fig. 2: Efficiency comparison of Au–Ag core-shell nanostructures vs Pt-based catalysts in plasmon-enhanced water splitting.

Fig.2 shows the efficiency comparison between Au–Ag core-shell nanostructures and conventional Pt-based catalysts, highlighting a 59.9% enhancement in light-driven WS performance.

2.1.1. Thermochemical WS

This method uses heat and redox cycles for water splitting, with nanocatalysts aiding intermediate regeneration. The thermochemical processes formulated for WS entail a progressive process. The technique involves using intermediary interactions and chemicals repeatedly repurposed throughout chemical-based alterations, leading to the breakdown of water molecules into H2. This technique theoretically necessitates thermal power. The thermochemical WS cycle (TCWSC) is an H2 generation mechanism that uses thermal energy to regenerate substances for further utilization. TCWSC may be driven only by heat energy and are thus classified as solely TCWSC. A combination of heating and other energy, like electrical or optical power, may also power them. In this instance, they are referred to as composite TCWSC. It denotes processes that facilitate WS by utilizing heat at temperatures under 2050◦C, often occurring in many stages.

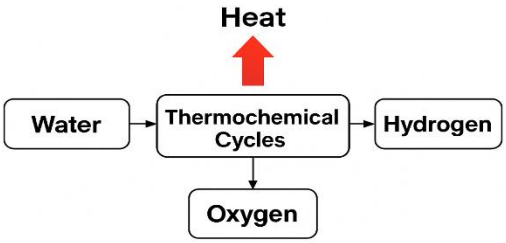


Fig. 3: Schematic of thermochemical water splitting cycles (TCWSC) for hydrogen generation using heat-driven reactions.

Fig.3, the thermochemical cycle includes multiple stages of heat-driven reactions involving reusable chemical intermediates.

2.1.2. Opto-biological WS

Opto-biological systems leverage light and biological agents, but face challenges from CO_2 by-products and catalyst stability. Opto-biological WS is classified into two main groups: biological and aquatic photolysis. The earlier process may degrade biological waste materials and produce H2. Nonetheless, it generates detrimental residues, such as CO2, which present environmental hazards. Conversely, the latter technique is ecologically sustainable owing to its unpolluted response process. The direct method entails using sunlight to dissociate water into H2 and O2, then transforming the acquired H2 ions into gas forms via hydrophilic enzymes. Nonetheless, due to the sensitivity of these catalysts to O2, it is essential to preserve a minimal oxygen concentration. Additionally, passive photolysis may be used, including bacteria or blue-green algal cells, to generate H2 from water.

Although opto-biological WS has potential due to its biological integration, its environmental sustainability is contested. The CO_2 by-products released during the degradation of biomass or biological waste introduce a carbon penalty that partially offsets its green credentials. Studies (Ayub et al., 2024; Elsapagh et al., 2024) emphasize the importance of managing these emissions using integrated CO_2 capture systems to preserve ecological balance. Additionally, the low quantum efficiency and enzyme instability under fluctuating oxygen levels present major challenges in scaling this approach for commercial deployment.

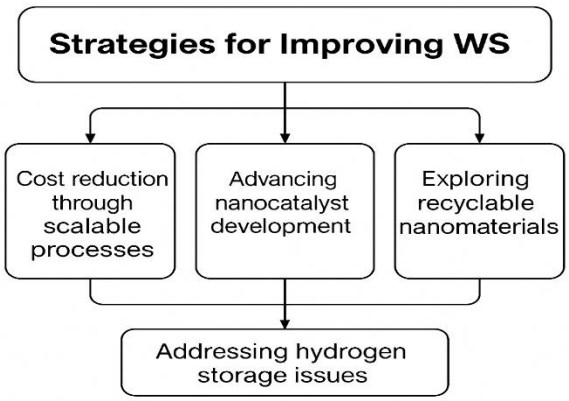


Fig.4: Environmental impact assessment of opto-biological WS showing CO_2 emissions from photolysis-based systems.

Fig.4 presents an environmental impact comparison, indicating that opto-biological WS, while renewable, may generate non-trivial CO_2 residues during biomass degradation.

In contrast, photolysis-based variants using algae or cyanobacteria show higher selectivity but suffer from slow kinetics and poor light absorption efficiency. Emerging approaches in 2024–2025 have demonstrated the utility of genetically engineered microalgae strains, which increase H_2 yields by 1.5x compared to natural strains (Liu & Kuang, 2024). However, these systems remain cost-prohibitive for large-scale applications.

2.1.3. Elevated temperatures electrolysis (ETE) WS

This high-efficiency method operates at extreme temperatures, enhanced by durable nanomaterials in the electrode setup. In ETE, the vapor is decomposed into H2 and O2 at temperatures ranging from 850 to 1250 °C. The entire procedure occurs inside a cell with electrodes. The method is very efficient, yielding H2 gas with excellent quality.

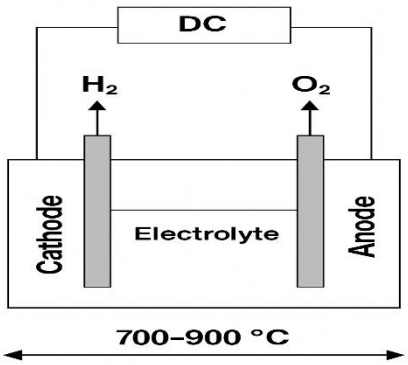


Fig. 5: Diagram of high-temperature electrolysis setup showing electrode configuration and operational temperature ranges.

Fig.5 outlines key components and illustrates the thermal environment required for efficient hydrogen production.
Despite the high H_2 purity, ETE is limited by its substantial energy demand, typically requiring 850–1250 °C, which may necessitate fossil-fuel-based heat in non-RES-supported infrastructures. According to recent life cycle assessments (Raman et al., 2024), the carbon footprint of ETE-based H_2 production exceeds that of alkaline electrolysis unless paired with concentrated solar thermal input or nuclear heat sources. Moreover, material degradation at extreme temperatures increases maintenance costs and reduces operational stability.

2.1.4. Photoelectrolysis (PE) of WS

Photoelectrolysis directly converts sunlight into chemical energy using semiconductor nanostructures. PE-WS is an efficient method for transforming solar power into chemical power. Numerous substances, including carbon graphite, metal transitions, and sulfur-doped cobalt-iron (oxy) nanosheets, have been considered photosensitive electrodes for PE-WS.
Numerous studies focus on improving the performance and reliability of photoelectrodes to facilitate effective WS and H2 generation. The PE-WS process, which entails the direct production of H2, is a viable technical approach that efficiently mitigates the storage challenges linked to our abundant but intermittent power source.

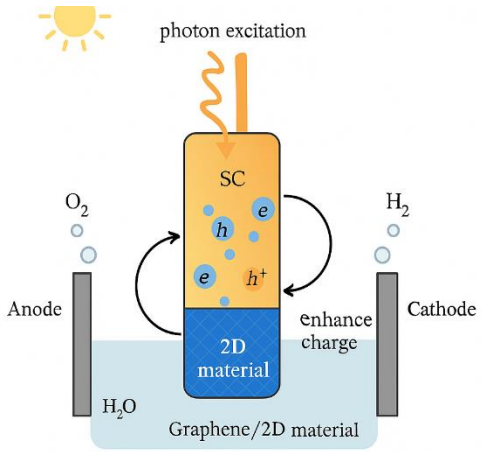


Fig.6: Illustration of the photo electrolysis mechanism showing photon excitation, oxygen generation at the anode, and hydrogen evolution at the cathode.

Fig.6 depicts photons trigger electron-hole pair separation in the semiconductor, enabling water-splitting reactions at the electrodes.
The possibility of H2 as an eco-friendly and green power source is exciting. Thermal separating, which entails the dissociation of water atoms into O2 and H2, depends on a fundamentally simple idea:

1) Photons excite holes and electrons in the semiconductor absorption material.
2) The activated hole in the valence region promotes water combustion, producing O2, referred to as the oxygen generation process. This occurs upon reaching the anode region.
3) The energized electron in the conductive layer converts water to H2 at the cathode, widely known as the H2 generation process.

2.1.5. PCS-WS

This hybrid method integrates thermal and light-based inputs, with layered nanocarbons improving charge separation. PCS-WS utilizes RES, including water and thermal power, to produce H2 fuel. Combining diverse 2D-layered photons and cathodes with nano-carbon catalysts has shown enhanced efficacy in thermal PE-WS systems (Boudart, 1991; Ertl, 1994) (Dalapati et al. (2020).

3. Future Research Directions

To enable widespread deployment of green hydrogen technologies, several targeted research directions must be prioritized:

Scalability and Cost Optimization: Future studies should address how nanoengineered catalysts (NCs) can be scaled for cost-effective, industrial-grade water splitting. For instance, “How can abundant materials like Ni, Fe, or Cu be engineered to match or exceed the catalytic performance of rare-earth metals like Pt or Ru in industrial settings?”

Catalyst Longevity and Stability: Most high-performance NCs degrade under prolonged thermal or electrochemical stress. This raises the question: "What synthesis strategies (e.g., core–shell structures or heteroatom doping) can improve NC durability across extended operating cycles?"
Next-Generation Nanomaterials: Emerging 2D materials such as MXenes, sulfur-doped graphene, and transition metal dichalcogenides (TMDs) show potential for dual functionality in both catalysis and hydrogen storage. Research should explore: "Which layered nanomaterials offer the best trade-off between charge mobility, surface area, and binding energy for H_2 evolution and retention?"
Hydrogen Storage Integration: A critical bottleneck is storing hydrogen efficiently for decentralized or mobile applications. This invites exploration of questions like: "What nanomaterials—e.g., MgH_2 composites or metal–organic frameworks (MOFs)—enable reversible, high-density hydrogen storage under mild conditions?"
Techno-Economic Assessment (TEA): Finally, all future material innovations must be evaluated through TEA models to ensure commercial feasibility, especially when considering lifecycle energy input and end-of-life recyclability.

4. Conclusion

Nanoengineering techniques at the nanoscale or microscale are especially intriguing since they enable the investigation of how activity varies according to factors such as size, material, structure, electrical characteristics, and interaction with substrates. This comprehension provides insights into structure–performance relationships in hydrogen production, enhancing efficiency and enabling the methodical advancement of Nanoengineering catalysts (NC) with specific functionalities and a focus on hydrogen generation. Conventional technologies produce substantial GHG emissions due to high production expenses and limited efficiency. Water separation (WS) is one of the most ecologically friendly manufacturing techniques when combined with renewable energy sources (RES). Despite its high cost, it is burdened with adverse effects that reduce efficiency. By clarifying physical parameters and structural correlations, NC methodologies significantly impact green H2 generation. Further investigation is required in storage facilities for resilient hydrogen for long-distance transportation networks with sufficient recharging stations while enhancing the performance of nitrogen compounds in renewable energy hydrogen-producing systems.

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