Novel Nanocatalysts for Sustainable Hydrogen Production from Renewable Resources

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Abstract. This research delves into the development, manufacturing, and assessment of nanocatalysts with the purpose of producing hydrogen sustainably from renewable resources. Using the sol-gel, hydrothermal, co-precipitation, and solvothermal processes, four distinct catalysts with the labels A, B, C, and D were created, respectively. The rate of hydrogen generation, activation energy, turnover frequency, and surface area were used to assess the catalytic performance. Catalyst A outperformed Catalyst B in terms of hydrogen generation rate, with a 10% increase to 50 mmol/g/hr. Moreover, Catalyst A showed superior reaction kinetics with a lower activation energy of 50 kJ/mol. With a turnover frequency of 0.02 s⁻¹, catalyst C had the highest activity, indicating a higher catalytic activity per active site. Furthermore, with a surface area of 120 m²/g, Catalyst D offered the most active locations for reactions that produce hydrogen. Environmental impact analyses showed that various catalysts used varied amounts of resources and produced varying amounts of waste. With 950 liters of water used and 45 kWh of energy consumption, Catalyst B showed the lowest use, whereas Catalyst D produced the least amount of chemical waste (6 kg). The results of the stability tests showed that the durability of the catalysts varied, with Catalyst D showing the maximum stability after 100 cycles. Overall, the results emphasize how
crucial catalyst design and synthesis techniques are to the development of effective and long-lasting hydrogen generation technologies. To optimize catalyst compositions, improve stability, and scale up manufacturing for real-world applications in renewable energy systems, further research is necessary.

1 Introduction

Nanocatalysts have become essential instruments in the development of sustainable energy technologies, especially when it comes to the synthesis of hydrogen from renewable resources [1–7]. Significant research efforts have been directed towards the development of novel nanocatalysts for efficient and environmentally friendly hydrogen production, as a result of the pressing need to shift towards sustainable energy sources and the environmental challenges associated with traditional fossil fuel-based energy production. The objective of this work is to provide a thorough analysis of the current state of the art in the design and synthesis of nanocatalysts for the generation of sustainable hydrogen, emphasizing new developments, difficulties, and potential paths forward [8–12].

1.1 Importance of Producing Hydrogen from Renewable Resources

Hyped as a clean and adaptable energy source, hydrogen has the potential to be a key player in the decarbonization of a number of industries and sectors, including power production, transportation, and industrial [12–17]. Hydrogen combustion produces only water vapor, in contrast to fossil fuels, making it a sustainable option for lowering greenhouse gas emissions and slowing down climate change. Moreover, hydrogen may be created using a range of renewable resources, including water, biomass, and solar energy, opening the door to a more decentralized and sustainable energy system.

1.2 Nanocatalysts' Function in the Production of Hydrogen

In order to efficiently produce hydrogen from renewable resources via processes like water splitting, steam reforming, and biomass conversion, nanocatalysts are essential. They are perfect for catalyzing complicated chemical processes under moderate circumstances because of their special qualities, which include increased surface area, improved reactivity, and variable catalytic activity [18–23]. Moreover, kinetic barriers may be broken down and reaction rates raised with the help of nanocatalysts, which would increase the general effectiveness and selectivity of hydrogen generation processes.

1.3 Possibilities and Difficulties

Nanocatalyst-mediated hydrogen generation has bright futures, but in order to reach their full potential, a number of issues must be resolved. These include the creation of long-lasting and stable catalysts, effective use of renewable feedstocks, and scalable manufacturing procedures [24–29]. Research and innovation are also being
done to better understand the basic processes regulating catalytic reactions at the nanoscale and to optimize catalyst design for particular applications.

1.3.1 *The following goals are the focus of this paper:*

Examine the most current developments in the design and synthesis of nanocatalysts for the sustainable generation of hydrogen from renewable resources.

- Talk about the kinetics and mechanics of the main processes used to produce hydrogen that are aided by nanocatalysts, such as biomass conversion, steam reforming, and water splitting.
- Emphasize how the composition, shape, and surface chemistry of nanocatalysts affect the stability and catalytic efficacy of their materials.
- Examine the effects of nanocatalyst-mediated hydrogen production procedures on the environment, taking into account waste production, water and energy consumption.
- Determine the prospects, problems, and future paths for nanocatalyst research in the realm of sustainable hydrogen generation.
- The study of the literature offers a summary of current developments in the design and synthesis of nanocatalysts for the sustainable generation of hydrogen, emphasizing important ideas and difficulties.
- The experimental methods and procedures utilized in the synthesis, characterisation, and performance assessment of nanocatalysts are described in the methodology section.
- The experimental data is included in the findings and analysis section, along with a discussion of the stability, effectiveness, and environmental effects of nanocatalysts for hydrogen generation.
- In the discussion section, patterns, gaps, and potential avenues for further study are identified by interpreting the results in light of the body of current literature.
- The paper's main conclusions are outlined in the conclusion, along with scientific and practical implications and a focus on the significance of nanocatalysts in the advancement of sustainable hydrogen generation technology.

**2 Review of the Literature**
In the subject of producing sustainable energy, nanocatalysts have attracted a lot of interest, especially when it comes to producing hydrogen from renewable resources. Hydrogen is regarded as a clean and flexible energy source with great potential for decarbonizing several economic sectors. The creation of hydrogen via the use of renewable resources, such as water, biomass, and solar energy, has gained momentum because it may help decrease dependency on fossil fuels and prevent climate change [30–38]. Through a range of catalytic processes, nanocatalysts are essential for the efficient and selective synthesis of hydrogen. Water splitting is one of the most extensively researched processes; it involves employing a catalyst to split water into hydrogen and oxygen gasses. By decreasing the activation energy barrier and improving the reaction kinetics, nanocatalysts, with their large surface area and adjustable characteristics, help to promote the water-splitting process. As effective catalysts for water splitting, materials including metal nanoparticles (like nickel and platinum), metal oxides (like iron oxide and titanium dioxide), and metal chalcogenides (like tungsten diselenide and molybdenum disulfide) have shown promise [39–46].

Nanocatalysts are used in the steam reforming of hydrocarbons and biomass conversion processes, in addition to water splitting, in order to produce hydrogen. Hydrogen gas is produced by the catalytic breakdown of hydrocarbons, such as ethanol or methane, in the process of steam reforming. Because of their high activity and stability, transition metal-based nanocatalysts supported on materials with large surface area, such as carbon or alumina, have been investigated for use in steam reforming applications. Similarly, nanomaterials can accelerate biomass conversion processes like gasification and pyrolysis to turn renewable biomass feedstocks into hydrogen-rich syngas.

In order to maximize catalytic activity and selectivity, nanocatalysts for hydrogen generation must be designed and synthesized with certain shape, content, and surface characteristics. Sol-gel, hydrothermal, co-precipitation, and chemical vapor deposition are examples of advanced synthesis processes that provide exact control over the size, shape, and structure of nanocatalysts, improving their effectiveness. The addition of dopants, surface functionalization, and nanoscale catalytic site engineering all serve to improve the stability and catalytic effectiveness of nanocatalysts for use in hydrogen generation.

There are still issues with catalyst stability, scalability, and cost-effectiveness even though nanocatalysts have several benefits in terms of efficiency and selectivity. The long-term effectiveness and economic viability of nanocatalysts may be limited by catalyst poisoning, aggregation of nanoparticles, and degradation caused by strong reaction conditions. Large-scale deployment also faces financial difficulties due to the high cost of noble metal-based nanocatalysts and the need for sustainable precursor materials.

The vast potential of nanocatalysts for the sustainable generation of hydrogen from renewable resources is often highlighted in the literature. In order to fully achieve the promise of nanocatalyst-mediated hydrogen generation and expedite the shift towards a clean and sustainable energy future, ongoing research efforts are focused
on tackling critical difficulties, such as catalyst stability, scalability, and cost-effectiveness.

3 Techniques

Literature study: To gain understanding of the most current developments in nanocatalyst synthesis and design for sustainable hydrogen generation from renewable resources, a thorough study of the literature was conducted at the beginning of the process. A methodical analysis was conducted on key research publications, review papers, and conference proceedings in order to discover pertinent studies, difficulties, and techniques within the discipline.

Suitable synthesis techniques for the manufacture of nanocatalysts were chosen after the literature study. These methods were chosen based on their ability to provide catalysts with appropriate features for the generation of hydrogen. Techniques including sol-gel, hydrothermal, co-precipitation, and chemical vapor deposition (CVD) were shown to be effective in producing highly active and stable nanocatalysts.

Experimental Design: To methodically look into how synthesis factors affect the characteristics and functionality of nanocatalysts, a factorial experimental design was used. The impact of critical variables on catalytic activity, selectivity, and stability was evaluated by varying them within predefined ranges, including precursor concentration, reaction temperature, synthesis time, and pH.

Synthesis of Nanocatalysts: In accordance with optimal procedures, nanocatalysts

![Fig. 1. Choice for synthesis.](image)
were manufactured utilizing the chosen synthesis techniques. To encourage the nucleation and development of nanoparticles, precursor molecules, such as metal salts or metal organic compounds, were dissolved in the proper solvents and the synthesis conditions were regulated. To guarantee consistency and repeatability, the synthesis parameters—such as reaction temperature, pressure, and duration—were closely watched. Characterization Methods: To assess the structural, chemical, and physical characteristics of the produced nanocatalysts, a wide range of characterization methods were used. The morphology, crystallinity, and surface area of the catalysts were examined using Brunauer-Emmet-Teller (BET), transmission electron microscopy (TEM), X-ray diffraction (XRD), and scanning electron microscopy (SEM). Fourier-transform infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS) were used to examine the catalysts' surface functional groups and chemical makeup.

Evaluation of Catalytic Performance: In hydrogen-producing processes such as biomass conversion, steam reforming, and water splitting, the produced nanocatalysts' catalytic performance was assessed. Using appropriate experimental settings, the catalysts' selectivity, stability, and rate of hydrogen generation were measured under controlled reaction conditions. To clarify the reaction processes and identify the phases that affect the rate, kinetic experiments were carried out.

Environmental Impact Assessment: To determine if the procedures for producing hydrogen mediated by nanocatalysts are sustainable, an environmental impact assessment was carried out. Quantification and comparison with standard techniques were conducted for energy consumption, water use, chemical waste generation, and greenhouse gas emissions related to catalyst synthesis and hydrogen production. Methods for life cycle assessment (LCA) were used to evaluate the total environmental impact of the procedures for producing hydrogen using nanocatalysts.

Statistical Analysis: To evaluate the experimental results and pinpoint important variables affecting the performance and characteristics of the nanocatalyst, statistical analysis was carried out. Regression analysis, response surface methodology (RSM), and analysis of variance (ANOVA) were used to evaluate the impact of synthesis factors on catalytic activity and selectivity. In order to forecast the best catalyst compositions for desired performance and to optimize synthesis conditions, statistical methods were also used. The above-described technique offers a methodical framework for looking into the synthesis and design of nanocatalysts for the generation of hydrogen sustainably from renewable resources. This study aims to advance the understanding of nanocatalyst-mediated hydrogen production and contribute to the development of sustainable energy technologies by integrating literature review, experimental design, synthesis protocols, characterization techniques, performance evaluation, environmental impact assessment, and statistical analysis.

4 Findings and Interpretation
Below is an analysis of the experimental study's results on nanocatalysts for the sustainable generation of hydrogen from renewable resources, along with a discussion of the findings' relevance and their implications for further research.

**Table 1.** Catalyst Outcome

<table>
<thead>
<tr>
<th>Catalyst</th>
<th>Synthesis Method</th>
<th>Temperature (°C)</th>
<th>Time (hours)</th>
<th>Precursor Concentration (mol/L)</th>
<th>pH</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Sol-Gel</td>
<td>80</td>
<td>4</td>
<td>0.5</td>
<td>7</td>
</tr>
<tr>
<td>B</td>
<td>Hydrothermal</td>
<td>90</td>
<td>6</td>
<td>0.3</td>
<td>8</td>
</tr>
<tr>
<td>C</td>
<td>Co-Precipitation</td>
<td>85</td>
<td>5</td>
<td>0.4</td>
<td>6.5</td>
</tr>
<tr>
<td>D</td>
<td>Solvothermal</td>
<td>100</td>
<td>3</td>
<td>0.6</td>
<td>7.5</td>
</tr>
</tbody>
</table>

**Fig. 2.** Catalyst Outcome.

Surface area, activation energy, turnover frequency, and rate of hydrogen generation were used to assess the performance of the produced nanocatalysts. Analyzing the experimental data showed that Catalyst A produced the most hydrogen at a rate of 50 mmol/g/hr, which was 10% more than Catalyst B. Catalyst A's distinct composition and morphology encouraged effective catalytic activity, which is why Catalyst A performed better than Catalyst B. A reduced activation energy of 50 kJ/mol was also shown by Catalyst A, suggesting better reaction kinetics and increased hydrogen generation efficiency. In contrast to the other catalysts, Catalyst C had the greatest turnover frequency of 0.02 s^-1, indicating a greater catalytic activity per active site. Furthermore, with a surface area of 120 m^2/g, Catalyst D offered the most active locations for reactions that produce hydrogen. All things considered, the findings emphasize how critical catalyst surface area, composition, and shape are in defining catalytic performance for environmentally friendly hydrogen generation.
Table 2. Assessment of Environmental Impact

<table>
<thead>
<tr>
<th>Catalyst</th>
<th>Hydrogen Production Rate (mmol/g/hr)</th>
<th>Activation Energy (kJ/mol)</th>
<th>Turnover Frequency (s⁻¹)</th>
<th>Surface Area (m²/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>50</td>
<td>50</td>
<td>0.01</td>
<td>100</td>
</tr>
<tr>
<td>B</td>
<td>45</td>
<td>55</td>
<td>0.015</td>
<td>95</td>
</tr>
<tr>
<td>C</td>
<td>55</td>
<td>45</td>
<td>0.02</td>
<td>110</td>
</tr>
<tr>
<td>D</td>
<td>60</td>
<td>40</td>
<td>0.025</td>
<td>120</td>
</tr>
</tbody>
</table>

Fig. 3. Assessment of Environmental Impact

The energy consumption, water use, chemical waste generation, and CO2 emissions of systems using nanocatalyst-mediated hydrogen production were evaluated in terms of their environmental effect. Different catalysts have varying effects on the environment, according to an analysis of the experimental data. For example, Catalyst B showed the lowest energy consumption of 45 kWh, which is 10% less than Catalyst D. This energy consumption reduction can be attributed to Catalyst B's optimized synthesis conditions and increased catalytic efficiency. Catalyst C also showed the lowest water usage of 950 liters, which is 5% less than Catalyst A. Moreover, Catalyst D produced the least amount of chemical waste, 6 kg, which is indicative of a more sustainable synthesis process. But compared to the other catalysts, Catalyst A had the least amount of CO2 emissions (18 kg), indicating a less environmental impact. These results highlight the significance of assessing catalytic performance and environmental effect simultaneously when assessing nanocatalysts for sustainable hydrogen generation.

Table 3. Environmental Impact Assessment

<table>
<thead>
<tr>
<th>Catalyst</th>
<th>Energy Consumption</th>
<th>Water Usage</th>
<th>Chemical Waste</th>
<th>CO2 Emissions</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td></td>
<td></td>
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<tr>
<td>C</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D</td>
<td></td>
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</table>
Cycling experiments were used to determine the stability of the produced nanocatalysts in order to evaluate their long-term performance and durability. Varied catalysts have varied levels of catalytic stability, according to an analysis of the experimental data. With a retention rate of 97%, Catalyst D, for example, had the maximum stability after 100 cycles, suggesting less deterioration and superior long-term efficacy. On the other hand, Catalyst B exhibited the least stability after 200 cycles, with an 85% retention rate, indicating a gradual reduction in catalytic activity. These changes in stability are explained by variations in the surface characteristics, shape, and composition of the catalyst. Overall, the findings highlight how crucial stability testing is in determining whether nanocatalysts are suitable for real-world uses in the generation of sustainable hydrogen.

<table>
<thead>
<tr>
<th>Catalyst</th>
<th>Stability After 100 Cycles (%)</th>
<th>Stability After 200 Cycles (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>95</td>
<td>90</td>
</tr>
<tr>
<td>B</td>
<td>90</td>
<td>85</td>
</tr>
<tr>
<td>C</td>
<td>92</td>
<td>88</td>
</tr>
</tbody>
</table>

Fig. 4. Environmental Impact Assessment
The experimental study's findings provide significant insights into the stability, environmental effect, and efficiency of nanocatalysts for the sustainable synthesis of hydrogen from renewable resources. Catalyst surface area, shape, and composition were shown to be important determinants of catalytic performance, with differences amongst catalysts. Environmental impact evaluations also emphasized how crucial it is to optimize synthesis conditions in order to reduce waste production and resource consumption. The necessity for strong catalyst design and synthesis techniques was highlighted by stability testing, which found variations in catalyst durability and long-term performance.

4.1 Implications for Upcoming Studies

The study's conclusions have a number of ramifications for future investigations into nanocatalysts for the creation of sustainable hydrogen. Initially, further research is necessary to clarify the fundamental principles controlling catalytic activity and stability, enabling the creation of more effective and long-lasting catalysts. Second, steps should be taken to scale up catalyst synthesis procedures and assess how well they function in actual operational environments. Furthermore, studies concentrating on cutting-edge characterisation methods, computational modeling strategies, and innovative catalyst formulations may provide insightful information about catalyst design and optimization. Overall, developing sustainable hydrogen production technologies and quickening the shift to a low-carbon energy future depend on ongoing research and innovation in nanocatalyst development.

5 Conclusion
To sum up, this study examined the development, synthesis, and assessment of nanocatalysts for the sustainable generation of hydrogen from renewable resources. The analysis and outcomes of the experiments have given important new information on the stability, environmental effect, and catalytic activity of the produced nanocatalysts. Significant differences in the catalysts' surface area, activation energy, turnover frequency, and rate of hydrogen generation were found during the performance test. The study revealed that catalyst shape, composition, and surface characteristics are significant determinants of catalytic performance. This underscores the significance of customized catalyst design in achieving efficient hydrogen generation. Environmental impact evaluations showed that alternative synthesis techniques and catalyst compositions differed in terms of resource usage, waste production, and greenhouse gas emissions. Sustainable hydrogen production methods may be supported and the environmental effect reduced by optimizing catalyst design parameters and synthesis conditions. The significance of evaluating catalyst durability and long-term performance for real-world applications was highlighted by stability test findings. Strong catalyst design and synthesis techniques are essential to guarantee stable and consistent hydrogen generation over long periods of time. This is because catalyst stability plays a critical role in these processes. In summary, the results of this investigation add to the expanding corpus of information on nanocatalysts for sustainable hydrogen production and provide significant perspectives for further investigation and advancement. To improve synthesis conditions, scale up catalyst manufacturing for practical uses, and clarify the underlying principles driving catalytic activity and stability, further research is necessary. The development of nanocatalyst technology may expedite the shift towards an energy future that is sustainable and clean.

Reference

1. S. Ahmad, W. A. Siddiqi, and S. Ahmad, J Environ Chem Eng 11, (2023)
3. Meenu, M. Rani, and U. Shanker, Environmental Pollution 340, (2024)
8. T. A. Saleh, RSC Adv 12, 23869 (2022)
18. L. Fereidooni, A. R. C. Morais, and M. B. Shiflet, Resour Conserv Recycl 203, (2024)
41. S. Dixit and A. Stefańska, Ain Shams Engineering Journal (2022)
42. M. Kumar, C. Mohan, S. Kumar, K. Epifantsev, V. Singh, S. Dixit, and R. Singh, MRS Adv 7, 939 (2022)