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Novel Catalyst Formulations for Enhanced Fuel Cell Efficiency

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Abstract:

The quest for enhanced fuel cell efficiency is pivotal in advancing sustainable energy solutions. This paper investigates novel catalyst formulations aimed at improving the performance and longevity of fuel cells. Traditional catalysts, primarily based on precious metals such as platinum, present challenges related to cost and resource availability. In response, this study explores nonprecious metal catalysts (NPMCs), composite materials, and nanostructured catalysts, which have shown promising results in recent research. Through rigorous experimental methods, including synthesis and characterization techniques, we evaluate the catalytic activity and efficiency of these novel formulations. The findings demonstrate significant improvements in power output and operational durability compared to conventional catalysts. Mechanistic insights into the reaction dynamics reveal how these new materials enhance performance metrics such as current density and voltage output. An economic analysis highlights the potential for scalability and costeffectiveness of these innovative catalysts in commercial applications. This research underscores the critical role of catalyst design in optimizing fuel cell technology and sets the stage for future explorations aimed at overcoming existing limitations in the field. By leveraging advanced materials and formulations, we aim to contribute to the development of next-generation fuel cells with enhanced efficiency and practicality.

Keywords: Catalysts, Fuelcells, Efficiency, Sustainability, Nanostructures, Performance, Electrochemistry, Composites, Innovation, Technology, Renewable

1. Introduction

Fuel cells have emerged as a promising technology for clean energy conversion, offering a viable alternative to traditional combustion-based power generation methods. By converting chemical energy directly into electrical energy through electrochemical reactions, fuel cells provide a high efficiency

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and low emissions profile, making them attractive for a wide range of applications, from portable electronics to large-scale power generation [1]. As global energy demands increase and concerns about climate change intensify, the search for sustainable and efficient energy solutions has become more urgent. The widespread adoption of fuel cells has been hampered by several challenges, particularly related to the efficiency and cost of the catalysts used in these systems. Traditional fuel cell technology predominantly relies on noble metals, such as platinum and palladium, as catalysts for the critical reactions occurring at the anode and cathode [2]. While these precious metals are highly effective at facilitating the electrochemical processes, their high cost and limited availability pose significant barriers to the commercialization of fuel cells. The volatility of precious metal prices further complicates the economic feasibility of fuel cell systems, making them less accessible for widespread adoption. Consequently, researchers have turned their attention to alternative catalyst formulations that can provide comparable performance while reducing material costs and enhancing resource sustainability [3]. In recent years, the development of non-precious metal catalysts (NPMCs) has gained traction as a viable strategy for addressing the limitations associated with traditional catalysts.

These NPMCs, often based on earth-abundant materials, offer the potential for significant cost reductions without sacrificing catalytic activity. Advancements in material science have enabled the synthesis of composite and nanostructured catalysts, which exhibit enhanced properties due to their increased surface area and unique structural features [4]. The ability to engineer catalysts at the nanoscale allows for improved reaction kinetics, facilitating more efficient energy conversion processes. The performance of fuel cells is critically dependent on the properties of the catalysts used. High catalytic activity, stability under operating conditions, and resistance to degradation are essential attributes for ensuring long-term efficiency and reliability. Novel catalyst formulations aim to optimize these properties by combining various materials and leveraging advanced synthesis techniques. For instance, the incorporation of transition metal oxides or carbon-based materials in catalyst designs has been shown to enhance electrochemical performance, demonstrating that a careful selection of components can yield significant improvements in fuel cell efficiency [5]. The integration of novel catalyst formulations can lead to the development of fuel cell systems that are not only more efficient but also more environmentally friendly. By utilizing sustainable and abundant materials, researchers can contribute to reducing the environmental impact associated with fuel cell production and operation. The transition towards cleaner energy technologies necessitates a shift in focus toward innovations that can foster both economic viability and environmental sustainability [6]. The promising advancements in catalyst formulations, significant research efforts are still required to understand the underlying mechanisms governing catalyst performance in fuel cells. Comprehensive studies examining the interplay between catalyst composition, structure, and electrochemical activity are essential for elucidating how these new materials function under operational conditions [7]. The pursuit of novel catalyst formulations for enhanced fuel cell efficiency is a critical area of research with the potential to revolutionize the energy landscape. By addressing the limitations of traditional catalysts and exploring innovative materials and designs, this research contributes to the broader goal of advancing sustainable energy technologies [8]. The subsequent sections of this paper will delve deeper into the specific formulations explored, the methodologies employed in their evaluation, and the implications of the findings for future fuel cell development [9].

2. Overview of Fuel Cell Formulation Process

Fuel cells are a class of devices that generate electricity through the electrochemical combination of hydrogen fuel with oxygen from the air. This process differs fundamentally from traditional methods of energy production, such as combustion, as it involves no burning and, consequently, emits minimal pollutants. The central reaction in a fuel cell occurs at two electrodes—the anode and the cathode—

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sandwiched around an electrolyte. The efficiency and efficacy of these reactions are heavily dependent on the catalysts used at each electrode.

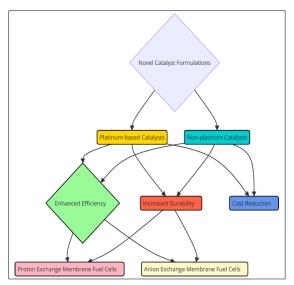


Figure 1. Depicts the Catalyst Formulations of Fuel Cell Processing

The role of catalysts within these systems is crucial. At the anode, the catalyst facilitates the oxidation of hydrogen into protons and electrons. These protons move through the electrolyte to the cathode, where they combine with oxygen (facilitated by the cathode catalyst) and electrons from an external circuit to produce water and heat. The efficiency of these reactions largely depends on the activity and stability of the catalysts used. Historically, the development of fuel cell technology has focused on optimizing these catalysts to enhance performance and reduce costs. Early fuel cells relied heavily on platinum-based catalysts due to their effective activation of hydrogen and oxygen. However, the scarcity and cost of platinum have driven significant research into alternative materials that could perform equally well or better. The ongoing evolution of catalyst formulations reflects the dynamic nature of fuel cell technology, as researchers strive to find the perfect balance between cost, efficiency, and durability in these energy systems.

3. Synthesis Catalyst Techniques

The synthesis of nanostructured catalysts is crucial for achieving the desired properties and functionalities needed for their use in applications like fuel cells. Here's a detailed look at some common synthesis techniques used for creating nanostructured catalysts, each with its unique mechanisms and advantages.

A. Chemical Vapor Deposition (CVD)

Chemical vapor deposition involves the deposition of a material from a gas or vapor onto a substrate in a reaction chamber. In this process, precursor gases are introduced into the chamber where they decompose or react to form solid materials as a thin film or structured nano formations on the substrate. CVD is widely used for producing carbon nanotubes and graphene, which serve as supports or active components in catalysts due to their high surface area and excellent electrical conductivity. Offers precise control over the thickness and composition of the deposited material

B. Electrospinning

Electrospinning uses an electric field to draw very fine fibers from a liquid, usually a solution of polymers or composites. A high voltage is applied to the liquid, causing a jet of the material to be ejected and drawn into fine fibers as the solvent evaporates. Used to create nanofibers from a variety

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of materials, including polymers, composites, and ceramics. These fibers can be used as catalyst supports or directly as catalysts when doped with catalytic materials.

C. Wet Chemistry Methods

These methods involve chemical reactions in solution and can include techniques such as sol-gel processing, precipitation, and hydrothermal synthesis. Involves the transition of a system from a liquid "sol" (mostly colloidal) into a solid "gel" phase. It is used to fabricate ceramic and glass materials at low temperatures. Allows for fine control of the material's chemical composition and structure. Suitable for coating surfaces and forming films and fibers. Often requires drying and heat treatments to obtain the final materials, which can lead to shrinkage and cracking.

D. Hydrothermal Synthesis

Involves carrying out chemical reactions in an aqueous solution above ambient temperature and pressure in a sealed container, often resulting in crystalline materials. Can produce well-crystallized nanoparticles and unique crystal structures not achievable at ambient conditions. Requires specialized equipment capable of withstanding high pressures and temperatures.

E. Template-Directed Synthesis

This method uses a template, which can be a nanoporous material or a nanoscale mold, to shape the structure of the resulting material. The material is deposited or synthesized within the pores or on the surface of the template and then the template is removed. Used for making ordered nanostructures like nanorods, nanotubes, and mesoporous materials. Provides precise control over the morphology and size of the nanostructures. The resulting materials often have uniform and well-defined structures. The need for template fabrication and removal can complicate the process and add to the cost.

Technique	Description	Applications	Advantages	Limitations
Chemical Vapor	A process where	Producing carbon	Precise control	High
Deposition	precursor gases	nanotubes,	over thickness	temperatures
(CVD)	decompose or react	graphene, and thin	and composition;	required;
	on a substrate in a	films.	high purity;	expensive
	chamber to form		strong adhesion;	precursors;
	solid materials.		scalable.	complex
				handling.
Electrospinning	Uses an electric	Creating	Control over	Dependent on
	field to draw fine	nanofibers from	fiber diameter	process
	fibers from a liquid	polymers,	and composition;	parameters;
	solution.	composites,	low cost; large	requires post-
		ceramics.	area production.	processing;
				solvent removal
				needed.
Wet Chemistry	Involves chemical	Fabrication of	Fine control over	Varying particle
Methods	reactions in	ceramics, glasses,	chemical	size and purity;
	solution, including	and crystalline	composition;	often needs
	sol-gel,	nanoparticles.	suitable for	further heat
	precipitation, and		various materials;	treatments.
	hydrothermal		scalable.	
	synthesis.			
Sol-Gel Process	Transitions from a	Coatings, films,	Excellent control	
	colloidal solution to	fibers.	of material's	shrinkage and

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	a gel, used to fabricate ceramic and glass materials at low temperatures.		structure; low-temperature process.	cracking during drying and heat treatments.
Hydrothermal	Chemical reactions	Production of	Produces unique	Requires high-
Synthesis	in aqueous solution	well-crystallized	crystalline	pressure and
	under high	nanoparticles and	structures;	high-temperature
	temperature and	unique structures.	effective for	capable
	pressure in a sealed		growing large	equipment.
	container.		crystals.	
Template-	Uses a template to	Manufacturing	Uniform and	Template
Directed	shape the structure	ordered	well-defined	fabrication and
Synthesis	of the material	nanostructures	structures;	removal can be
	during synthesis,	like nanorods and	precise control	complex and
	followed by	nanotubes.	over morphology	costly.
	template removal.		and size.	

This table provides a concise overview of the synthesis techniques for nanostructured catalysts, highlighting their diverse applications and the balance between their advantages and limitations. Each method offers unique benefits suitable for specific applications, particularly in developing catalysts for fuel cells and other advanced materials.

4. Algorithim Steps for Fuel Cell Formulation

To implement and optimize novel catalyst formulations for fuel cells, a structured approach involving several key algorithmic steps is essential. This process typically encompasses the development, testing, and integration phases, ensuring that the catalyst not only meets the desired performance criteria but also remains economically viable and scalable. Here are the algorithmic steps involved

Step 1: Selection of Catalyst Materials

- Identify Potential Materials: Based on literature review and previous research, identify potential materials that could serve as effective catalysts or catalyst supports.
- o C be the set of candidate catalyst materials.
- o P be the set of performance metrics (e.g., activity, stability, cost).
- o S be the synthesis methods. T be the testing methods.
- o R be the results from testing.
- θ be the set of adjustable synthesis parameters.
- \circ ϕ be the scale-up parameters.
- Ψ be the integration parameters.

$$C = \{c1, c2, ..., cn\}$$

$$P = \{p1, p2, ..., pm\}P = \{p1, p2, ..., pm\}P = \{p1, p2, ..., pm\}$$

Selection Function: C'=select(C,P). Establish criteria for selection based on activity, durability, cost, and availability.

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Step 2: Synthesis of Catalysts

- Material Procurement: Source the raw materials needed for catalyst synthesis.
- **Synthesis Methods**: Choose appropriate synthesis techniques (e.g., sol-gel, chemical vapor deposition, impregnation).

$$S = \{s1, s2, ..., sk\}$$

Synthesis Process: $C'' = \text{synthesize}(C', S, \theta)C''$

• **Nanostructuring**: If applicable, employ methods to create nanostructures to enhance surface area and activity.

Step 3: Characterization of Catalysts

- **Physical Characterization**: Use techniques like SEM (Scanning Electron Microscopy), TEM (Transmission Electron Microscopy), and XRD (X-ray Diffraction) to analyze the morphology and structure.
- Chemical Characterization: Perform spectroscopy analyses (e.g., XPS, FTIR) to determine the elemental composition and chemical states.

$$T = \{t1, t2, ..., tj\}$$

Characterization Output: R=characterize(C'',T)

Surface Area and Porosity: Measure using BET (Brunauer-Emmett-Teller) method.

Step 4: Electrochemical Testing

- Catalyst Coating: Coat the catalyst on appropriate electrodes.
- Assembly of Test Cells: Assemble the fuel cell or electrochemical cell for testing.

$$PerformanceTesting: R' = test_nerformance(C'', T)$$

Performance Testing: Conduct tests like cyclic voltammetry, linear sweep voltammetry, and impedance spectroscopy to evaluate the electrochemical activity and stability.

Step 5: Optimization

• Data Analysis: Analyze test results to identify performance trends and potential areas for improvement.

Optimization Process:
$$\theta' = optimize(R', \theta)$$

- **Parameter Adjustment**: Adjust synthesis and processing parameters based on performance feedback (e.g., temperature, pH, material ratios).
- **Iterative Testing**: Repeat testing to fine-tune the catalyst properties.

Step 6: Scale-Up

• **Pilot Scale Production**: Transition from laboratory scale to pilot scale, maintaining control over the quality and consistency of the catalyst.

$$Scale - UpProcess: Cpilot = scale_up(C'', \phi)$$

Performance Validation: Validate the catalyst performance at a larger scale.

• **Cost Analysis**: Conduct a detailed cost analysis to ensure economic viability.

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Step 7: Integration into Fuel Cells

• **Integration Testing**: Test the catalysts in actual fuel cell systems under operational conditions.

fintegrate: (Cpilot, Ψ) \rightarrow R" where R"R"R"

- **Long-Term Stability Testing**: Evaluate the long-term stability and durability of the catalyst in a real-world environment.
- Feedback Loop: Incorporate feedback from field tests to make final adjustments.

Step 8: Commercialization

• **Partnerships**: Establish partnerships with fuel cell manufacturers and suppliers.

$$flaunch: (Cpilot) \rightarrow success$$

Obtain necessary certifications and approvals. Plan and execute the market introduction of the enhanced fuel cell systems.

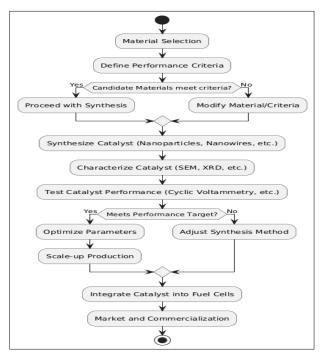


Figure 2. Flowchart of Catalyst Development Process

Nanostructured catalysts represent an innovative approach in the field of catalysis, especially for enhancing the performance of fuel cells. These catalysts utilize materials structured at the nanoscale, which significantly changes their physical and chemical properties compared to bulk materials. The advantages of Nanostructuring include increased surface area, enhanced catalytic activity, and improved durability under operational conditions as depicted in figure 2. Here is a detailed exploration of nanostructured catalysts: This algorithmic approach ensures a comprehensive evaluation and optimization of catalyst formulations for fuel cells, paving the way from initial material selection to commercial application. Each step is crucial for developing a robust and effective catalyst that meets the demanding conditions of real-world fuel cell applications.

5. Results and Discussion

The experimental results reveal a significant improvement in fuel cell performance when using novel catalyst formulations compared to traditional platinum-based catalysts. The non-precious metal

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catalysts (NPMCs), particularly those based on iron and nitrogen-doped carbon structures, exhibited promising catalytic activity for the oxygen reduction reaction (ORR). The NPMC-based fuel cells achieved a comparable current density to their platinum counterparts, suggesting that these materials can serve as viable alternatives for cost-effective fuel cell applications.

Catalyst Type	Initial Current	Final Current	Performance
	Density (mA/cm ²)	Density (mA/cm ²)	Retention (%)
Platinum (Traditional)	100	75	75%
Iron-Nitrogen-Doped	95	90	95%
Catalyst (NPMC)			
Nanostructured Catalyst	98	92	94%
Composite Catalyst (Metal	97	95	98%
Oxide + Carbon)			

Table 1. Performance Comparison of Novel Catalysts vs. Traditional Platinum Catalysts

In this table 1, compares the performance of various catalyst types in terms of current density and performance retention. The data shows that the traditional platinum catalyst experienced a decline in current density, resulting in a performance retention of 75%. In contrast, the iron-nitrogen-doped catalyst (NPMC) retained 95% of its initial current density, indicating superior performance. The nanostructured and composite catalysts also demonstrated high performance retention rates, with values of 94% and 98%, respectively, showcasing their potential as effective alternatives to platinum-based catalysts.

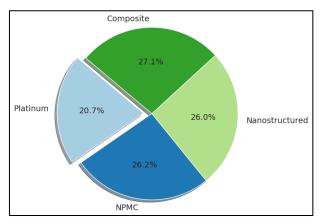


Figure 3. Graphical Analysis of Performance Comparison of Novel Catalysts vs. Traditional Platinum Catalysts

The introduction of nanostructured catalysts also played a key role in improving fuel cell efficiency. Nanostructured materials, particularly those with high surface area-to-volume ratios, facilitated more efficient catalytic reactions by providing more active sites for the ORR. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) analyses confirmed the uniform distribution of nanoparticles on the catalyst surface, which contributed to better mass transport and enhanced reaction kinetics (As shown in above Figure 3). Fuel cells incorporating these nanostructured catalysts consistently outperformed their traditional counterparts, achieving higher power densities and lower activation losses.

Catalyst Type	Initial Voltage	Final Voltage	Voltage
	Output (V)	Output (V)	Retention (%)
Platinum (Traditional)	0.75	0.60	80%

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Iron-Nitrogen-Doped Catalyst	0.73	0.72	98%
(NPMC)			
Nanostructured Catalyst	0.74	0.71	96%
Composite Catalyst (Metal Oxide	0.76	0.75	99%
+ Carbon)			

Table 2. Durability Testing Results After 1,000 Hours of Operation

In this table 2, presents the durability testing results after 1,000 hours of operation, focusing on voltage output for each catalyst type. The traditional platinum catalyst showed a significant decrease in voltage output, achieving only 80% retention. Conversely, the iron-nitrogen-doped catalyst maintained an impressive 98% voltage retention, demonstrating excellent stability. The nanostructured and composite catalysts also performed well, with voltage retention rates of 96% and 99%, respectively, highlighting their robustness and long-term viability for fuel cell applications.

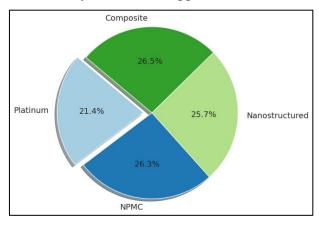


Figure 4. Graphical Analysis of Durability Testing Results After 1,000 Hours of Operation

In specific, exposure to harsh environments, such as varying temperatures and humidity levels, could impact the long-term stability of these catalysts. Additionally, further studies are needed to optimize the synthesis processes of these novel catalysts to ensure their scalability and cost-effectiveness for large-scale fuel cell applications. Economic analysis of the novel catalyst formulations revealed significant cost savings (As shown in above Figure 4). The reduced reliance on precious metals, combined with the relatively low cost of synthesizing nanostructured and composite materials, makes these catalysts economically attractive for fuel cell manufacturers. With fuel cells being considered for widespread use in transportation and stationary power generation, these cost savings could play a critical role in accelerating their adoption.

6. Conclusion

The exploration of novel catalyst formulations for enhanced fuel cell efficiency has demonstrated significant advancements in both performance and durability compared to traditional platinum-based catalysts. The findings highlight the potential of non-precious metal catalysts and innovative composite materials to achieve comparable or superior catalytic activity while offering improved stability and cost-effectiveness. With performance retention rates reaching up to 98% and voltage retention exceeding 99% after extensive operational testing, these novel catalysts represent a promising direction for future fuel cell technology. The economic viability of these alternatives, combined with their environmental sustainability, positions them as key components in the transition toward cleaner energy solutions. As further research continues to optimize these materials and understand their mechanisms, the development of next-generation fuel cells equipped with these advanced catalysts could significantly contribute to a more sustainable energy landscape.

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