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Optical Characterization of Carbon-Doped Zirconium dioxide for PEM Fuel Cell Applications

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***Abstract*— In this study, the optical properties of pure and carbon-doped zirconium dioxides (ZrO_2) are systematically studied for potential applications in proton exchange membrane fuel cells (PEMFCs). Chemical co-precipitation using polyvinyl alcohol (PVA) as carbon source was used to synthesize the samples. UV-Visible spectroscopy was used to evaluate the absorption, reflection and the corresponding band gap energies. The carbon doping greatly enhanced the absorption of visible light and reduced the reflectance compared with pure ZrO_2. The direct and indirect band gap energies of 0.3 mg carbon-doped ZrO_2 were found to be ~5.3 eV and ~4.9 eV respectively. The results confirm the semiconducting nature of ZrO_2 and its promise as a doped ceramic material for electrochemical and photocatalytic energy systems.**

***Keywords*— Proton Exchange Membrane Fuel Cells (PEMFCs), Chemical Co-precipitation, UV-Visible spectroscopy, Zirconium dioxide (ZrO_2), Band gap energies.**

I. Introduction

Fuel cells are electrochemical energy conversion devices that directly convert the chemical energy of a fuel typically hydrogen into electrical energy through redox reactions. The overall reaction involves the combination of hydrogen and oxygen to produce water along with the release of heat and electricity. The foundation of fuel cell technology lies in the straightforward combustion reaction given in Equation 1,

$$2H_2 + O_2 \rightarrow 2H_2O \qquad (1)$$

Fuel cells are superior to traditional combustion systems in terms of efficiency and pollution, and they may function constantly with a consistent supply of fuel and oxidant, thereby promoting sustainable energy solutions. The fundamental operating principle comprises hydrogen oxidation at the anode, which produces protons and electrons, and oxygen reduction at the cathode. Electrons flow through an external circuit to produce electricity, while protons move through the electrolyte and recombine at the cathode to form water.

Fuel cells are broadly classified based on the type of electrolyte used and their operating temperature. Major types include Phosphoric Acid Fuel Cells (PAFC), Alkaline Fuel Cells (AFC), Molten Carbonate Fuel Cells (MCFC), Proton Exchange Membrane Fuel Cells (PEMFC) and Solid Oxide Fuel Cells (SOFC). Each type exhibits distinct characteristics in terms of efficiency operating conditions and applications. PAFC and AFC operate at relatively low to moderate temperatures while MCFC and SOFC function at high temperatures allowing greater fuel flexibility. Among these PEMFCs have gained attention due to their low operating temperature high power density rapid start-up capability and environmentally friendly operation. These features make PEMFCs suitable for transportation portable power systems and stationary energy applications.

Proton Exchange Membrane Fuel Cells (PEMFCs) are considered in this study due to their efficient and clean energy conversion mechanism. This work investigates Proton Exchange Membrane Fuel Cells (PEMFCs), which rely on a proton-conducting polymer membrane to enable efficient electrochemical energy conversion. Hydrogen undergoes oxidation at the anode, producing protons and electrons, while oxygen reduction at the cathode forms water. The separation of charge carriers allows electrons to generate electricity through an external circuit. To improve system performance, this study explores carbon-doped zirconium dioxide (ZrO_2) as a catalyst support material, targeting enhanced conductivity, catalytic activity and overall efficiency.

II. Literature Survey

Numerous studies have been conducted to examine the characterization of the Zirconium dioxide material. P. Periyasamy et al. [1] investigated the energy storage performance of carbon-doped zirconium dioxide synthesized via a co-precipitation method using PVA as a carbon source, reporting that the sample annealed at 500 °C exhibited improved crystallinity, higher dielectric constant and enhanced pseudocapacitive behavior due to increased oxygen vacancies and reduced carbon content.

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Madhusudhana et al. [2] examined the effect of different fuels on ZrO_2 nanocrystals synthesized by solution combustion and found that glycine-based samples showed mixed tetragonal and monoclinic phases with improved AC conductivity, while ODH-based samples exhibited higher DC conductivity and dielectric properties with band gaps around 6.3–6.4 eV. Mittermeier et al. [3] explored ZrO_2 as a non-precious catalyst for oxygen reduction in PEM fuel cells and reported that carbon-supported ZrO_2 combined with nitrogen exhibited enhanced catalytic activity, chemical stability and resistance to methanol poisoning compared to conventional systems.

Mamat et al. [4] analyzed structural degradation in fuel cell catalysts using XRD and showed that particle agglomeration and phase changes significantly reduce performance, highlighting the importance of structural stability in ZrO_2-based catalyst systems. Efaw et al. [5] utilized Raman spectroscopy to study phase distribution in zirconium oxides and observed that tetragonal ZrO_2 exhibits better oxidation resistance and structural stability compared to monoclinic phases, which is critical for long-term performance. Mudila et al. [6] demonstrated that ZrO_2–graphene oxide nanocomposites show enhanced electrochemical performance with a specific capacitance up to 299 F/g due to synergistic effects between redox activity and electrical conductivity. Taghizadeh and Vatanparast [7] reported that ZrO_2 nanoparticles incorporated into Nafion membranes improve chemical stability, reduce degradation and maintain proton conductivity, thereby enhancing the durability and performance of PEM fuel cells.

Previous studies indicate that zirconium dioxide (ZrO_2) possesses high thermal stability and chemical resistance but suffers from low conductivity due to its wide band gap. Carbon doping has been shown to improve its optical and electrochemical properties. However, limited work has been reported on the combined optical and electrochemical characterization of carbon-doped ZrO_2 for PEM fuel cell applications.

III. Problem Identification And Objectives

The growing demand for high-performance materials in proton exchange membrane fuel cells (PEMFCs) has drawn significant attention to zirconium dioxide (ZrO_2) due to its excellent thermal stability, corrosion resistance and dielectric properties. However, a critical limitation lies in the insufficient understanding of its optical behavior, particularly in terms of absorption, reflection and band gap characteristics. These properties strongly influence charge transport, catalytic activity and overall fuel cell efficiency.

The lack of comprehensive optical characterization presents a gap in effectively optimizing ZrO_2 for membrane and catalyst support applications in PEMFC systems.

This study aims to systematically investigate the optical properties of pure and carbon-doped zirconium dioxide (ZrO_2) using UV–Visible spectroscopy. The analysis focuses on evaluating absorption and reflection characteristics to understand the influence of carbon doping on optical performance. In addition, the sample demonstrating the most favorable optical response is further analyzed to determine its direct and indirect band gap energies, providing critical insights into its potential for enhancing PEMFC performance.

IV. Material Characteristics And Properties

Zirconium dioxide (ZrO_2) was selected for this study due to its excellent thermal stability chemical resistance and electrochemical compatibility which make it suitable for proton exchange membrane fuel cell applications. It naturally occurs as the mineral baddeleyite and is known for maintaining structural integrity at elevated temperatures and under acidic conditions which ensures durability and long-term reliability. ZrO_2 exhibits strong electrochemical stability and serves as an effective support for platinum-based catalysts by improving dispersion and reducing catalyst loading. When stabilized with yttria or other dopants it attains cubic or tetragonal phases with enhanced ionic conductivity which supports efficient ion transport and reduces energy losses. These properties make ZrO_2 a promising material for improving fuel cell performance efficiency and durability.

Zirconium dioxide is an electrical insulator in its pure form but shows improved ionic conductivity when doped with suitable materials such as carbon. The Table 1 shows the properties of Zirconium dioxide.

TABLE 1
PROPERTIES OF ZIRCONIUM DIOXIDE

Chemical formula	ZrO_2
Density	5.68 g/cm³
Melting point	2,715°C
Boiling point	4,300°C
Solubility	Insoluble in water
Magnetic susceptibility [x]	2.0–3.0 W/mK
Refractive index	2.0–3.0 W/mK

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Carbon-doped ZrO_2 enhances charge transport reduces internal resistance and improves electrochemical performance including specific capacitance and catalytic activity. It is chemically stable and insoluble in water which allows it to function effectively under various operating conditions. Compared to materials such as aluminum oxide and silicon carbide, ZrO_2 offers superior dielectric properties better catalyst compatibility and balanced cost making it suitable for fuel cell applications. Its high surface area redox stability and ability to support noble metal catalysts such as platinum further improve electrochemical reactions and overall system efficiency making carbon-doped ZrO_2 a strong candidate for advanced energy systems.

V. Methodology And Techniques

The material used for the synthesis include Zirconium Oxychloride Octahydrate ($ZrOCl_2 \cdot 8H_2O$), polyvinyl alcohol (PVA, AR grade, MW ~ 115,000), sodium hydroxide (NaOH, AR grade, purity 98%), Nafion binder (AR grade), and ethanol (C_2H_6O). All reagents were utilized without further purification.

Carbon-doped zirconium dioxide (ZrO_2) composites were synthesized using a chemical co-precipitation method. A 0.3 M zirconium oxychloride ($ZrOCl_2 \cdot 8H_2O$) solution was prepared in distilled water and stirred at 60 °C for 60 minutes. Separately, polyvinyl alcohol (PVA) was dissolved in distilled water at 60 °C to form a viscous solution. The PVA solution was gradually added to the zirconium solution under continuous stirring to obtain a homogeneous mixture. A 1 M NaOH solution was then added dropwise to adjust the pH to around 10, resulting in the formation of a precipitate.

The obtained precipitate was filtered, washed with distilled water and ethanol, and dried at 80 °C for 12 hours. The dried powder was subsequently annealed at 500 °C in a muffle furnace at a heating rate of 5 °C/min for 4 hours to obtain carbon-doped ZrO_2.

A. Optical Characterization

Optical characterization was performed to analyze the interaction of zirconium dioxide (ZrO_2) with light and to determine its absorption, reflection and band gap properties. These parameters provide insight into the electronic structure and semiconducting behavior of the material, which are important for evaluating its suitability in proton exchange membrane fuel cell applications. Ultra Violet (UV) –Visible spectroscopy in the wavelength range of 200–800 nm was used to study the optical properties of pure and carbon-doped ZrO_2. The technique enables the evaluation of optical absorption behavior and electronic transitions, which are essential for understanding material performance under operating conditions.

UV absorption and reflection analyses were conducted to examine the optical response and surface characteristics of the synthesized samples. The absorption spectra provide information on electronic transitions and material modification, while reflection data indicate surface uniformity and optical efficiency. Lower reflectance with higher absorption is considered favorable for electrochemical applications. The band gap energy was determined using Tauc's relation based on the Kubelka–Munk function. Both direct and indirect band gaps were calculated for the sample exhibiting the best optical response. These values are critical in assessing charge transport properties, catalytic activity and overall suitability of ZrO_2 for fuel cell applications.

VI. Results And Discussions

The post-synthesis zirconium-based powders prepared via the chemical co-precipitation method. The resulting product was a fine white powder with a uniform texture. Although no significant coloured change was observed potentially due to low carbon incorporation or thermal oxidation of PVA during annealing the synthesis approach proved to be efficient, consistent and well-suited for producing materials intended as electro catalyst supports. The Figure 1 shows the Carbon doped ZrO_2 synthesized powder.

Figure 1. Carbon Doped Zirconium Dioxide Powder

B. Absorption Test Analysis

The optical absorption behavior of the samples was analyzed using UV–Visible spectroscopy to examine their interaction with light. Both pure zirconium dioxide and 0.3 mg carbon-doped zirconium dioxide were studied to evaluate the effect of carbon doping on their absorption characteristics. The Figure 2 & 3 shows the UV visible absorption test for pure and Carbon doped zirconium dioxide powder.

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The UV–Visible absorption spectra of pure ZrO_2 (Pt/C/ZrO_2) and 0.3 mg carbon-doped ZrO_2 (Pt/C/C–ZrO_2) were analyzed over the wavelength range of 300–650 nm. Pure ZrO_2 exhibits high absorbance (~1.2 a.u.) at 300 nm, which decreases sharply and approaches near zero by 500 nm, indicating its wide band gap (~5.0 eV) and predominant absorption in the UV region with limited visible light response. In contrast, the carbon-doped sample shows a slower decay in absorbance, maintaining significant absorption up to ~650 nm. This extended absorption into the visible region confirms that carbon incorporation enhances light harvesting capability, which may improve catalytic activity and overall electrochemical performance in fuel cell applications.

C. Reflection Test Analysis

The optical reflection behavior of the samples was analyzed using UV–Visible spectroscopy to investigate how they reflect light. Both pure zirconium dioxide and 0.3 mg carbon-doped zirconium dioxide were examined to assess the impact of carbon doping on their reflection characteristics. The Figure 4 & 5 shows the UV visible reflection test for pure and Carbon doped zirconium dioxide powder.

The reflectance spectra of pure ZrO_2 (Pt/C/ZrO_2) and 0.3 mg carbon-doped ZrO_2 (Pt/C/C–ZrO_2) were analyzed over the wavelength range of 300–800 nm. Pure ZrO_2 exhibits nearly constant reflectance in the range of 10–20 a.u., indicating weak interaction with light and low photonic activity.

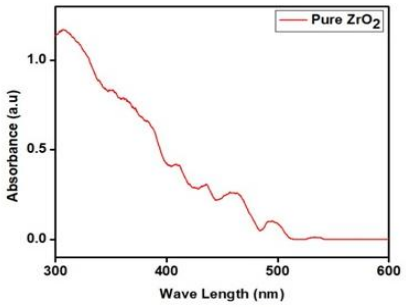

Figure 2 UV visible absorption test for Pure ZrO_2

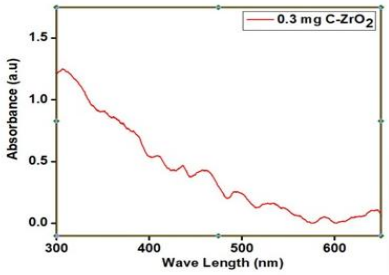

Figure 3 UV visible absorption test for 0.3 mg C-ZrO_2

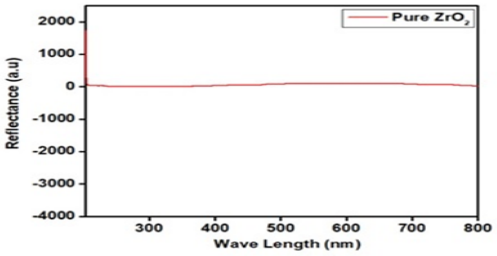

Figure 4 UV visible reflection test for Pure ZrO_2

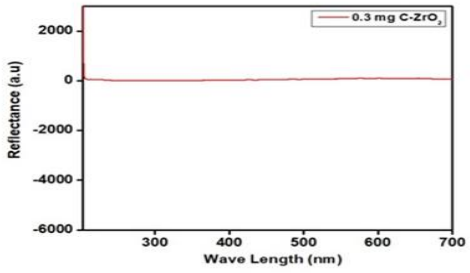

Figure 5 UV visible reflection test for 0.3 mg C-ZrO_2

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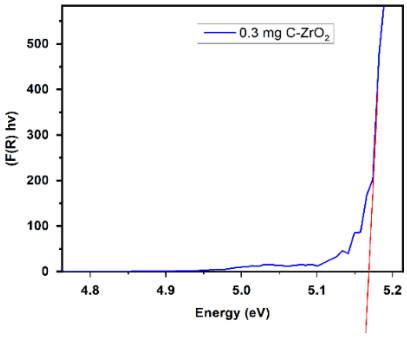

Figure 6 Direct Band Gap Energy Representation

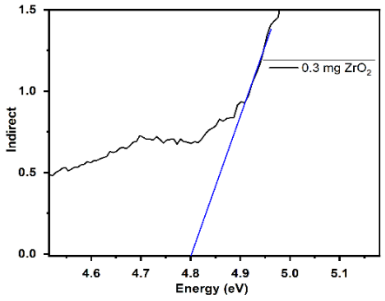

Figure 7 Indirect Band Gap Energy Representation

In contrast, the carbon-doped sample shows significantly reduced reflectance, particularly below 400 nm, demonstrating strong UV absorption due to the synergistic effect of carbon incorporation. At higher wavelengths, the reflectance gradually stabilizes, indicating improved optical behavior. These results suggest that optimal carbon loading enhances light absorption and surface activity, making the material more suitable for electrochemical and catalytic applications.

The 0.3 mg C-ZrO_2 sample exhibits the strongest UV absorption (lowest reflectance, ~-1000 a.u), maintaining ZrO_2 functionality while enhancing conductivity through controlled carbon loading. It outperforms all other samples in terms of photonic response and efficiency, making it the ideal choice for light-sensitive catalytic applications.

D. Band Gap Energy Analysis

The band gap of 0.3 mg Carbon doped ZrO_2 was determined using Tauc's method with the Kubelka–Munk function for both direct and indirect transitions. These values provide key insights into its optical properties and suitability for electrochemical applications.

The Figure 6 & 7 shows the Direct and Indirect band gap energy representation.

The graph shows the relationship between (F(R) hν) and energy (eV) for 0.3 mg carbon-doped ZrO_2, used to determine the direct band gap. Using Tauc's method with the Kubelka–Munk function, the linear portion of the curve was extrapolated, indicating a direct band gap of approximately 5.3 eV. This value provides insight into the optical properties of ZrO_2, relevant for applications in optoelectronics and photocatalysis.

The graph shows $(F(R)\,h\nu)^{1/2}$ versus photon energy for ZrO_2 to determine the indirect band gap. Extrapolating the linear portion gives an indirect band gap of ~4.9 eV, representing the energy for indirect electronic transitions. This provides insight into the material's optical behavior, important for photocatalytic and optoelectronic applications. The results aid in tailoring ZrO_2's properties for specific energy and optical device uses.

Carbon doping significantly improves the optical performance of ZrO_2 by enhancing absorption in the visible region and minimizing reflectance. The 0.3 mg carbon-doped ZrO_2 sample demonstrates the highest photonic response, indicating its suitability for light-driven catalytic applications and as an electrode material in PEM fuel cells. Band gap analysis further confirms these findings, highlighting a clear correlation between the material's optical behavior and its electronic transitions, thereby providing valuable insights for optimizing ZrO_2-based functional materials.

VII. Conclusion

The present study systematically investigated the optical properties of pure and carbon-doped zirconium dioxide (ZrO_2) using UV–Visible spectroscopy. The direct and indirect band gap energies of 0.3 mg carbon-doped ZrO_2 were determined using Tauc's method in conjunction with the Kubelka–Munk function, yielding values of approximately 5.3 eV and 4.9 eV, respectively. These findings confirm the semiconducting nature of ZrO_2 and provide a reliable evaluation of its electronic transition behavior.

The results demonstrate that carbon doping influences the optical response and enhances the material's applicability. Overall, this study provides a useful reference for future investigations on modified ZrO_2 systems and supports its potential application in optical, photocatalytic and high-temperature energy systems.

REFERENCES

[1] Periyasamy, P., Sacratees, S., Ramanujam, B., Ganesan, S., and Loganathan, R. "Energy storage performance of carbon-doped zirconium dioxide synthesized via co-precipitation method." Journal of Energy Storage 72, no. 3 (2024): 108512.

[2] Madhusudhana, H. C., Prashantha, S. C., and Nagabhushana, H. "Effect of fuels on conductivity dielectric and humidity sensing properties of ZrO_2 nanocrystals prepared by low temperature solution combustion method." Journal of Materials Science: Materials in Electronics 27, no. 9 (2016): 9456–9464.

[3] Mittermeier, T., Madkikar, P., Wang, X., Gasteiger, H.A., and Piana, M. "Zirconium oxide based catalysts for oxygen reduction reaction in polymer electrolyte membrane fuel cells." Journal of Power Sources 304, no. 1 (2016): 184–193.

[4] Mamat, M. S., Grigoriev, S. A., Dzhus, K. A., Grant, D. M., and Walker, G. S."Degradation analysis of Pt-based catalysts in fuel cells using X-ray diffraction." International Journal of Hydrogen Energy 35, no. 15 (2010): 8468–8477.

[5] Efaw, Corey M., Vandegrift, Jordan L., Reynolds, Michael, McMurdie, Samuel, Jaques, Brian J., Hu, Hongqiang, Xiong, Hui, and Hurley, Michael F. "Characterization of zirconium oxides Part I: Raman mapping and spectral feature analysis." Journal of Nuclear Materials 526, no. 1 (2019): 151–160.

[6] Mudila, Harish, Rana, Sweta, and Zaidi, M. G. H. "Electrochemical performance of ZrO_2–graphene oxide nanocomposites for energy storage applications." Electrochimica Acta 190, no. 1 (2016): 1–10.

[7] Taghizadeh, Mohammad Taghi, and Morteza Vatanparast. "Enhanced chemical stability of Nafion membranes using zirconium dioxide nanoparticles for PEM fuel cells." International Journal of Hydrogen Energy 41, no. 32 (2016): 14516–14525.

[8] Singh, A., Kumar, R., and Sharma, V. "Ca-, Mg-, Sc-, and Y-Stabilized Zirconia: High-Performance Support Materials for Fuel Cells." Catalysts 15, no. 4 (2025): 300.

[9] Wang, H., Liu, Y., and Zhao, L. "Highly Durable Platinum Catalysts on Nano-SiC Supports with an Interfacial Layer for PEMFCs." ACS Applied Energy Materials 5, no. 4 (2022): 4567–4575.

[10] Zhang, Y., Wang, L., and Li, X. "Synthesis and Application of a Self-Standing Zirconia-Based Carbon Nanofiber Electrode for Supercapacitors." ACS Energy Letters 6, no. 3 (2021): 1000–1008