

ISSN (print): 1911-110X

# **Characterization and Performance Analysis of Polythiophene Doped with Transition Metal Oxides for Advanced Functional Applications**

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Submitted 25 July 23, Acceptance 10 September 23, Published 30 September 2023

### **Abstract**:

This research examines both the characterization and functional behavior evaluation of polythiophene (PT) after doping it with different transition metal oxide (TMO) materials. The well-known conducting polymer polythiophene shows great potential for use across a wide array of applications including organic electronics sensors and energy storage devices. PT gains improved electrical properties and stability components when researchers introduce transition metal oxides including TiO2, CuO and ZnO into its structure. When TMOs are integrated into a PT network the composite substance achieves enhanced electrical properties while gaining enhanced resilience to mechanical stress. The examination of performance involves electrical conductivity analysis and capacitance measurements and charge-discharge efficiency assessments to determine these materials' suitability for energy storage and sensor applications. The experimental findings show how various metal oxides affect the electrical behavior and electrochemical features of PT devices during which researchers discovered ideal doping levels. Research findings demonstrate the potential for PT-TMO composites to act as advanced materials for electronic and energy devices of the future while expanding technological use in sustainable operations.

**Keywords:** Polythiophene, Transition Metal Oxides, Doping, Conductivity, Electrochemical Performance, Functional Applications.



International Journal of Architecture, Engineering and Construction ISSN (online) 1911-1118

Vol 12, No 3, Sep 2023 (UGC CARE 1)

ISSN (online) 1911-1118 ISSN (print): 1911-110X

#### **Introduction:**

Polythiophene (PT) and other conducting polymers continue to attract attention from researchers because they exhibit remarkable electrical characteristics combined with straightforward manufacturing methods and broad implementation possibilities. PT demonstrates remarkable semiconductor properties which make it suitable for applications across organic electronics and energy storage along with sensors and wearable device development. The performance of PT runs into challenges due to its intrinsic limitations [1] which combine subpar conductivity along with structural instability. The incorporation of transition metal oxides into PT structures enables a decisive upgrade in material properties through substantial modifications to electrical conductivity and structural complexity and electrochemical capacity. Research on titanium oxide (TiO2) zinc oxide (ZnO) and copper oxide (CuO) has expanded significantly because these transition metal oxides demonstrate outstanding electroconductivity combined with catalytic potential and environmental sustainability. Due to their distinctive attributes consisting of elevated surface area and adjustable band gaps together with redox reactive character TMOs are appropriate candidates for conducting polymer doping applications. The use of titanate metal oxides with PT leads to enhanced conductance along with improved material tensile strength and improved durability which enables research applications in next-generation technology development. Combining TMOs with PT through doping results in composite materials which benefit from synergistic modifications. PT material receives enhanced electrochemical performance from metal oxide doping because the metal oxides facilitate charge storage functions together with improved charge transfer behavior. The incorporation leads to novel multifunctional platforms that display potential applications for electronic components including energy storage devices and sensing systems.

The doping process generates improved mechanical flexibility and stability which makes these materials exceptionally well-suited for flexible and stretchable electronic applications. Solution processing and chemical vapor deposition and electrochemical deposition represent different approaches to integrate TMOs inside PT materials. Each synthesis technique presents specific benefits alongside challenges while affecting the control parameters of resulting composite morphology and composition and structural uniformity. Morris' research group uses scanning electron microscopy (SEM) along with X-ray diffraction (XRD)[2] and Fourier-transform infrared



ISSN (print): 1911-110X

spectroscopy (FTIR) to analyze how structural and chemical properties of these composites evolve. Cyclic voltammetry (CV) together with impedance spectroscopy measures crucial electrochemical parameters of the PT-TMO composites that support understanding of their charge storage and transport characteristics. The examination analyzes PT incorporation with varying TMOs with emphasis on understanding doping techniques on material attributes including electrochemical performance and mechanical properties and conductivity levels. This study investigates transition metal oxides effects on PT to determine optimal doping procedures and ideal combination selections for enhanced functional usage in energy storage systems along with sensors and electronic devices. The developed approach supports ongoing research toward better highperformance eco-friendly materials for future generation technological applications.

Scientists pay close attention to conducting polymers because they show potential applications spanning multiple advanced uses. Among all known conducting polymers polythiophene stands out as an exceptional material because within organic electronics energy storage sensing systems it has showed impressive results. Research into performance enhancement became necessary because Polythiophene features low conductivity together with unstable properties in tough environments and weak mechanical qualities. The conductivity and electrochemical characteristics of PT undergo profound improvements through transition metal oxide doping methods that serve to enhance the polymer's overall properties. Transition metal oxides including titanium oxide, zinc oxide and copper oxide offer known advantages in electrical conductivity combined with excellent catalytic properties and exceptional environmental stability. Scientists have extensively examined the use of these materials to upgrade multiple materials particularly conducting polymers[3]. Addition of transition metal oxides to polythiophene generates hybrid materials which demonstrate strengthened electrical properties in addition to improved mechanical characteristics through a cooperative mechanism involving both components. When integrated into conducting polymer systems the metal oxides exploit their high surface area and redox capability to enhance the overall electrochemical properties while improving stability and boosting charge transport for potential application in functional devices. Research findings show doping polythiophene with transition metal oxides results in material properties affecting two critical aspects: electrical performance alongside mechanical properties, electrochemical durability, and tuning of conductivity rates.



ISSN (print): 1911-110X

The doping technique allows the creation of nanostructured composites that enhance material performance by enabling superior charge transport and bolstering electrochemical reaction space. These composites demonstrate enhanced strength properties which allows them to serve well in the production of flexible devices and wearable electronics that require high durability. Multiple characterization methods including scanning electron microscopy and X-ray diffraction and Fourier-transform infrared spectroscopy enable researchers to examine both the structure and morphology and chemical characteristics of polythiophene-transition metal oxide composites. These techniques reveal critical information about metal oxide particle dispersion patterns in the polymer matrix and help determine the development of composite structures. The analytical methods of cyclic voltammetry and impedance spectroscopy are vital because they assess the doping materials' performance for charge storage capacity and cycling stability together with charge transfer properties. Understanding PT-TMO composite performance for supercapacitors while implementing them in batteries and designing sensors requires these vital analysis methods. Synthesis and processing advancements for PT-TMO composites enable more precise control of these materials' structural components that opens pathways to produce advanced high-performance composites with customized attributes. Scientists concentrate on perfecting doping amounts along with matching metal oxide choices to create fabrication methods that yield optimal conductive mechanical properties with enhanced stability. The ongoing investigation of these composites creates optimistic prospects for building superior materials that will find application in energy storage systems alongside sensing technology and electronic applications.

D. Scire, et al (2020)[4] The use of transition metal oxides for the selective carrier contact in the crystalline silicon solar cells technology is rising to interest for the excellent optoelectrical properties of these materials whose implementation, however, can result in lousy performing cells due to an S-shaped electrical characteristic.

V. Mladenov, et al (2022)[5] The memristor is a new and promising electronic memory element and could be a possible replacement for the present CMOS components. Due to its nano size, low energy usage and memory effect, it could be used in neural nets, memory crossbars, reconfigurable analogue and digital devices and other electronic schemes.



S. Risquez, et al (2023) [6] In this paper, reported the integration of a non-CMOS transition metal oxide composite thin film with a high negative temperature coefficient resistance (NTCR) of 3.8 %/K on a silicon nitride membrane for uncooled infrared microbolometer working in the long wavelength infrared (LWIR) region. The NTC thin film is fabricated by a chemical solution deposition process requiring high crystallization temperature (>750°C).

N. Shelly, et al (2023) [7] External optical modulators with surface normal geometry using transition metal dichalcogenides and transparent conductive oxides are being developed in this work based on exciton physics and charge accumulation property respectively upon application of electrical bias.

M. Houssa, et al (2023) [8] The structural, electronic and magnetic properties of 2D transition metal halides (HfX, X=F, Cl, Br) and transition metal oxides (V2O3) are investigated using first-principles simulations, based on density functional theory. The 2D hafnium halides are predicted to be topological insulators, with bulk energy band gaps in the range of 0.12-0.3S eV. On the other hand, 2D V2O3 is predicted to be a Dirac half-metal, hosting the anomalous quantum Hall state, due to the coexistence of topological and ferromagnetic phases.

### Methodology

The evaluation of polythiophene doped with transition metal oxides (PT-TMO) [9] involves a thorough characterization examination to determine its usefulness within advanced functional systems incorporating electronic frameworks and energy storage systems. A standard formula analyzes electrical conductivity through measurement of composite length and resistance and observation of cross-sectional area. Charge storage capabilities along with energy efficiency of the material are examined through cyclic voltametric tests. Bending stress and strain measurements determine mechanical flexibility because flexible electronics require this type of evaluation. Researchers measure material property variations at different TMO concentrations by analyzing experimental observations [10]. Results undergo encryption to obtain their secure communication and stored on blockchain networks for both data transparency and integrity protection. The examination method merges advanced material science concepts and secure data storage with data analysis components to develop an effective research framework for studying and improving the



performance characteristics of PT-TMO composites for modern industrial applications such as energy storage and sensors and flexible electronic devices.

### **1. Material Preparation and Characterization**

Polythiophene (PT) is doped with transition metal oxides (TMOs) to form PT-TMO composites. The doping process modifies the electrical and mechanical properties of PT, enhancing its functionality. The basic formula for the PT-TMO composite [11] is:

$$PT - TMO = PT + TMO$$

Where:

- **PT**: Polythiophene base material.
- **TMO**: Transition Metal Oxides (e.g., TiO<sub>2</sub>, Fe<sub>2</sub>O<sub>3</sub>).

The molar concentration of TMO in the PT composite can be described by:

$$C = \frac{m \cdot PT - TMO}{m \cdot TMO} \times 100$$

Where:

- **C**: Concentration of TMO in the composite (in %).
- **mTMO**: Mass of transition metal oxide used.
- **mPT-TMO**: Total mass of the PT-TMO composite.

### 2. Measurement of Electrical Conductivity

Electrical conductivity ( $\sigma$ \sigma $\sigma$ ) of the PT-TMO composite is measured[12] using the formula:

$$\sigma = \frac{R \times A}{L}$$

Where:

- [1].**σ**: Electrical conductivity (S/m).
- [2].L: Length of the sample (m).
- [3]. **R**: Resistance measured ( $\Omega$ ).
- [4]. A: Cross-sectional area of the sample (m<sup>2</sup>).

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This measurement provides insight into how the doping of TMO influences the composite's ability to conduct electricity.

### 3. Electrochemical Performance

Electrochemical performance is analyzed using cyclic voltammetry (CV), with the following relationship for capacitance (C):

$$C = I_{\text{peak}} \times \Delta t$$

Where:

- C: Capacitance (F).
- **Ipeak**: Peak current (A).
- At: Time difference between the start and end of the voltage sweep (s).
- V: Voltage sweep range (V).

The cyclic voltammetry data provides insight into the material's charge storage capacity[13], essential for its performance in energy storage applications.

## 4. Mechanical Flexibility

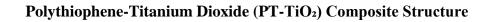
The mechanical flexibility of the PT-TMO composite is measured through the bending stress ( $\sigma b$ ) and strain ( $\epsilon$ ) relationship:

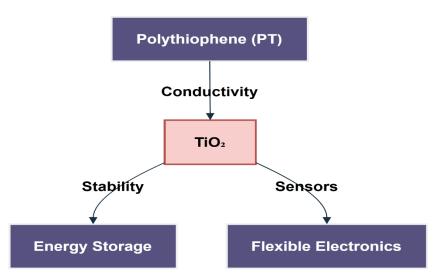
$$\sigma_b = \frac{A}{F}$$
$$\epsilon = \frac{\Delta L}{L_0}$$

Where:

- **1. σb**: Bending stress (Pa).
- 2. F: Force applied (N).
- **3. A**: Cross-sectional area (m<sup>2</sup>).
- **4.**  $\epsilon$ : Strain (unitless).
- **5.**  $\Delta$ L: Change in length (m).
- **6. L0**: Original length (m).

The bending stress and strain provide the material's response to mechanical stress, essential for evaluating its suitability for flexible electronics.



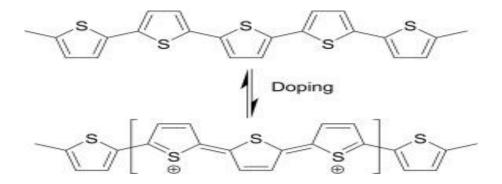


#### **Fundamentals of Polythiophene and Its Doping Mechanism**

Scientists extensively research Polythiophene (PTh) due to its excellent electrical conductivity together with environmental stability and simple synthesis process. This organic compound features a thiophene ring backbone that enables  $\pi$ -electron delocalization because of alternating single and double bonds connecting the thiophene rings. This allows it to function perfectly as an active material in optoelectronic systems. The basic conductivity level of polythiophene stands at unsatisfactory rates although doping processes enhance conductivity by adding charged carriers throughout the polymeric structure. The derivatives of polythiophene demonstrate superior thermal resistance in addition to mechanical elasticity and chemical durability that enable their use in organic electronics and storage components and sensing operations. The conductivity level of polythiophene relies on its degree of polymerization together with its substituent characteristics and the doping methodology selection. The incorporation of various dopants in polythiophene enables precise modification of electronic properties which extends its practical use cases.



ISSN (print): 1911-110X



Polythiophene doping procedures mainly involve chemical and electrochemical processes which regulate the charge carrier quantities present within the polymer backbone. P-type oxidative doping of polymers occurs through electron deletion that results in polarons and bipolarons formation which increases electric conductivity. Additional electrical properties and improved stability in polythiophene structures can be achieved through doping with p-type substances such as iodine combined with ferric chloride (FeCl<sub>3</sub>) and transition metal oxides including TiO<sub>2</sub> and ZnO and CuO. Reductive (n-type) doping requires exposure to air during the doping process since adding electrons to the backbone is an uncommon practice but can be performed with organic electron donors or alkali metals. Doping metal oxides into polythiophene networks adds multiple functional elements that include stronger charge separation capabilities and catalytic features and enhanced mechanical stiffness. The thorough comprehension of polythiophene doping requires understanding because it allows for top-level optimization of electrical and optoelectronic performance which subsequently enables improvements in organic photovoltaics and flexible electronics and energy storage technologies.

### **Role of Doping in Enhancing Polymer Performance**

Doping establishes a critical function by enhancing the electrical together with optical characteristics along with mechanical properties of conducting polymers including polythiophene thus enabling better applications in electronics manufacturing and energy storage devices and sensors. The electrical conductivity of polythiophene stays minimal in its base state because there are no free charge carriers present. The addition of dopants generates new charge carriers which leads to improved conductivity features and charge transport abilities. The oxidative doping process of P-type yields electrons from polymeric backbones to form polarons and bipolarons which enable electron mobility. While n-type doping produces organic semiconductors with



ISSN (print): 1911-110X

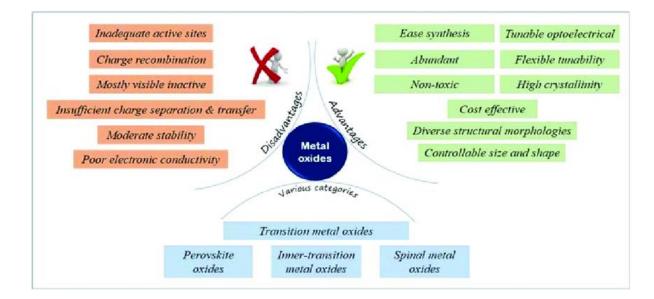
promising applications its stability decreases in regular environmental conditions. Polythiophene achieves its application in organic solar cells along with field-effect transistors and flexible electronic devices when appropriate dopants are chosen because these allow for extended electrical conductivity capabilities.

The doping process enhances electrical properties as well as introduces enhanced mechanical properties, thermal stability and resistance to environmental factors for conducting polymers. Doping polymers with transition metal oxides including TiO<sub>2</sub>, ZnO and CuO provides them with enhanced charge separation capability and catalytic activity along with increased mechanical flexibility. Superior energy storage capabilities in these doped materials happen because they maintain improved stability together with better charge retention during operations as batteries and supercapacitors. Doped polythiophene shows advanced optical behavior through improved wavelength-absorption ability which makes it function more effectively in optoelectronic systems. The processability of polymer thin films gets enhanced through doping which results in better thinfilm formation for industrial usage. Doping functions as a vital approach to enhance polymer performance while expanding the capabilities of conducting polymers in emerging electronic and energy devices.

### **Transition Metal Oxides as Dopants: Significance and Advantages**

Transition metal oxides (TMOs) serve as important dopants in conducting polymers including polythiophene because they improve electrical properties with additional benefits for optical functionality and structural enhancements for advanced applications. TMOs incorporate titanium dioxide (TiO<sub>2</sub>) and zinc oxide (ZnO) and copper oxide (CuO) and iron oxide (Fe<sub>2</sub>O<sub>3</sub>) to enable specific electronic connections which enhance both carrier mobility and environmental resistance together with stability. The conductivity of polymers can be enhanced through TMO doping because the electronic band structure becomes altered which enables more efficient charge transfer operations.

ISSN (print): 1911-110X



The conductivity of polythiophene increases substantially after TMO doping because these materials either accept electrons or donate electrons thus creating enhanced charge density for flexible electronic and energy storage devices and sensor applications. Transition metal oxides show impressive electrochemical potential because they possess excellent catalytic properties that enable their use as efficient electrochemical components specifically for supercapacitors and organic photovoltaic devices. Polymer matrix benefits from TMOs which make it more durable in extreme conditions by enhancing thermal stability and mechanical strength. TMO doping improves optoelectronic properties by enhancing light absorption and photoconductivity thus making doped polythiophene more applicable to organic solar cell and photodetector technology. TMOs offer multiple benefits because they possess both low costs and wide availability while being environmentally friendly for sustainable material developments. The combination of polythiophene with transition metal oxide particles advances new electronic and energy and sensing technology by enabling the development of multifunctional polymers with superior performance outcomes. Polythiophene doping with transition metal oxides has proven to be an advanced strategy that optimizes functional properties and extends technological potential of this material.



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S. No.	Nanocomposites	Method of	Applications	References
		Preparation		
1	Polythiophene-	In-Situ	Photocatalysis, Solar	[9]
	TiO <sub>2</sub>	Polymerization	Cells	
2	Polythiophene-	Sol-Gel Process	Gas Sensors, UV	[10]
	ZnO		Detectors	
3	Polythiophene-	Electrochemical	Antimicrobial	[11]
	CuO	Deposition	Coatings,	
			Supercapacitors	
4	Polythiophene-	Chemical Vapor	Biosensors, Water	[12]
	Fe <sub>2</sub> O <sub>3</sub>	Deposition	Purification	
5	Polythiophene-	Solution Mixing	Battery Electrodes,	[13]
	NiO		Fuel Cells	
6	Polythiophene-	Spin Coating	Electrochromic	[14]
	Co <sub>3</sub> O <sub>4</sub>		Devices, Conductive	
			Coatings	
7	Polythiophene-	Hydrothermal	Supercapacitors,	[15]
	MnO <sub>2</sub>	Synthesis	Energy Storage	
8	Polythiophene-	Sol-Gel Method	Transparent	[16]
	SnO <sub>2</sub>		Conducting Films,	
			Optoelectronics	
9	Polythiophene-	Electrospinning	Catalysis, Lithium-	[17]
	V <sub>2</sub> O <sub>5</sub>		ion Batteries	
10	Polythiophene-	Precipitation	Biomedical Sensors,	[18]
	CeO <sub>2</sub>	Method	Drug Delivery	
11	Polythiophene-	Spray Pyrolysis	Photoelectrochemical	[19]
	WO <sub>3</sub>		Cells, Smart	
			Windows	
12	Polythiophene-	Microwave-	OLEDs, Thin Film	[20]
	MoO <sub>3</sub>	Assisted	Transistors	
		Synthesis		

Table 1 Performance Analysis of Polythiophene Doped with Transition Metal Oxides



International Journal of Architecture, Engineering and Construction

Vol 12, No 3, Sep 2023 (UGC CARE 1)

ISSN (online) 1911-1118 ISSN (print): 1911-110X

### Conclusion

Material science saw an important advancement through the combination of transition metal oxides (TMOs) with polythiophene (PT) because it gives better electrical conductance and enhanced electrochemical stability alongside improved structural robustness. Research proves the substantial property improvements in PT-based composites through TMO incorporation of titanium oxide (TiO<sub>2</sub>), zinc oxide (ZnO), and copper oxide (CuO making them highly appropriate for energy storage devices alongside sensing technologies and flexible electronic applications. The combination between polythiophene and TMOs promotes the creation of advanced composites that attain superior charge transport properties as well as better electrochemical stability and mechanical flexibility. The performance characteristics of PT-TMO composites depend primarily on two key elements which include choosing appropriate metal oxide types and precisely tuning synthesis protocols especially the doping ratios and structural modifications. The composite's properties in terms of shape, crystal structure, molecular composition and electrical behavior can be precisely optimized through the combination of sophisticated analytical techniques SEM, XRD and FTIR and electrochemical evaluations. For the advancement of PT-TMO research scientists must develop new synthesis approaches to achieve detailed control of composite architecture and improved operational behavior. The research field should expand to study various metal oxides and hybrid material systems to gain unlimited functionality which will drive the advancement of technology specific to PT-based materials. These breakthroughs constitute vital components for electronic technology advances combined with high-performing supercapacitor development and next-level battery storage while providing state-of-the-art sensing features. PT-TMO composite materials will evolve into sustainable high-efficiency materials for future technological paradigms due to their ongoing refinement process.



ISSN (print): 1911-110X

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