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Int. Jr. of Contemp. Res. in Multi. *PEER-REVIEWED JOURNAL* *Volume 5 Issue 1 [Jan- Feb] Year 2026*

Research Article

Frequency Dependent Energy Gap and Polarization Effects in ZnO Doped Polypyrrole

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DOI: https://doi.org/10.5281/zenodo.18831114

Abstract

The frequency-dependent energy gap and polarization effects in ZnO-doped Polypyrrole (PPy) nanocomposites with ZnO loadings of 4% and 5% were investigated exclusively under polarised conditions. Temperature-dependent electrical behaviour was examined using Arrhenius-type plots of the natural logarithm of resistance (LnR) versus inverse temperature (1/T) over a frequency range of 100–5000 Hz. The apparent activation energy and effective energy gap were evaluated to understand polarisation-assisted charge transport mechanisms. Both compositions exhibit thermally activated conduction characteristic of semiconducting behaviour, with effective energy gap values lying in the range of approximately 0.62–0.99 eV. Polarisation leads to a reduction in the effective energy gap, attributed to dipole alignment, enhanced polaron formation and improved hopping pathways for charge carriers. The 4% ZnO doped PPy nanocomposite shows a comparatively lower energy gap than the 5% ZnO sample, indicating more efficient interfacial polarisation and stronger polymer nanofiller interactions at this concentration. Frequency-dependent behaviour suggests that interfacial and dipolar polarisation mechanisms dominate at lower frequencies, while higher frequencies restrict carrier response, resulting in minor variations in the energy gap. Deviations from ideal Arrhenius linearity imply non-Arrhenius conduction involving hopping transport, trap-assisted mechanisms and structural disorder. The results highlight the significant role of polarisation and ZnO concentration in tailoring the electronic structure and charge transport properties of ZnO/PPy nanocomposites for advanced dielectric and electronic applications.

Manuscript Information

- **ISSN No:** 2583-7397
- **Received:** 10-12-2025
- **Accepted:** 23-02-2026
- **Published:** 28-02-2026
- **IJCRM:**5(1); 2026: 843-847

- **Plagiarism Checked:** Yes
- **Peer Review Process:** Yes

How to Cite this Article

Devi T S. Frequency Dependent Energy Gap and Polarisation Effects in ZnO Doped Polypyrrole. Int J Contemp Res Multidiscip. 2026;5(1):843-847.

Access this Article Online

www.multiarticlesjournal.com

KEYWORDS: Energy gap, Polarisation, ZnO/PPy nanocomposites, Arrhenius equation, Hopping conduction.

1. INTRODUCTION

Nanocomposites made using polymer have been extensively studied because their electrical, dielectric and mechanical properties can be tailored, therefore finding application in sensors, energy storage, electromagnetic interference shield, actuators and flexible electronics [15,3]. One such conducting polymer is polypyrrole (PPy), which has been the subject of much attention because it is simple to prepare, does not pollute the environment and has moderate transport capability of electrical and charge conduction as well as the ability to transport many models of charge transportation, such as polaron conduction and bipolaron conduction [6,13]. However, the structural disorder and charge transporting localisation limit the electrical and dielectric potentials of unmodified PPy in the majority of instances and need to be changed by the usage of nanofillers. One method that has been demonstrated to be effective in enhancing charge carrier mobility, interfacial polarization and dielectric response is the addition of inorganic semiconducting oxide, such as zinc oxide (ZnO), to the PPy Matrix [1,4]. Proposed ZnO colorless high dielectric constant and high thermal stable wide band gap semiconductor is that which would
provide additional conduction mechanisms and high interfacial forces when they are added to the polymer matrices [11]. Such areas of interfaces have significance to determination of frequency related dielectric behavior in addition to effective energy gap in polymer nanocomposites.

Energy gap (Eg) is one of the fundamental parameters that define the conductivity of the electronics, polarization process and a dielectric relaxation characteristic. A good insight into the processes which dominate the charge transport that occur in the sample can be provided by temperature-dependent measurements of dielectric constant or resistance [10,5]. Arrhenius-type resistance analysis in the form of lnR versus 1/T plots, is commonly employed in estimating the activation energy as well as testing ideal behaviour of semiconducting structural disordering, interfacial traps and trapped states [14, 7].

Electrical properties of the polymer nanocomposites are also influenced by the effects of polarization in which polarization of the dipoles in the nanocomposites decreases the potential barriers and triggering polaron formation that subsequently alters the effective energy gap [9,16]. This type of materials is extremely frequency dependent and
interfacial (Maxwell Gauge Sillars) and dipolar polarization mechanisms at lower frequencies and inhibits charges carrier interaction at higher frequencies respectively [8,12].

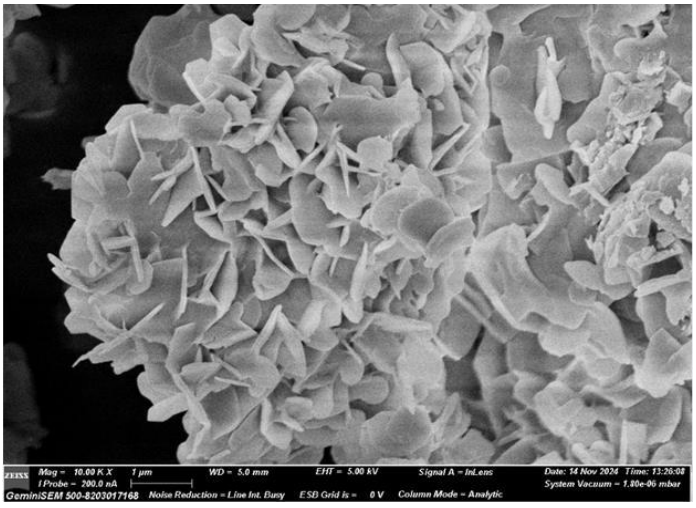
Polarization rate and ZnO concentration which are deposited on PPy nanocomposites are paramount factors in determining polarization related variability to the energy gap and conduction mechanism in frequency dependent nature characteristic of the conductivity in a sample of nanocomposite. These effects are significant to learn so as to create materials in optimum dielectric as well as electronic execution. Accordingly, the presented work is dedicated to the systematic study of the polarization dependent energy gap dynamics (as well as the frequency) of the ZnO doped PPy nanocomposites through the Arrhenius analysis within the context of the additional insight into the charge transport of the composites and their dielectric properties as an electronic approach.

2. Experimental Procedure:

Synthesis of Zinc Oxide (ZnO) Nanoparticles:

The synthesis of the nanoparticles of zinc oxide (ZnO) using a combination of the basic chemical precipitation technique. In this case, the following reaction
was taken 2.0g of sodium hydroxide (NaOH) was dissolved in 40mL of distilled water and 10g of zinc sulphate (ZnSO4) was dissolved in 120mL of distilled water. The two solutions were then mixed together and they were stirred to ensure that the solutions are mixed fluently with the help of a magnetic stirrer at a uniform period of time of one hour. PH of solution collected was maintained with a lot of caution and maintained at approximately 7.5.

The formed gel was allowed to kept an aging process for 48 hours. In this process Sulphate impurities were removed using repeated washing of the gel with distilled water. The purified gel after which it dried naturally in a Petri dish. This sample was dried and then annealed in the muffle furnace at a temperature 500°C for 4h. The cooled ZnO fine powder was obtained on the room temperature.



FESEM Image of Zinc Oxide

The dimensions of the crystallites (ZnO nanoparticles) were evaluated using the obtained findings in the X-ray diffraction (XRD) analysis of the test with the aid of the Debye-Scherrer equation:

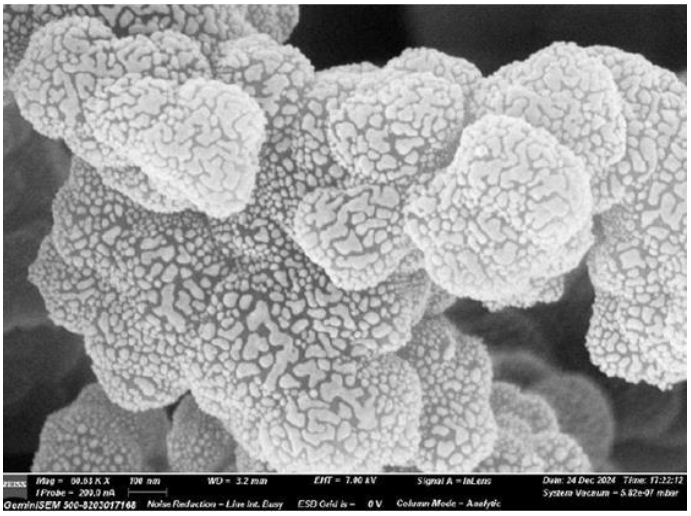
$$D = \frac{K\lambda}{\beta cos\theta}$$

where D is the average crystallite size, K is the shape factor, λ denotes the wavelength of the incident X-ray radiation, β represents the full width at half maximum (FWHM) of the diffraction peak, and θ is the Bragg diffraction angle. The

calculated average crystallite size was 41.37 nm for the (002) crystallographic plane. The corresponding interplanar spacing (*d*) was found to be 2.5938 Å, with a lattice parameter value of *a* = 3.2417 Å.

2.1 Synthesis of Polypyrrole (PPy):

In the chemical oxidative polymerization method, the oxidising agent was ammonium persulphate (APS) to form Polypyrrole (PPy). In this procedure 1.0mL of pyrrole monomer was mixed in 70mL of 1.5M solution of hydrochloric acid (HCl). 2.04 g of APS was dissolved in 20mL of deionized water.



FESEM Image of Polypyrrole (PPy

The pyrrole solution was stirred over a period of time, the APS solution had been added in similar drop portions into the pyrrole solution. The reaction of polymerization was allowed to proceed and was extended until the full polymerizing was achieved and it took 5 hours. The obtained black precipitate was filtered and washed thoroughly with a lot of ethanol and deionized water in order to remove any remaining monomer and oxidizing species. Finally, the polypyrrole powder was obtained by drying the product using a hot air oven, at 60℃. Nanoparticles used in this study are both the inorganic (ZnO) and organic (Polypyrrole) based particles which are casted to create nanocomposites films.

2.2 Casting of ZnO/Polypyrrole Nanocomposite Films:

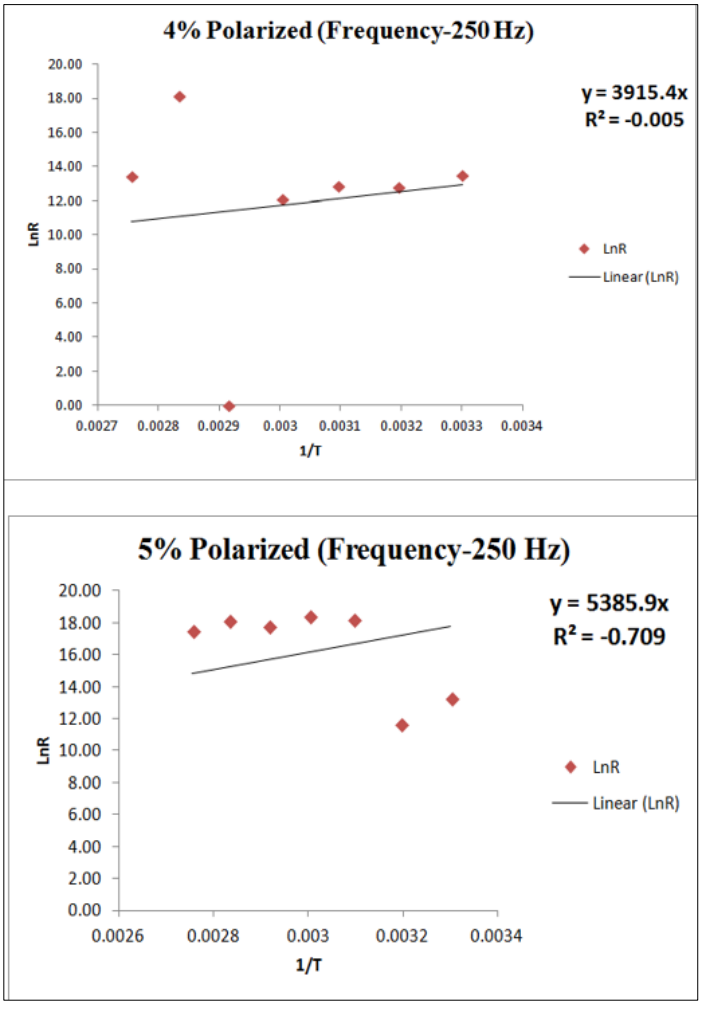
ZnO/polypyrrole nanocomposites films were prepared by the solution casting technique method. ZnO/PPy nanocomposites powder was fixed and spread to form some quantity of particles in a desired quantity of polyvinyl alcohol (PVA) solution. The mixture of solution was kept for 5 hours with a magnetic stirrer that ensured that there was a uniform mixture. In another attempt of enhancing the homogenization of the nanoparticles of ZnO in the polymer matrix, the solution was sonicated for 30 minutes.

The mixture was then smoothly left as a discrete solution on a clean flat glass surface. To remove the moisture content, it was dried in the room temperature and dried in the oven at 60℃ some hours to remove the solvent left behind. The free Standing film of ZnO/PPy nanocomposites was then removed carefully once the whole film was dry.

The thickness of the prepared films was measured with a digital micrometer screw gauge and then prepared films became the measures of dielectric and electrical properties.

3. RESULTS AND DISCUSSION:

The electrical activity of polarized ZnO doped polypyrrole nanocomposites were analyzed by plots of Arrhenius of lnR Vs 1 /T and at 250 Hertz and the nature of charge transfer by output and by the number of countenances of the activation energy. Strongly polarised composites significantly alter the electrical characteristics of the composites since it influences the orientation of dipoles, accumulation of charge and localized pathways of transport between interfaces. The research established that in all the polarized samples, the resistance decreased with an increase in temperature, which indicated that the samples were condensing thermo activated, as is characteristic of the semiconducting polymer composites



The slope of the lnR versus 1/T curve of the polarized 4% ZnO doped PPy composite is relatively low (3915.4), indicating that

the activation energy of movement charge is low. It means that polarization will facilitate the flow of carrier by minimizing potential barriers in the composite. The polarization sorting of dipoles at the ZnO / PPy interfaces applied and the polarization of interfaces enhance the hopping of charge carriers between local energies at the interfaces of the nanotubes. However, the value of R^2 (-0.005) is very low and therefore, a clear sign of non-optimal Arrhenius instincts. This deviation is used to show that there is a multiple number of conduction processes and not just a thermally activated process. Interfacial polarization, localized states and trap assisted hopping are contributions of process of transport which is dominated by presence of ZnO nanoparticles.

From the result, the data points are scattered, which is the reaction to the inclusion of the energetic and structural disorganization in the polarizing composite.

The slope of the lnR versus 1/T curve showed that the apparent activation energy is relatively high in the case of polarized 5% ZnO doped PPy composite (5385.9). This trend suggests that an increase in the ZnO composition and polarization will cause an enhancement in the interaction among the dipoles, will improve the interfacial barriers that can at least partially inhibit the passage of charges. Polarization of the dipoles might also lead to confinement of carriers along the interfaces of ZnO and consequently, a more thermal energy should be applied to free the carrier. The greater energy of activation however results in an R^2 value of (-0.709) although with bad consistency, this is an improvement compared to the lower ZnO concentration where the conduction would be more consistent.

The data points of ZnO are fused around in the polarized 5% sample as compared to the 4% sample demonstrates that the polarization of the sample using a larger filler material in the disseminated sample enables easier conduction channels. This tendency can be donated by an increased contact of the ZnO particles with the PPy matrix which leads to stabilized interfacial sites which control the flow of charge. Non-linearity of Arrhenius plots in both polarized samples, however, confirms the fact that the conduction mechanism is non-Arrhenius in nature and it cannot be accounted with such a single band type of transport.

Overall, it is possible to describe the polarized nanocomposites of ZnO and PPy as semiconducting materials the conductivity of which is controlled by thermal conduction during hopping, polarization at the interface and the conduction by traps. At the high loading ZnO polarization decreases the activation energy between the low ZnO content and the high ZnO loading due to the higher interfacial effects. This indicates that polarization makes a strong impact on the energetic scenario as well as charge transportation pathways of ZnO/PPy nanocomposites that forms a major factor in regulating their dielectric and electrical activities under varying thermal conditions.

The results of energy gap (Eg) measurement of the polarized ZnO/PPy based nanocomposites at various frequencies of

Frequency (Hertz)	4% Polarized	5% Polarized
100	0.6834	0.9808
250	0.6754	0.9791
1000	0.6628	0.9761
5000	0.6409	0.9596

100- 5000 Hz under the load of 4% and 5% of ZnO provides a clear indication on the reliance of the nanofiller and frequencies contents on the processes of charge transport and polarization. The values of the E_g of all the samples are lower than of the semiconducting range (0.64-0.98 eV), which, once again, demonstrates that polarized ZnO/PPy composites exhibit electrical behavior of a semiconductor that can be used in dielectric or electronic applications.

At 4% polarized ZnO/PPy composite, the energy gap implies that the 4% polarized sample always has the same low energy gap over the whole range of frequencies compared to the 5% polarized sample. E_g decreases from 0.6834 eV at 100 Hz to a minimum of 0.6409 eV at 5000 Hz. The fact that polarization has a pronounced increase in the charge carrier mobility in the 4% composite can be viewed as evidence of such a sharp decrease. The minimized band gap gives an indication to the effective orienting of the dipole, facilitate the establishesment of polarons and evolved hopping of a localization between conditions. Slow decay in E_g with frequency implies that although space-charge effects and interfacial polarization of higher frequency may still occur and charge carriers can effectively respond at high frequencies. The mentioned effect means that the optimum concentration of ZnO is 4% where the dispersion or contact of a nanoparticle and the PPy panel is the maximum and there are no longer any potential barriers to the transfer of charges. On the other hand, the composites containing a higher concentration of polarized ZnO/PPy have much higher Eg values which are ranging between 0.9808 eV and 0.9596 eV at 100Hz and 5000Hz respectively. Although there is a slight tendency of E_g decreasing with the frequency increase, the band gap particularly is fairly large. It refers to the fact that excessive loading of ZnO might lead to additional carrier localization and further nanoparticle agglomeration to offer another trapping location and an interfacial interface. As a result, there is increased thermal consumption of charge excitation and transport. When compared to the 4% polarized sample, the 4% polarized sample is better electrically favored and has a smaller, more frequency-dependent energy gap which show high projectability and better conduction efficiency of the polarization mediated charge transfer. The polarized sample (5% polarised) remains semiconducting and less delocalised of charges due to the influences of overloading. Overall, the current results show that polarization and an ideal concentration of ZnO (4%) plays a significant role in decreasing the energy gap, and electronic efficiency of ZnO/PPy nanocomposites.

4. CONCLUSION

The frequency-dependent energy gap and polarization experiment of ZnO doped polypyrrole nanocomposites with a 4% and 5% ZnO load ratio ratios ratifies that the electrical transport of the ionomeric filler could be highly dependent on

the polarization as well as the concentration of the filler. Throughout the two compositions that have the conduction thermally adjusted, there are clear semiconducting properties. The polarization, on the contrary, transforms the energetic landscape to give rise to non-Arrhenius transport characterized by hopping, polarization at the interfaces and trap-assisted instead of the direct band conduction. To achieve a superior electricity functionality, it is worthwhile to achieve the optimum balance between content of ZnO and polarization. The polarized 4% ZnO/PPy nanocomposite is more behaved uniformly in the respect of electrical behaviour in the sense that it has reduced Arrhenius slope, reduced apparent activation energy and lesser value of energy gap in the frequency range investigated. It implies efficient process of dipole orientation, a better establishment of polarons and a more pronounced establishment of hopping pathways due to the adequate dispersion of the nanoparticle and existence of an excellent interfacial communication between ZnO and PPy. On the other hand, polarized 5% ZnO / PPy composite is observed to possess high activation energy, higher energy gaps, which is defined by the overfiller material, which bring stronger interfaces interfaces, carrier localization and other trapping sites. In contrast to 5% polarizing achieving uniformity of conductors, it has no effect on the concept of overloading.These results show the potential potential of polarized ZnO/PPy nanocomposites particularly with 4% of ZnO components loaded and applied in the electronic appliances that are temperature and frequency sensitive. They can be quantified by their capability to tune the gap in energy between the electrons, high conductivity and polarization-assisted charge transport and are applicable as sensors, dielectric capacitors, flexible electronics and energy storage. Controlled polarization and optimum ZnO content is an effective way towards the moulding of the PPy based nanocomposites to a better functional purpose in electronics.

Acknowledgement: Authors gratefully acknowledge XRD support from Manipur University, FESEM facilities from NECBH–IIT Guwahati and the valuable guidance and encouragement provided by Dr. A. Joy Singh throughout this research work and technical assistance.

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