

Preparation and Optical Characterization of PAAm/TiO₂ Nanocomposites for Optoelectronic Applications

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Abstract:

The synthesis and optical characterization of PAAm/TiO₂ nanocomposites made using the solution casting method for optoelectronic applications are the main objectives of this work. Improved light-matter interaction inside the polymer matrix is indicated by the optical research, which shows a discernible increase in ultraviolet (UV) absorption with increasing TiO₂ nanoparticle loading. Additionally, when the concentration of TiO₂ nanoparticles increases, the optical constants of the nanocomposite films, such as the refractive index and extinction coefficient, show a consistent rise. On the other hand, when nanoparticle loading increases, the PAAm/TiO₂ nanocomposites' optical transmittance and optical energy band gap diminishes. This can be explained by the creation of localized states and enhanced charge carrier interactions. These results demonstrate that the incorporation of TiO₂ nanoparticles effectively tailors the optical properties of PAAm, highlighting the potential of PAAm/TiO₂ nanocomposites for optoelectronic device applications.

Keyword: PAAm, TiO₂ NPs, Optical properties, optoelectronic device

1. INTRODUCTION

Polymer nanocomposites (PNCs) are an advanced class of functional materials in which nanoscale fillers are introduced into polymer matrices to improve performance above ordinary composites. Nanoparticles improve optical, electrical, mechanical, and thermal properties significantly because of their high surface-to-volume ratio and strong interfacial interactions with polymer chains [1, 2]. Such materials have received a lot of attention in optoelectronic technologies, which need precise control over light absorption, transmission, and electrical band structure [3, 4].

Polyacrylamide (PAAm) is a hydrophilic polymer that is widely utilized in scientific and industrial applications due to its outstanding film-forming ability, chemical stability, and strong interaction with inorganic fillers via its amide functional groups. These properties enable PAAm to serve as an excellent host matrix for metal oxide nanoparticles, allowing for uniform dispersion and stable nanocomposite formation [5, 6]. Furthermore, PAAm-based nanocomposites display tunable optical characteristics, making them intriguing candidates for optoelectronic and photonic applications [7, 8].

Titanium dioxide (TiO₂) is a widely studied metal oxide semiconductor with a wide band gap, high refractive index, significant UV absorption, and great chemical and thermal durability. TiO₂ is mostly found in anatase and rutile crystalline phases, which are ideal for optoelectronic applications such UV detectors, photovoltaic devices, and optical coatings [9]. Nanoscale TiO₂ exhibits size-dependent optical characteristics, including band gap alteration and improved light absorption, which are particularly useful when introduced into polymer matrices [10].

Integrating TiO₂ nanoparticles into polymer matrices alters optical behavior, resulting in increased absorbance, reduced band gap, and improved refractive index. These alterations are the result of nanoparticle-induced localized

states and enhanced charge transfer at the polymer-nanoparticle interface [11]. Increasing nanoparticle concentration in polymer/TiO₂ nanocomposites enhances light-matter interaction, improving optoelectronic device performance [12].

While polymer/TiO₂ nanocomposites have been studied extensively, there has been less focus on analyzing the optical properties of PAAM/TiO₂ systems for optoelectronic applications. Understanding the link between nanoparticle concentration, structural traits, and optical properties such as absorbance spectra, optical band gap, and refractive index is critical for optimizing these materials for device integration [13]. To assess their potential in future optoelectronic technologies, PAAM/TiO₂ nanocomposites must be synthesized and optically characterized. This study aims to synthesize PAAM/TiO₂ nanocomposite films with different TiO₂ nanoparticle concentrations using casting process and analyze the applicability of PAAM/TiO₂ nanocomposites for optoelectronic applications by observing optical improvements relative to virgin PAAM.

2. MATERIALS AND METHOD

The casting procedure was utilized to create PAAM/TiO₂ films with varying amounts of PAAM and TiO₂ nano powder. The PAAM films were created by dissolving 1 g of PAAM in 50 mL of distilled water and mixing the polymers with a magnetic stirrer to obtain a more homogeneous solution. TiO₂ NPs were introduced to PAAM solution at concentrations of 1.3%, 2.6%, and 3.9%, resulting in a 130 µm thickness. The UV-1800 OA-Shimadzu was used to test optical qualities.

The absorption coefficient (α) is given as [14]:

$$\alpha = 2.303 \frac{A}{t} \quad (1)$$

The energy gap is calculated by [15]:

$$(\alpha h\nu)^{1/m} = B (h\nu - E_g) \quad (2)$$

The refractive index (n) can be determined using [16]:

$$n = \frac{1 + \sqrt{R}}{1 - \sqrt{R}} \quad (3)$$

The reflectance is denoted by R . This describes the extinction coefficient (k) [17]:

$$k = \frac{\alpha \lambda}{4\pi} \quad (4)$$

Real (ϵ_1) and imaginary (ϵ_2) components of the insulator continuous are provided by [18]:

$$\epsilon_1 = n^2 - k^2 \quad (5)$$

$$\epsilon_2 = 2nk \quad (6)$$

The optical conductivity (σ_{op}) is calculated by [19]:

$$\sigma_{op} = \frac{anc}{4\pi} \quad (7)$$

2. RESULTS AND DISCUSSION

The data in Figure 1 show that absorbance values vary significantly with wavelength. It is interesting to note that, despite its narrower range compared to the visible wavelength, UV absorption is higher. This supports the presence of perfumed mixes with protracted π -electron schemes, recognized to absorb UV light, rather than protracted conjugate groups in the resulting precipitate, which absorb visible light. TiO₂ exhibits unusual behavior in terms of light absorption. This absorption can be determined using UV-visible (UV-vis) spectroscopy. As a result, the absorbance increases while the conduction reductions, as seen in Figure 2. The results match [20].

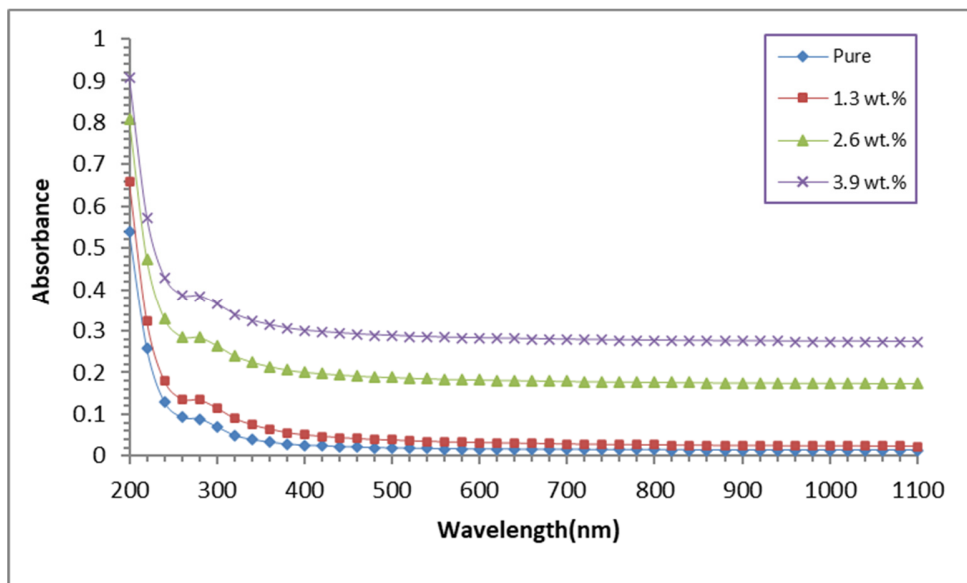


FIGURE 1. Absorbance scales of PAAm/TiO₂ NCPs.

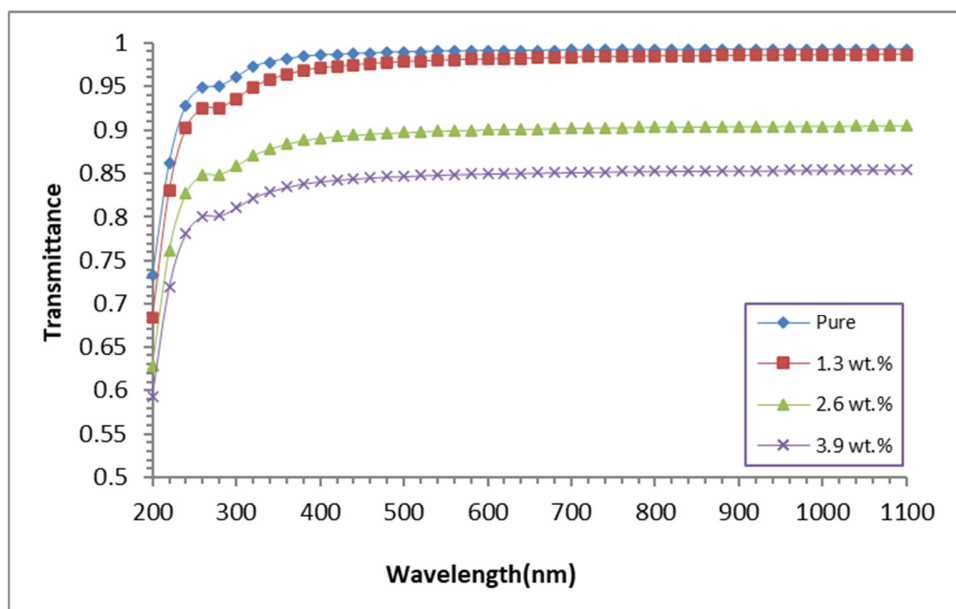


FIGURE 2. Transmittance of (PAAm/TiO₂) PNCs

The (α) for PAAm/TiO₂ with light energy is shown in Figure 3. With their inclined posture, TiO₂ NPs showed an increase in α . An indirect transition is indicated by $\alpha < 10^4 \text{ cm}^{-1}$. The rise in values may be related to the notable drop in inter-bond changes [22, 23]. Over a broad range of wavelengths, PAAm/TiO₂ alloys show enhanced UV spectra uptake. This characteristic makes nanostructures suitable for optoelectronic nanodevices.

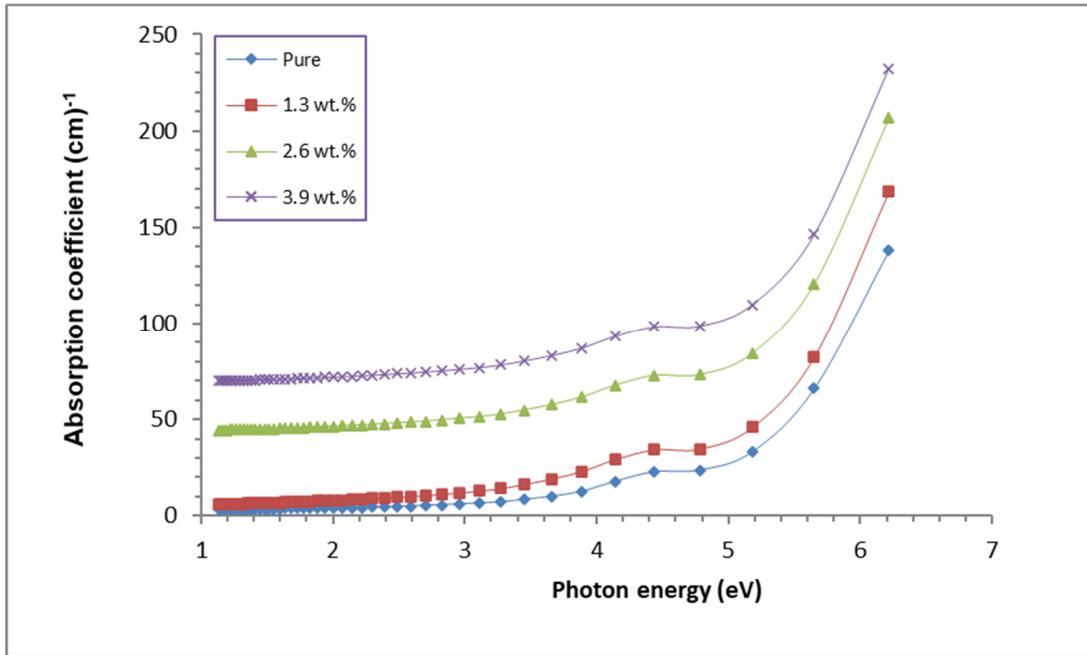


FIGURE 5. α of the (PAAm/TiO₂) PNCs

Figures 6 and 7 show the wavelength-dependent fluctuations in the (n) and (k) of PAAm/TiO₂ nanocomposites. The n values of PAAm/TiO₂ NCs increase as the TiO₂ NP content increases. This phenomenon is caused by the aggregation of nanoparticles within the PAAm matrix. The k values of PAAm/TiO₂ nanocomposites increase as the concentration of TiO₂ NPs increases. Because of TiO₂ NP dispersion and absorption, the k values of PAAm/TiO₂ NCs increase, demonstrating momentous light indulgence. Strong interaction between PAAm and TiO₂ NPs causes crystallinity alterations, which result in modifications in band structure and absorbance percentage [24].

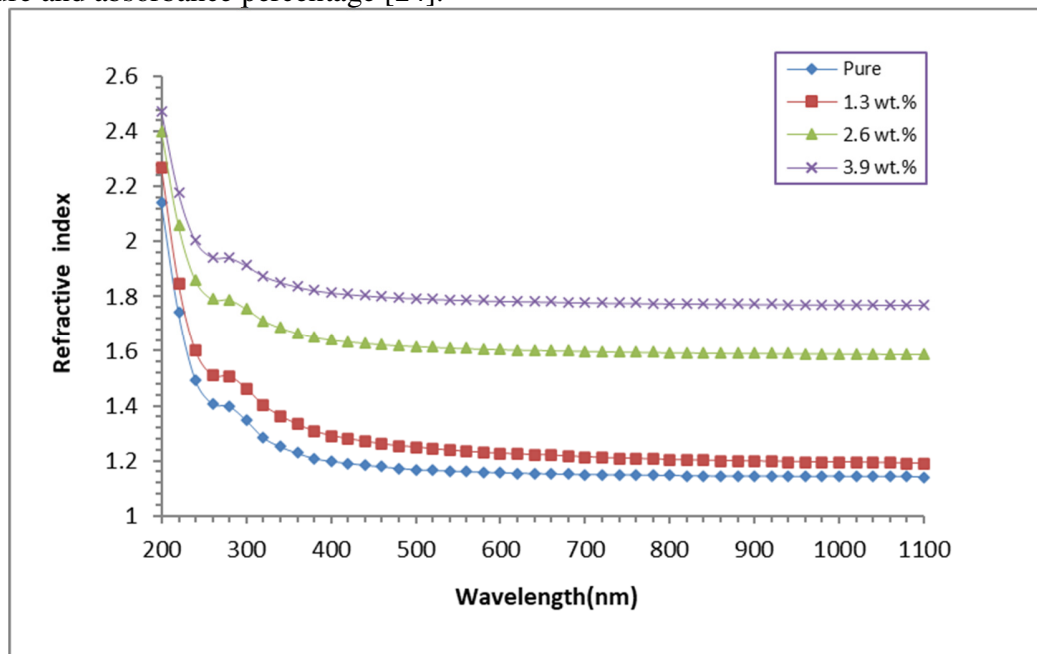


FIGURE 6. The n of (PAAm/TiO₂) PNCs

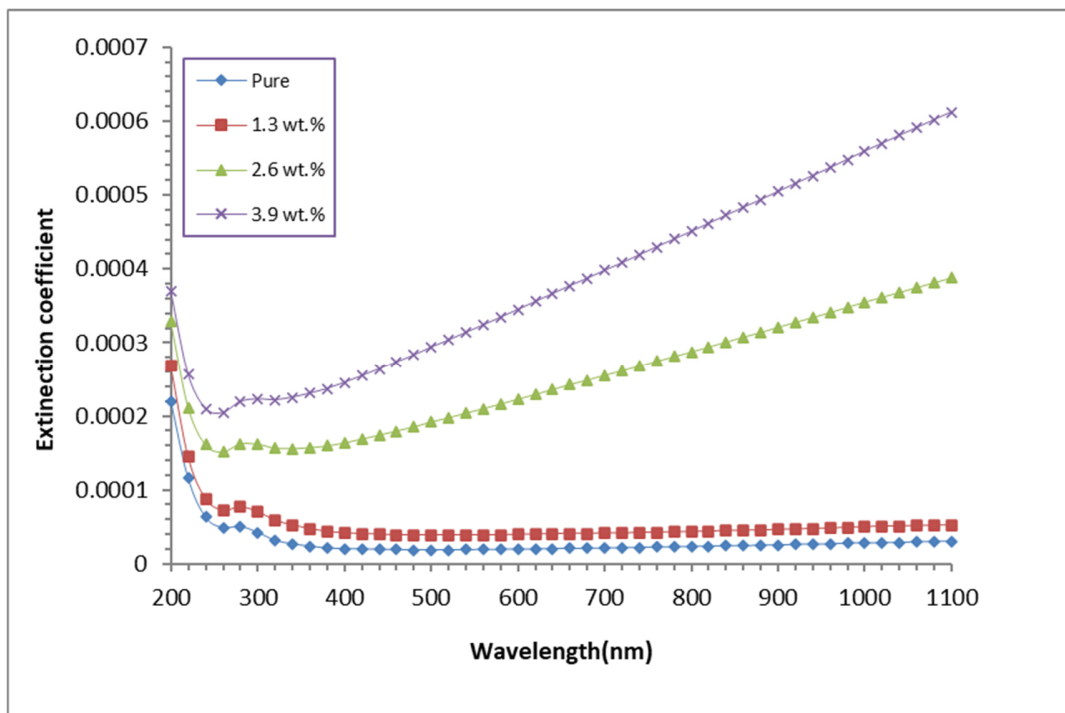


FIGURE 7. The K of (PAAm/TiO₂) PNCs

The energy difference in permitted and prohibited unintended changes for PAAm/TiO₂ is displayed in Figures 8 and 9. As the ratio of TiO₂ NPs rises, the values of E_g for PAAm diminution due to the creation of custody program complexes between the atoms of TiO₂ NPs and the practical gatherings of PAAm. By generating an interior band inside the PAAm structure, the injected TiO₂ NPs lower the nanocomposites' E_g . In order to generate a local level in the nanocomposites' edifices that led to the reduction in E_g values, the drop in E_g values is permitted to increase with a specific degree of disruption [25].

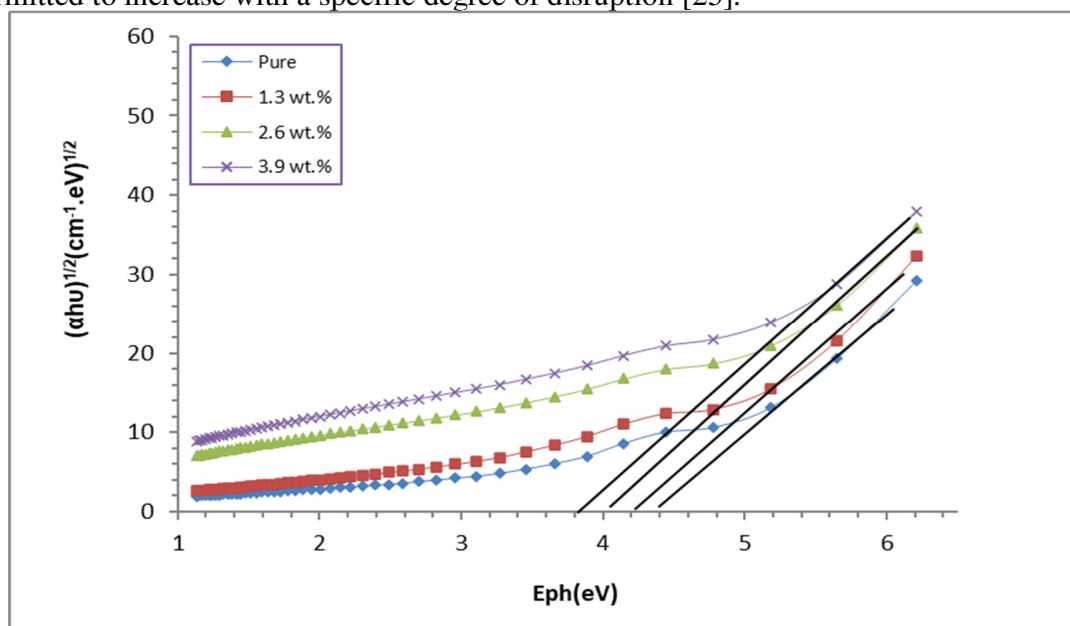


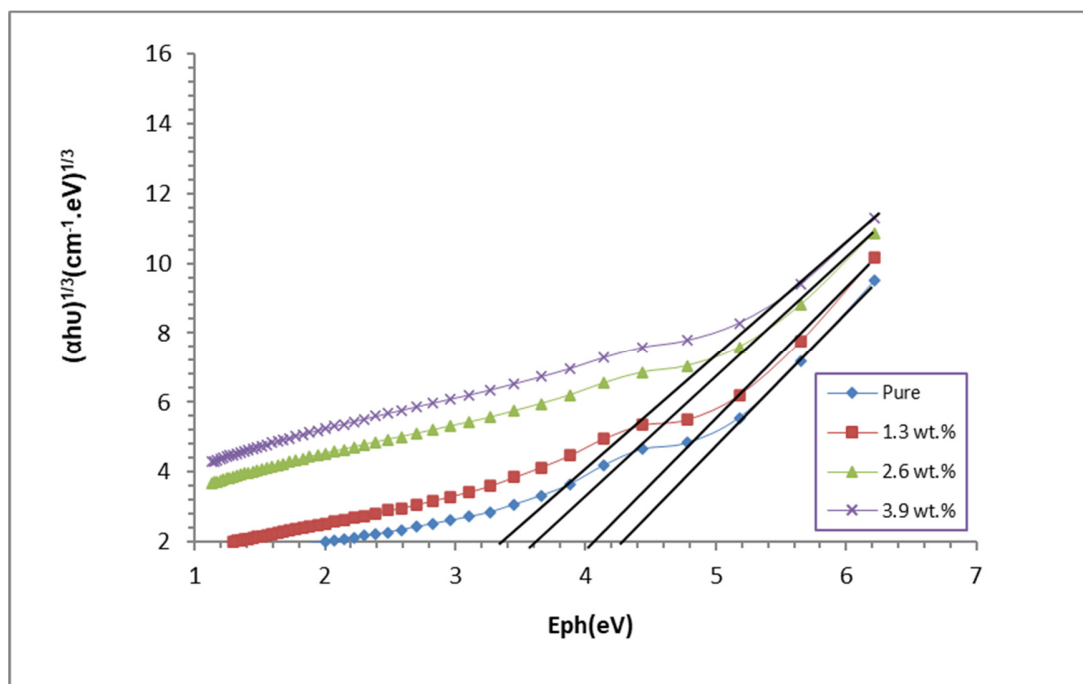
FIGURE 8. The $(\alpha h\nu)^{1/2}$ for (PAAm/TiO₂) PNCs

FIGURE 9. The $(\alpha h\nu)^{1/3}$ for (PAAm/TiO₂) PNCs

TABLE 1. standards for the Eg of PAAm/TiO₂ PNCs

wt.% of TiO ₂	Allowed Eg (eV)	Forbidden Eg (eV)
0	4.4	4.24
1.3	4.2	4
2.6	4	3.8
3.9	3.8	3.4

Figures 10–11 show the actual and fantasy sections of the insulator continuous behaviors for PAAm/TiO₂ films with wavelength. Increased TiO₂ NP content leads to higher ϵ_1 and ϵ_2 dielectric constants. Vagaries in the motion of charge carriers and local charged particles impacted the dielectric dispersion properties, affecting the performance of ϵ_1 . Defects that cause charge transference between polymer manacles and dopants in nanoparticles lead to an increase in ϵ_2 [26].

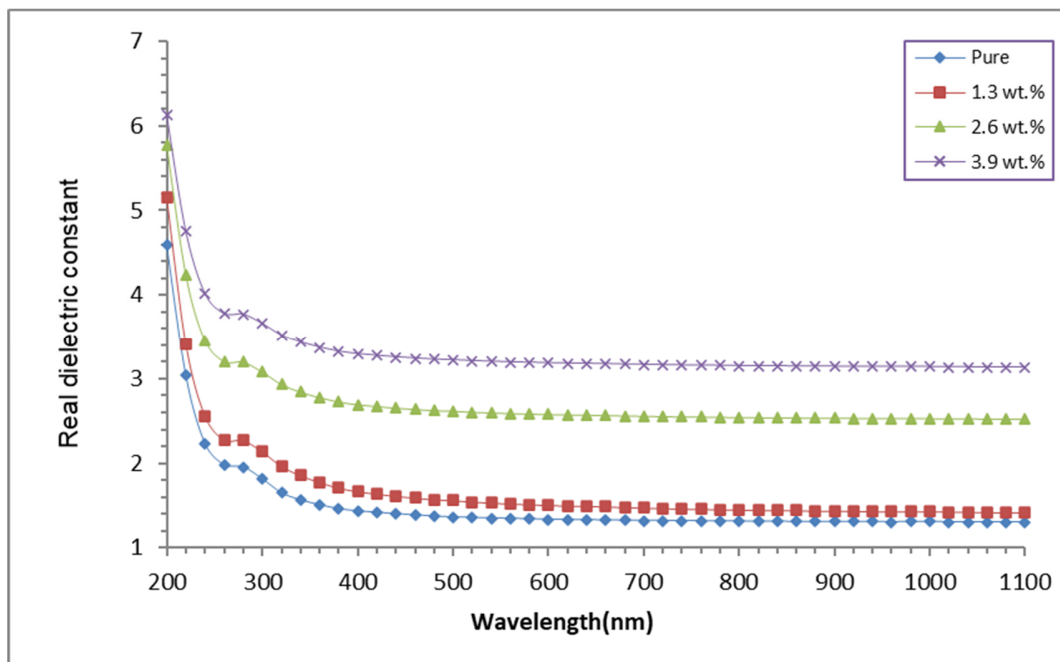


FIGURE 10. The ϵ_1 for (PAAm/TiO₂) PNCs

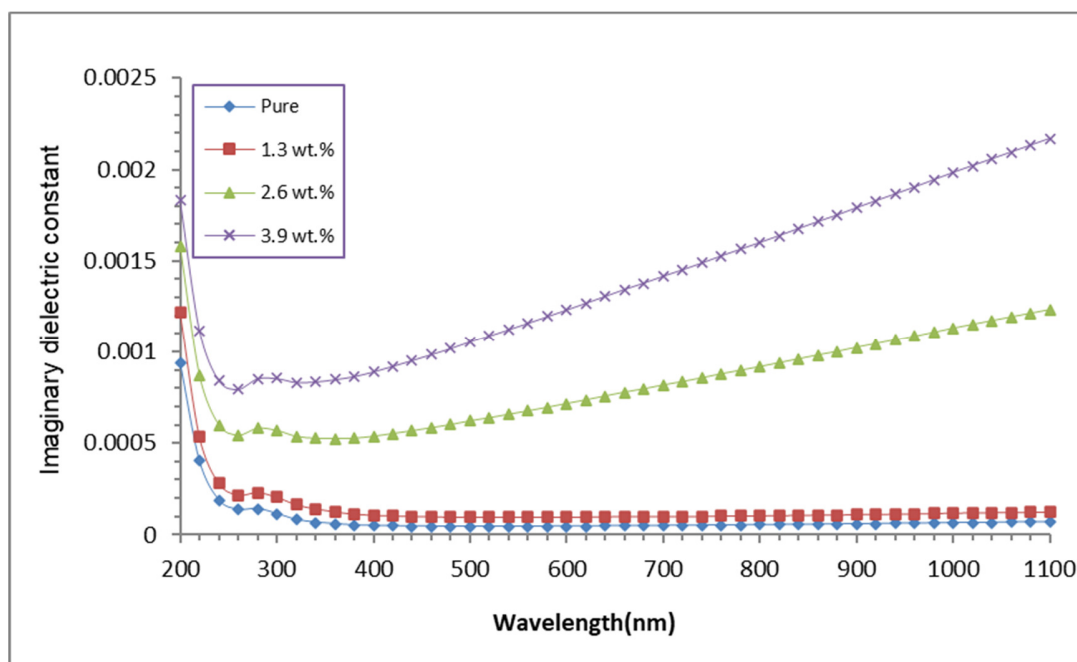


FIGURE 11. The ϵ_2 of (PAAm/TiO₂) PNCs

Figure 12 illustrates how PAAm/TiO₂ nanostructures' optical conductivity changes with wavelength. Because the absorption value encourages charge transference excitations, PAAm/TiO₂ nanostructures show higher optical conductivity at in-height photon energies. Increased optical conductivity in the presence of TiO₂ nanoparticles is correlated with higher restricted level concentrations in the gang construction. The optical conductivity of PAAm rises with the concentration of TiO₂ NPs; this phenomenon can be explained by either an growth in density and preoccupation factor or a reduction in the optical band gap [27].

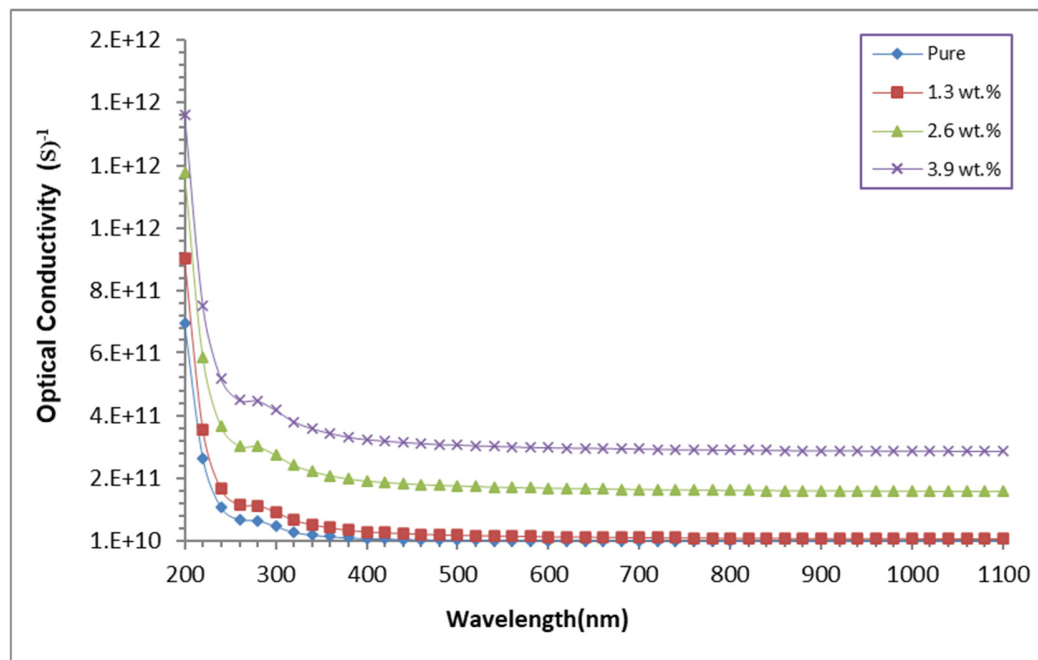


FIGURE 12. Optical conductivity for (PAAm/TiO₂) PNCs

4. CONCLUSION

PAAm/TiO₂ nanocomposites were made using the solution casting process, and their optical characteristics were thoroughly studied. Adding TiO₂ nanoparticles to the polymer matrix improves UV absorption, indicating stronger light-matter interaction. Increasing the concentration of TiO₂ nanoparticles leads to a rise in optical constants including refractive index and extinction coefficient, indicating greater interfacial polarization and nanoparticle-polymer interactions. Higher TiO₂ loading resulted in a reduction in optical transmittance and energy band gap. This conduct is linked to the creation of localized energy states and increased charge carrier interactions in the nanocomposite structure. The study found that adding TiO₂ nanoparticles improves the optical characteristics of PAAm, making it suitable for use in optoelectronic devices such as UV sensors and optical components.

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