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Optical properties for (Polystyrene-zinc oxide) nanocomposite for optoelectronic application

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Abstract
It was essential to investigate the features of overlapping nanocomposites because of the significance they have in the fields of science, industry, electricity, and medicine. As a result, it garnered a lot of attention and led a lot of scientists and researchers in the direction of studying the features of nanocomposite. Investigations have been conducted into the fabrication of (polystyrene (PS)-zinc oxide (ZnO)) nanocomposites and the examination of the optical characteristics of these nanocomposites for use in optoelectronic applications. Various concentrations for PS polymer & ZnO NPs were used in the fabrication of the nanocomposites using the solution casting process. The results of the experiments performed on (PS-ZnO) nanocomposites appear that each of the absorbance(A), absorption coefficient(α), extinction coefficient(K), refractive index(n), real and imaginary dielectric constants$(\varepsilon_r \;\&\; \varepsilon_i)$, and optical conductivity (σ_{opt}) of polystyrene increase by increasing ZnO NPs concentrations. On other hand, the transmittance (T) and energy gap (E_g) decrease by increasing ZnO NPs concentrations. Nanocomposites made of zinc oxide have a high absorption in the ultraviolet spectrum.

Keywords: Polystyrene, ZnO nanoparticles, optical properties, nanocomposites

1. Introduction
The concept of a nanocomposite material has greatly expanded over the years to embrace a wide range of different types of systems, like 1-dimensional, 2-dimensional, 3-dimensional, & amorphous materials, which are made of clearly different components and blended in the nanoscale range [1]. This expansion has occurred as a result of the increasing popularity of nanotechnology. Nanocomposite materials, created by mixing two or in sometimes more than two from the distinguished building constituents into one material, exhibit unique characteristics. These qualities most likely originate from the nanocomposite materials' tiny size, huge area for the surface, of course, interfacial reaction that occurs among phases. Extraordinary effort efficiently used for improving the biological effort of great number of medicines, biomaterials, and catalysts, as well as in several high-value added materials [2]. The existence or absence the polymeric materials in the nanocomposite might be used as a categorization criteria for the components in question. The non-polymeric nanocomposite indicate to the nanocomposite where neither polymers nor components generated from polymers in their compositions are exist, this nanocomposite called inorganic nanocomposite [3]. The dispersion of filler in the matrix is the step in the production of polymer-based nanocomposites that is considered to be the most essential phase. This goal can be accomplished through the application of a variety of mechanochemical techniques, such as sonication via ultrasound [4]. Nanocomposites are a type of material that is created by incorporating nanoparticles into the matrix of a more traditional substance. The incorporation of nanoparticles into a material results in a dramatic enhancement of the attributes of the material, which may include an increase in its mechanical strength, tensile strength, and electrical or thermal conductivity. Because of the remarkable efficacy of the nanoparticles, the amount of additional substance that is often required is only between 0.5 and 5% by weight [1]. The flexural and compressive properties of polymer nanocomposite materials are both more effectively resisted by these materials.

Nanocomposite materials offer excellent electrical conductivity, which is an important property for wide variety from technological applications. The use of a polymer nanocomposite that possesses better electrical conductivity has allowed for the construction of a multi-walled carbon nanotube [5]. Nanocomposites have a surface to volume ratio that is exceedingly high, which results in a significant shift in their properties when compared to the bulk-sized analogues of the same substance. Additionally, the way in which the nanoparticles bind with the bulk material is altered as a result of this process. As a consequence of this, the composite has the potential to be significantly improved in comparison to its component elements. It has been demonstrated that certain nanocomposite materials are one thousand times more durable than the bulk component components [1]. Nanocomposite materials are utilised in a variety of applications throughout the automotive and industrial sectors. Nanocomposites are having a profound effect on the world of materials thanks to their significantly improved functionality and wide range of potential applications. The development of biosensors makes use of a wide variety of nanostructural nanocomposites, also known as functional nanomaterials; these nanobiosensors have applications in the monitoring of biological, chemical, and environmental systems [6].

2. Theoretical part

The following equation [7] can be used to determine the transmittance, abbreviated as (T):

$$T = 10^{-A} = e^{-\alpha d} \tag{1}$$

Where A represents the amount of absorbance, d refers to the length of light path, Reflectance (D) can be obtained by [8] doing the following:

$$D = 1 - A - T \tag{2}$$

It is possible to express the absorption coefficient (α) at a fundamental absorption edge using the notation [9]:

$$\alpha = \frac{2.303}{t} A \tag{3}$$

Where t represents sample thickness measured in centimeters. We can calculate the extinction coefficient (K) by utilizing the equation that is presented here [10]:

$$K = \frac{\alpha\lambda}{4\pi} \tag{4}$$

Where λ refers to incident light wavelength.

Refractive index (n) calculated depending on the equation [11]:

$$n = \frac{1+\sqrt{D}}{1-\sqrt{D}} \tag{5}$$

Real & imaginary dielectric constant $(\varepsilon_r \;\&\; \varepsilon_i)$ can be calculated from the equations [12]:

$$\varepsilon_r = n^2 - K^2 \tag{6}$$

$$\varepsilon_i = 2nK \tag{7}$$

Absorption coefficient values indicate that the transition is indirect, and with the help of Tauc's equation [13]:

$$\alpha h\nu = L(h\nu - E_\circ)^z \tag{8}$$

Where $h\nu$ represent the photon energy, L refers to proportionality constant, $E_\circ$ indicate to optical energy gap [14, 15].

Optical conductivity, denoted by (σ_{opt}) can be determined through the application of the following equation [16]:

$$\sigma_{opt} = \frac{\alpha n c}{4\pi} \tag{9}$$

Where c refers to speed of light through space.

3. Materials and methods

Polystyrene (PS) was employed as the matrix, while zinc oxide nanoparticles (ZnO NPs) were used as the filler in this study's research materials. Casting was used to create nanocomposites of polystyrene and zinc oxide nanoparticles in varying quantities, and the nanocomposites were made using the casting method. A magnetic stirrer was used to dissolve two gram of PS in thirty milliliters of 1,2-dichloroethane ($C_2H_4Cl_2$) solvent for a period of thirty minutes. This was done in order to produce films of nanocomposites. After that, several concentrations of ZnO nanoparticles were put into the polymer solution. These concentrations were 0, 0.6, 1.2, 1.8, and 2.4 weight percent. The thickness of the nanocomposites samples that have been created is 0.25 millimeters. Optical characteristics for (PS-ZnO) nanocomposites evaluated from employing a double beam UV-Vis spectrophotometer / scinco / Mega-2100, and measuring the spectrum of wavelengths from 220 to 800 nm.

4. Results and Discussion

The fluctuation in absorbance that is seen in Figure (1) is for PS polymer that has varied concentrations of ZnO nanoparticles. This polymer was given different wavelengths. This behavior can be related to donor electrons excitations to the conduction band (C.B) in these energies, as seen in Figure, which shows that the absorbance increases as it moves towards the UV area, this return to the sufficient photons energy for interacting with atoms. When electron absorbs photon of a known energy, it is excited to move to upper energy level. Alterations in radiation that is absorbed and transmitted can provide clues as to the types of electron transitions that are feasible. Transition from band to band or transition by excitation is what is meant when someone talks about the absorbance spectrum [17]. In addition, the picture demonstrates that increases zinc oxide nanoparticles concentration leads to absorbance increase. This return to zinc oxide nanoparticles aggregation, which happen when the concentration of the nanoparticles is increased, as well as charge carriers number increasing [18].

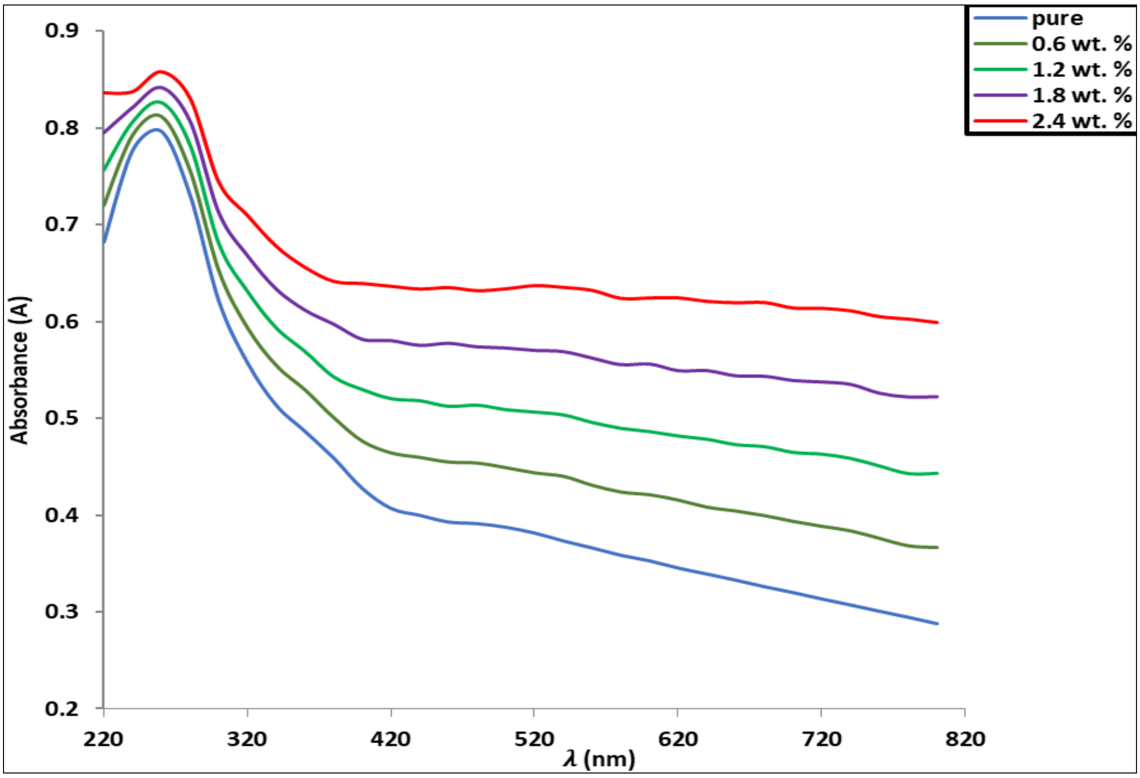

Fig 1: Absorbance variance with wavelength for (PS-ZnO) nanocomposites.

Figure (2) exhibit transmittance spectrum for (PS-ZnO) nanocomposites. When there was a higher ZnO NPs concentration in PS polymer, reduction in amount of light that could pass through into the UV spectrum will take place. The increased surface roughness is the likely cause of the lower transmittance that was found. Because ZnO nanoparticles generate Rayleigh scattering, the transmittance of the nanocomposite material is decreasing. This is owing to the fact that ZnO nanoparticles cause the scattering [19].

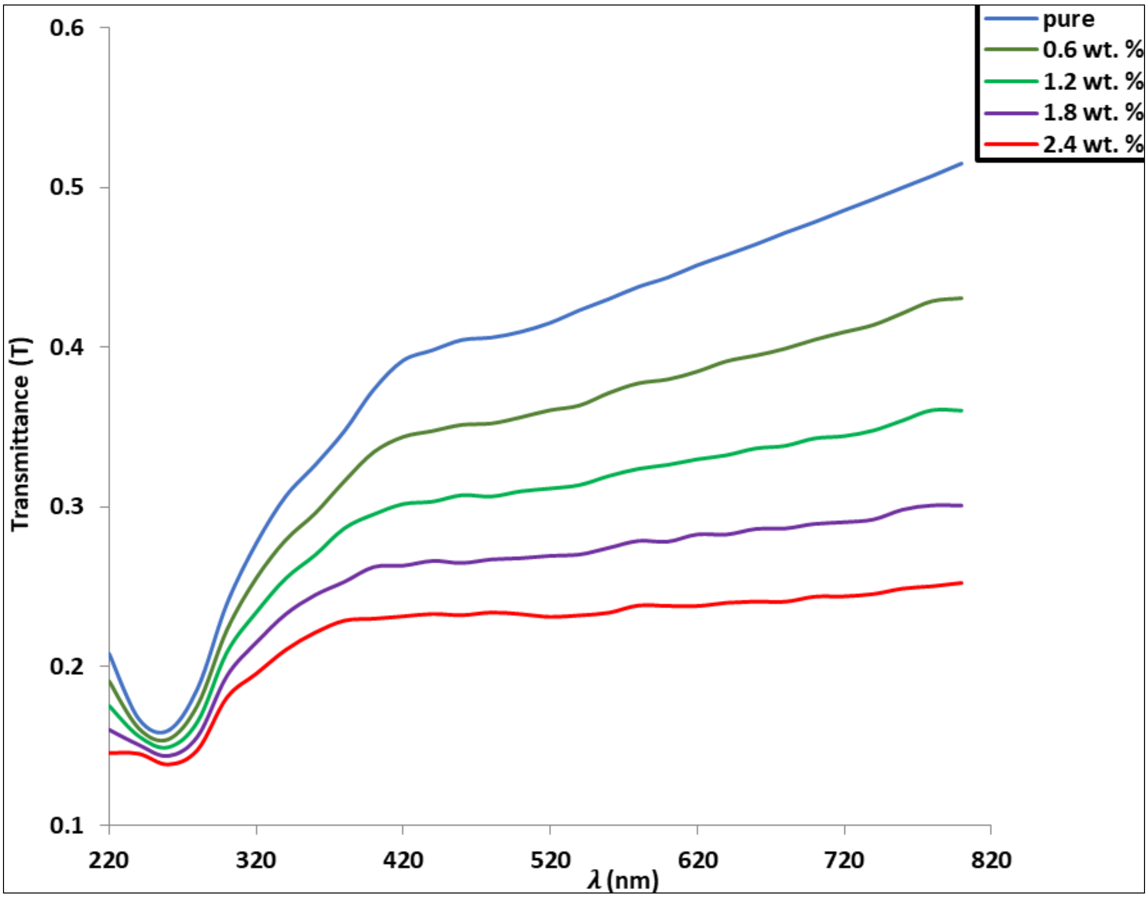

Fig 2: Transmittance variance with wavelength for (PS-ZnO) nanocomposites.

The reflectance of the (PS-ZnO) nanocomposites inversely proportional with incident light wavelength illustrated at Figure (3). Reflectance increase when ZnO nanoparticles concentration increases and increases when incident photon wavelength decrease for all nanocomposites [20].

The variance of absorption coefficient with photon energy are shown in the Figure (4) for PS polymer that contains zinc oxide nanoparticles in varying concentrations. This demonstrates the following, at low energy, absorption also being low for low transition of the electrons. However, when the energy is very high, a considerable amount of it is absorbed because transition the electron is a greater possibility. Absorption coefficient for nanocomposites can be made to be higher by increasing the amount of ZnO NPs addition. The aim of the absorption coefficient is to draw a conclusion about the nature of the electronic transitions that are taking place. Low absorption coefficient refers to indirect transition can take place, which ensures the conservation of energy and momentum. Photons can also be involved. Only phonons are responsible for the conservation of momentum. Based on the findings, absorption coefficient values for the nanocomposites are lower than ($10^4 cm^{-1}$), refers to the energy gap of these nanocomposites being indirect [21].

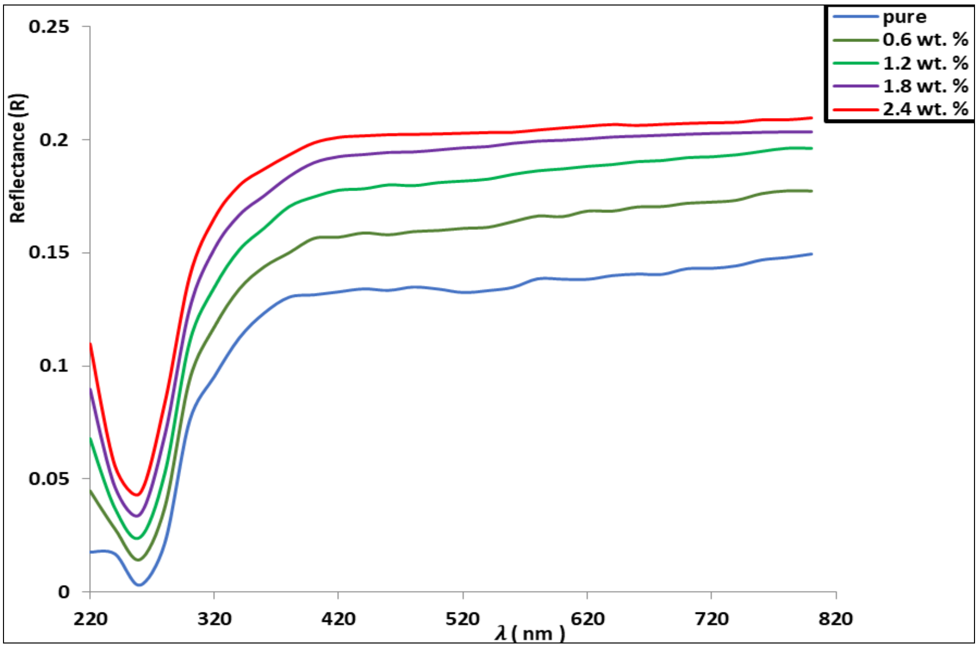

Fig 3: Reflectance variance with wavelength for (PS-ZnO) nanocomposites.

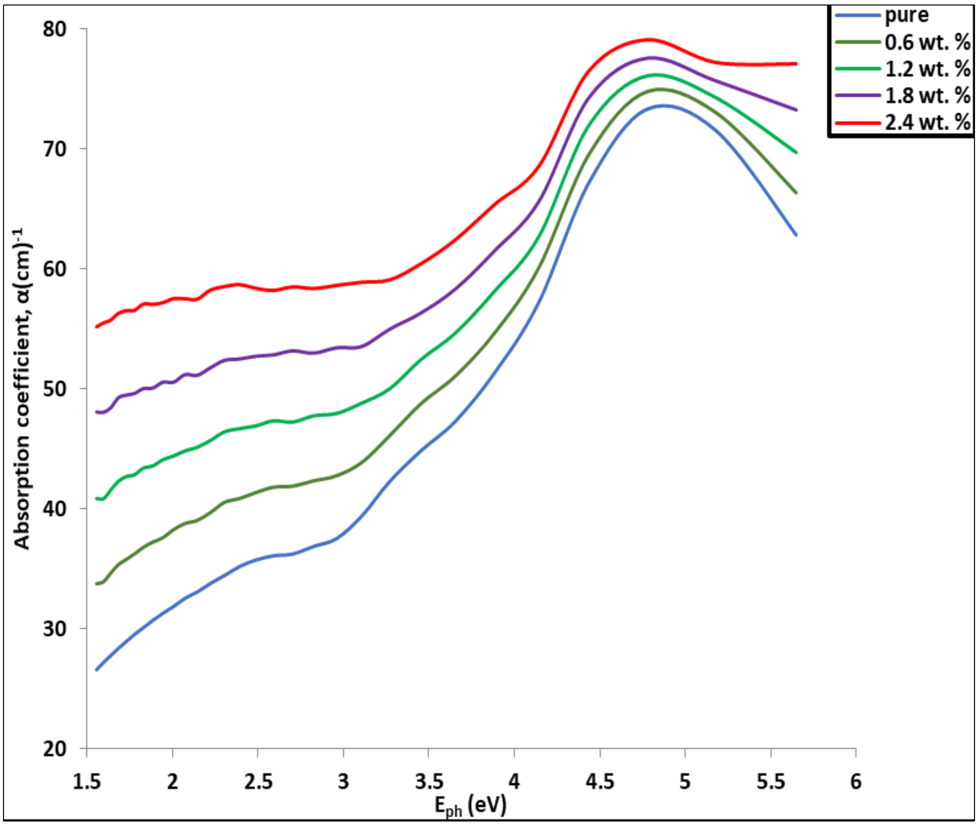

Fig 4: Absorption coefficient variance with photon energy for (PS-ZnO) nanocomposites.

Figure (5) illustrates how extinction coefficient variance with light wavelength. The amount of energy that is lost as a result of molecules and particles in the material scattering or absorbing light is indicated by the extinction coefficient. Extinction coefficient increases when ZnO nanoparticles concentration increases. As shown in Figure (5), extinction coefficient decreases as wavelength gets shorter in the range from 267 to 420 nm. This could be owing to the fact that the photon that caused the incident had enough amount of energy for electron excitations from one state to another. This is evidence that the amount of energy that has been lost has decreased, which indicates that the extinction coefficient has also decreased. According to Figure (5), the extinction coefficient also dramatically increases at wavelength (420-800) nm. This is because the energy required for excitation the electrons at these wavelengths are unavailable. Because of this, a significant quantity of energy was dissipated, which resulted in a significant extinction coefficient [22].

Refractive index changes with wavelength for (PS-ZnO) nanocomposites is shown in Figure (6). ZnO NPs concentration increases is attributed to intensity increase of (PS-ZnO) nanocomposites [23]. This is demonstrated by polystyrene refractive index increases. As well as causing incident photons scattering increase, and consequently increase the reflectance and refractive index of nanocomposites [24].

Real & imaginary dielectric constant fluctuation with wavelength is shown in Figures (7) and (8). Figures appear real & imaginary dielectric constant of PS increases by ZnO NPs concentration increase. The explanation for this behavior is due to increasing the electrical polarization due to nanoparticle concentration contribution at the sample [25].

Figures (9) and (10) demonstrate, respectively, absorption edge for allowed & forbidden indirect transition variance with photon energy. As shown in the Figures, energy gaps decreases when ZnO nanoparticle concentration increases (Table (1)) [26]. The decrease in energy gap value that occurs in PS as a result of the embedding of ZnO nanoparticles makes these materials effective for use in optoelectronic devices. This is because the stability of the energy gap is essential for the operation of these devices [27].

Optical conductivity variance with wavelength is illustrated in Figure (11). It is clear from the Figure that, optical conductivity decrease when wavelength increases. ZnO NPs addition leads to local states creation at energy gap, and with NPs concentration increasing, local states density will increase, and this increases the absorption coefficient, and thus the electrical conductivity increases [28].

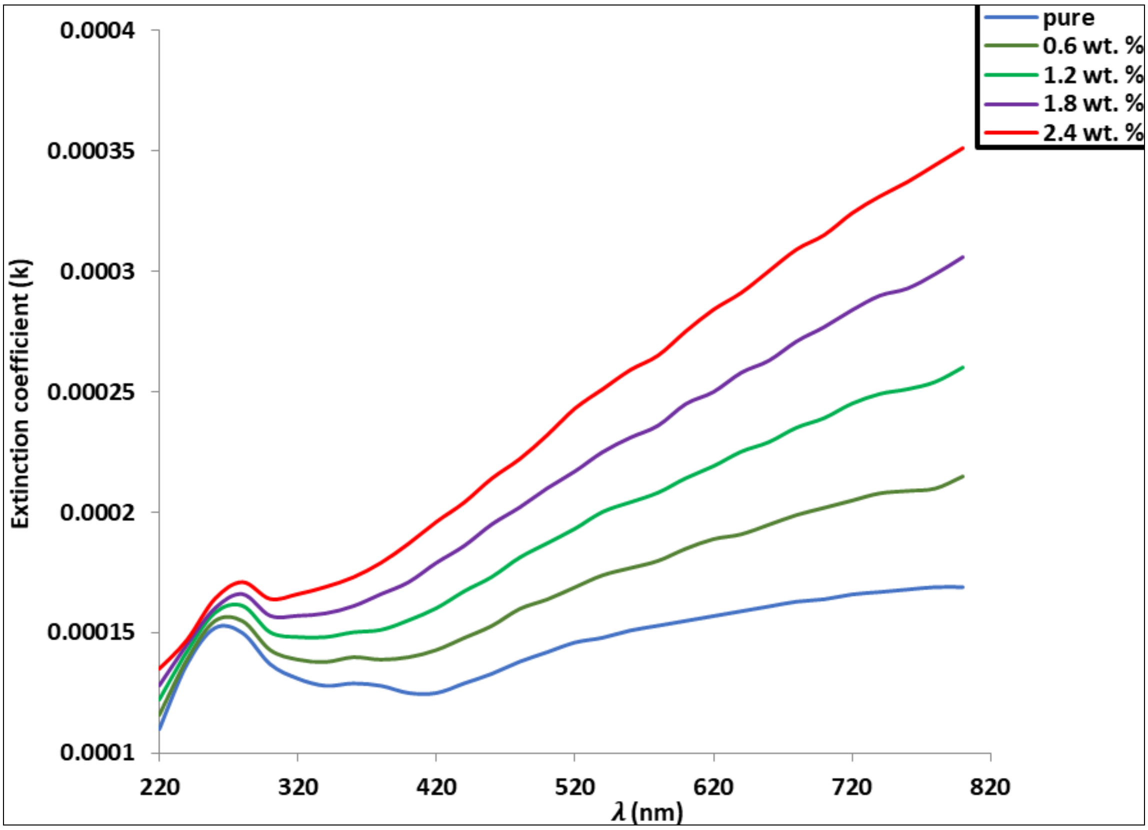

Fig 5: Extinction coefficient variance with wavelength for (PS-ZnO) nanocomposites.

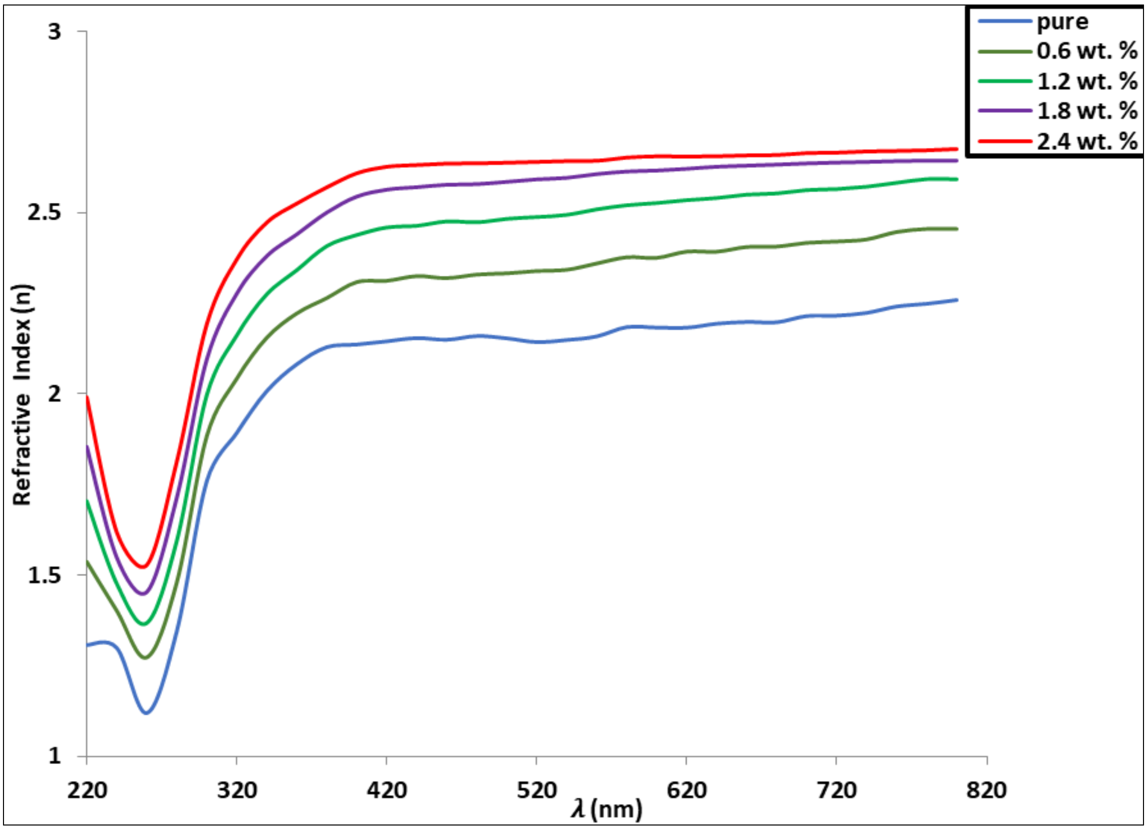

Fig 6: Refractive index variance with wavelength for (PS-ZnO) nanocomposites.

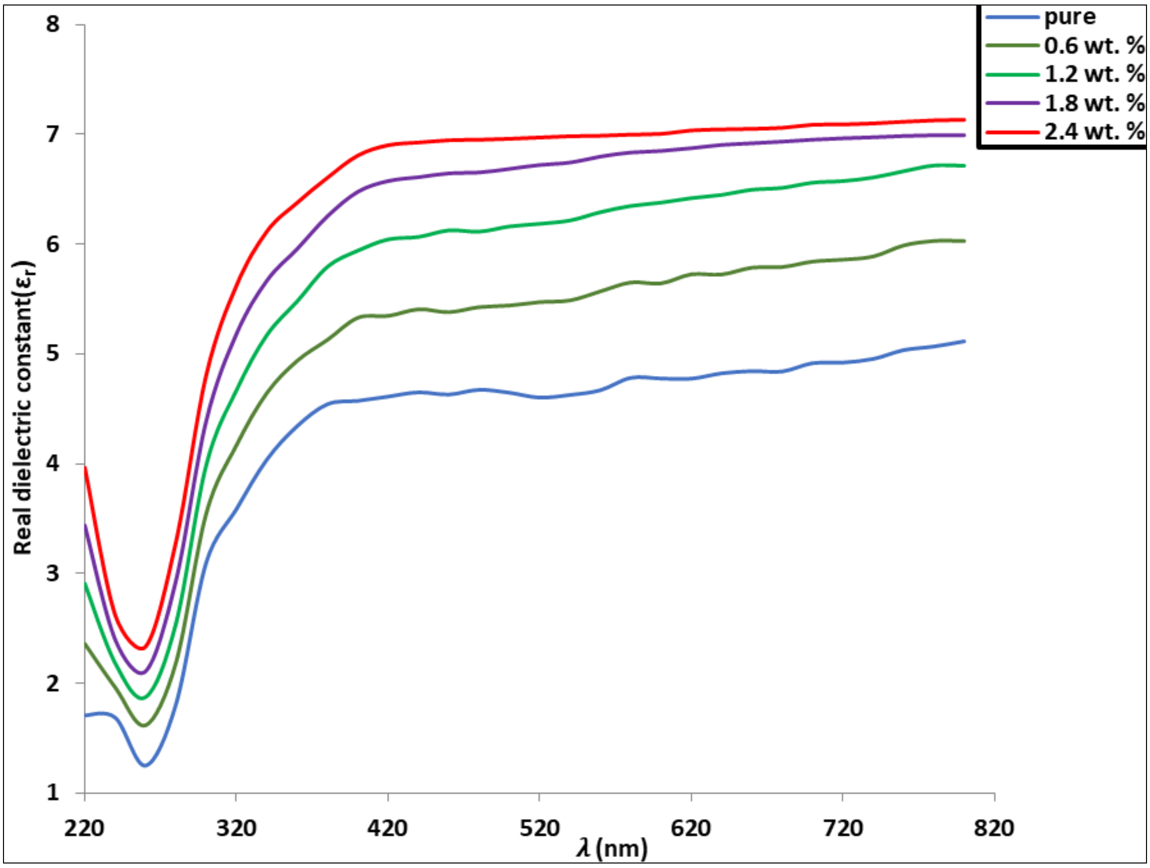

Fig 7: Real dielectric constant variance with wavelength for (PS-ZnO) nanocomposites.

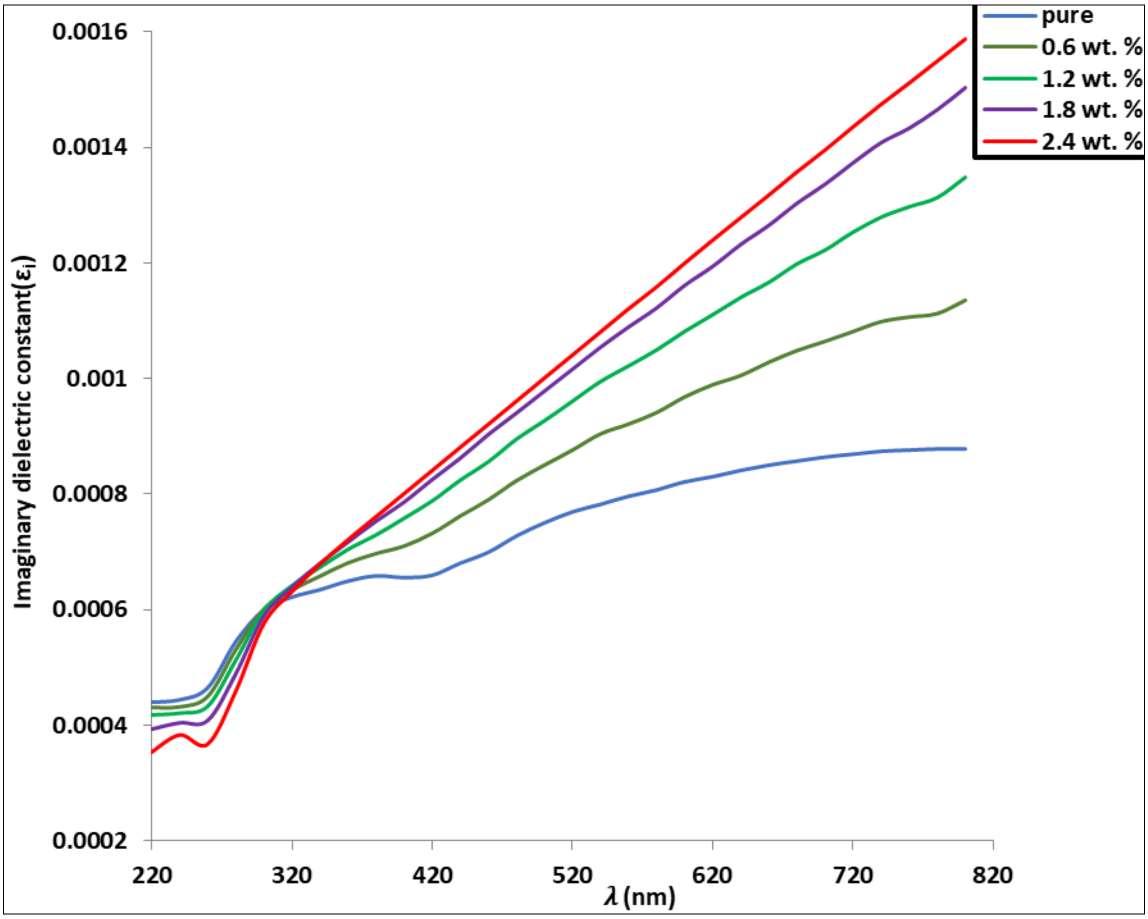

Fig 8: Imaginary dielectric constant variance with wavelength for (PS-ZnO) nanocomposites.

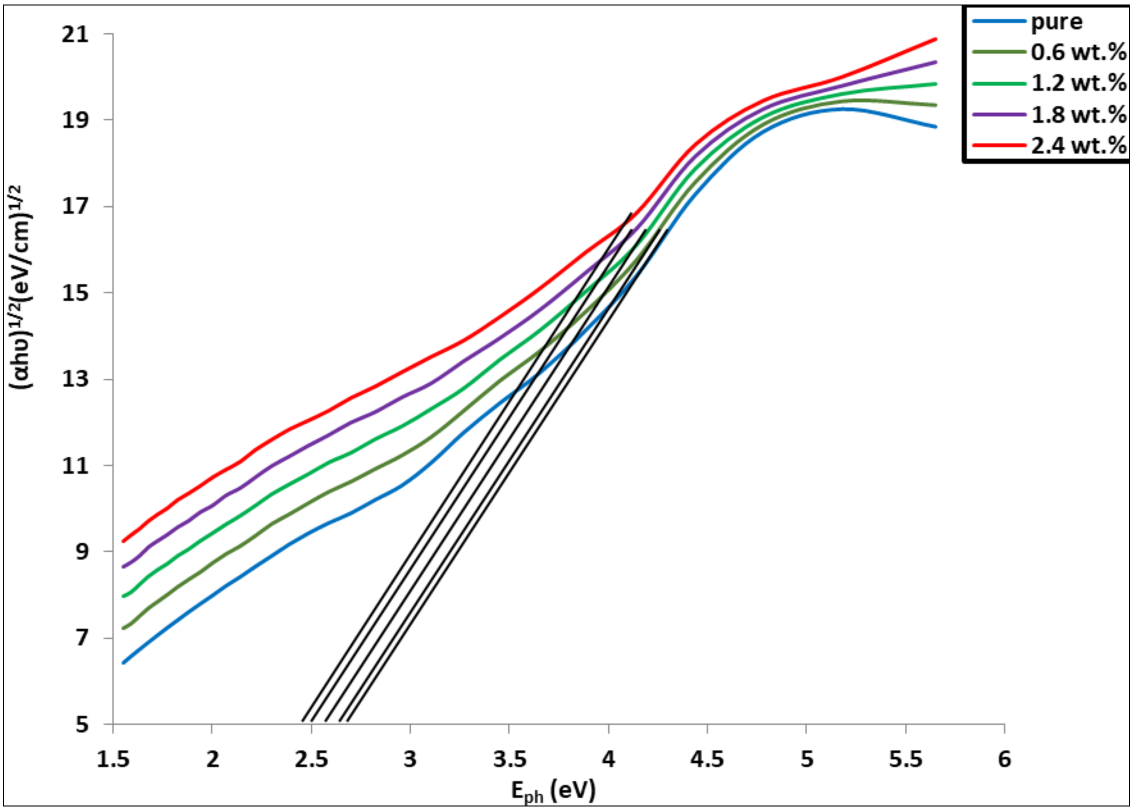

Fig 9: $(\alpha h\upsilon)^{1/2}$ variance with photon energy for (PS-ZnO) nanocomposites.

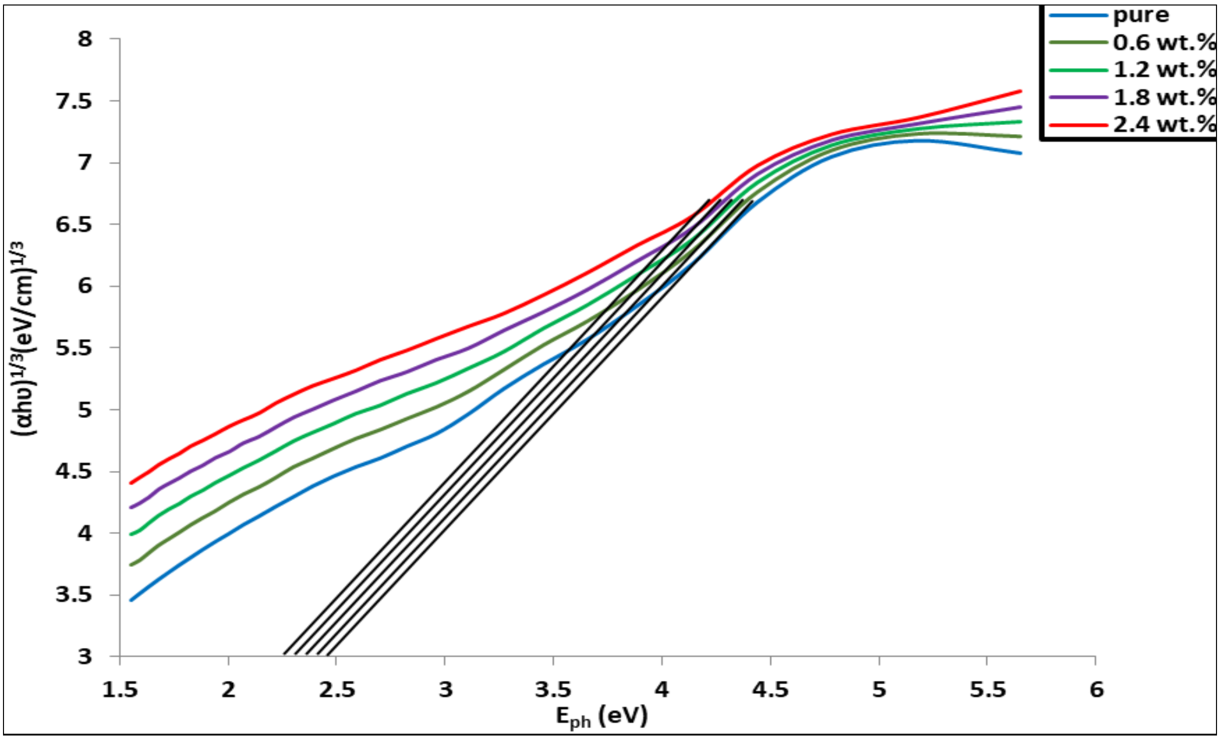

Fig 10: $(\alpha h\upsilon)^{1/3}$ variance with photon energy for (PS-ZnO) nanocomposites.

Table 1: Energy gap values for (PS-ZnO) nanocomposites.

ZnO NPs wt.%	$E_g\,(eV)$	
	Allowed	**Forbidden**
0	2.66	2.46
0.6	2.62	2.42
1.2	2.56	2.38
1.8	2.5	2.34
2.4	2.44	2.30

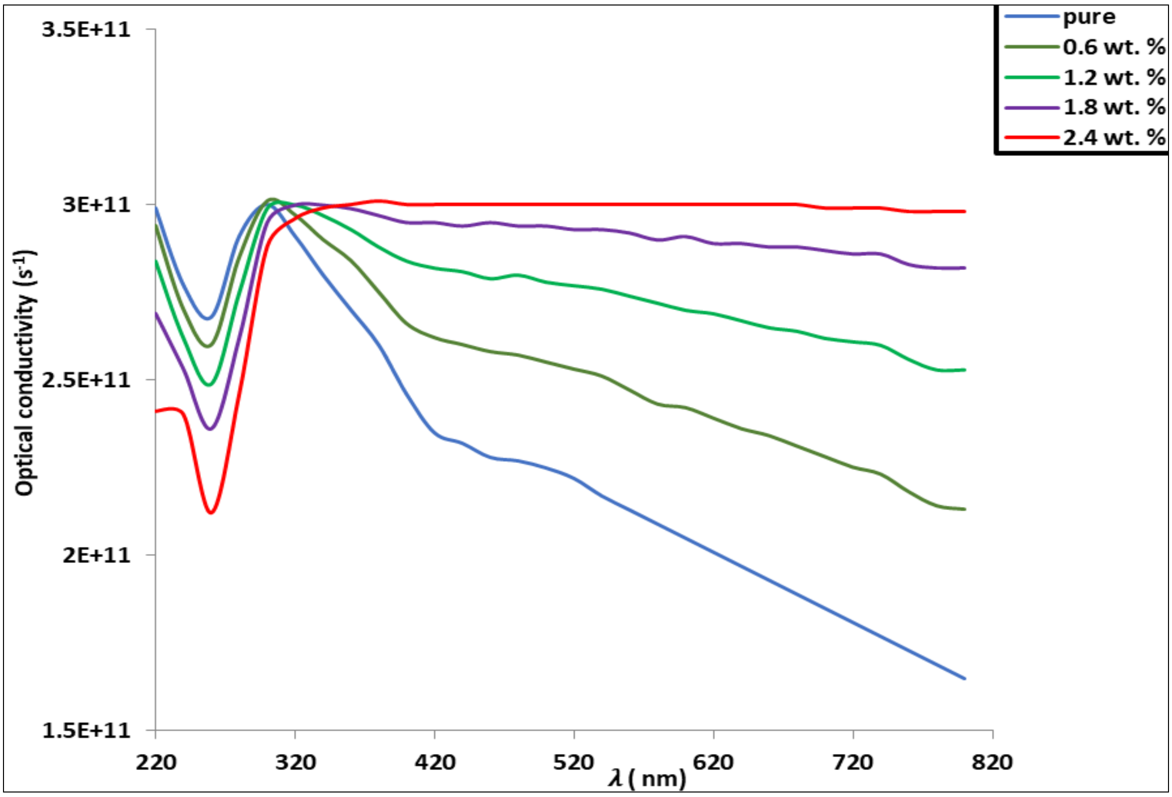

Fig 11: Optical conductivity variance with wavelength for (PS-ZnO) nanocomposites.

5. Conclusion

ZnO NPs adding leads to an increases in (A) as well as optical constants for the polystyrene polymer. These constants include (R), (α), (K), (n), $(\varepsilon_r \& \varepsilon_i)$, and (σ_{opt}), on the contrary, (T) and (E_g) will decreases. (PS-ZnO) nanocomposites possess higher absorption capacity at UV spectrum. According to the findings, (PS-ZnO) nanocomposites have the chance to be utilized in group of diverse optoelectronics application.

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