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RESEARCH ARTICLE

OPTICAL BAND GAP STUDIES OF POLYPYRROLE DOPED WITH NIZNFE$_2$O$_4$ NANO PARTICLES

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ABSTRACT

Polypyrrole/NiZnFe$_2$O$_4$ nanocomposites were synthesized by in-situ polymerization with Ammonium persulphate as an oxidising agent. Optical band gap of chemically synthesized polypyrrole and Polypyrrole-NiZnFe$_2$O$_4$ (10% - 50%) nanocomposites have been studied at room temperature and normal pressure. Energy band gap of these materials are determined by UV-VIS absorption spectra in the wavelength range 264 –1936 nm by spectrophotometer. In this work the experimental results obtained from the optical absorption spectra are reported for nanocomposites of different wt percentages (10% -50%). Characteristic peak around 800 nm (1.552eV) was observed in all the nanocomposites confirming the formation of polypyrrole. The optical properties of this conducting polymer make them a suitable candidate for optoelectronic devices.

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INTRODUCTION

In recent years Polymer nanocomposites have become one of the most extensively studied materials all over the world due to their unusual properties. Owing to their unusual combination of properties they have wide range of applications in various fields such as sensors, electronic devices, memory devices, lithium batteries, energy storage, microwave absorbers, electromagnetic shielding, optoelectronic devices etc.; (Paul and Robeson, 2008; Arami *et al*., 2007). In a number of applications the control of band gap is essential, be it for light emitting diodes (LED) transparency in the visible region combined with high electrical conductivity etc. (Shaktawat *et al*., 2007) The optical band gap is the characteristic of the materials and it depends on the crystallinity and stoichiometry of the material. UV–VIS diffuse reflectance spectroscopy is one of the most employed characterization technique that describes the electronic behaviour present in the structure of the solid. Through the absorption spectra, UV–VIS spectroscopy gives information about the electronic transitions of the different orbitals of a solid. The optical excitation of the electrons from the valence band to the conduction band is evidenced by an increase in the absorbance at a given wavelength, which corresponds to the band gap energy. Polypyrrole (PPy) is one of the most attractive conducting polymers due to its special transport properties, facile synthesis, tunable conductivity and good environmental stability (Ritu P. Mahare *et al*., 2014). Nano crystalline ferrites are materials of considerable interest due to their unique dielectric, magnetic and optical properties. We have selected Nickel zinc ferrites (Nickel zinc iron oxide) nanoparticles due to their importance in wide range of applications in lithium batteries, high-density information storage devices, radar absorbing materials, magnetic fluids etc. (Anjaneyalu *et al*., 2013) In this work we report optical band gap of pure Polypyrrole and polypyrrole doped with copper zinc iron oxide (NiZnFe$_2$O$_4$) nanoparticles.

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MATERIALS AND METHODS

Synthesis of Polypyrrole and PPy/NiZnFe$_2$O$_4$ Nanocomposites

Chemicals - The monomer pyrrole, oxidising agent Ammonium persulphate, nanopowder Nickel zinc iron oxide, acetone were purchased from Sigma Aldrich. All chemicals were of analytical grade and used as received without any further treatment.

PPy and PPy/ $NiZnFe_2O_4$ Nanocomposites were synthesized by in-situ polymerization of monomer Pyrrole using ammonium persulphate as oxidising agent. 0.3M pyrrole taken in a round bottomed glass flask was placed in an ice tray mounted on a magnetic stirrer. 0.6M Ammonium persulphate was added drop wise using a burette to the above 0.3M Pyrrole. The reaction was carried out for 5 hours under continuous stirring maintaining temperature of 0 to 5 degree Celsius. The resulting precipitate was removed by filtration by suction. The Polypyrrole powder thus obtained was then dried in a hot air oven and subsequently in a muffle furnace at a temperature of 100 degree Celsius. The yield was 2.15 g, taken as 100wt. % The nanocomposites are also prepared by the same method reported in detail elsewhere (Shanthala *et al*., 2016).

UV-VIS Spectroscopy Measurements

The optical properties of the nanocomposites were studied using UV-Vis spectrometry. The optical absorption data of the polymer samples were recorded in the range of 264 nm to 1936 nm by using *Cary 300* spectrophotometer.

RESULTS AND DISCUSSION

UV-VIS spectra of PPy and PPy-$NiZnFe_2O_4$ nanocomposites are shown in Fig.1. A major peak at 846 nm was observed for pure (undoped) polypyrrole which is attributed to transitions of the valence to polaron and bipolaron/polaron states. and is characteristic peak of conducting polypyrrole. Small humps in the spectrum indicates polaron bipolaron transitions for all the samples. A shift in characteristic wavelength is observed after doping. The wavelength is shifted from 846nm to 810nm for nanocomposites of 30wt.% and 40wt.%. For nanocomposites of 50wt% the wavelength is shifted from 846nm to 874nm,indicating a decrease in band gap, These observed shifts are due to dopant-polymer interaction (Mahnaz *et al*., 2012; Chakrabarty, 2013). The energy gap Eg can be determined by applying the Kubelka–Munk (K–M) method. The K–M method is based on the following equation

$$\alpha = \frac{(1-R)^2}{2R}.$$

where 'R, is the reflectance; It can be seen from the graph that the absorbance changes with the addition of nanoparticles for nanocomposites of 30% and 40%, there is an increase in the absorbance but decrease in the absorbance is observed for nanocomposites of 50%, which results in variation in the energy gap. The energy band gap of these materials has been calculated with the help of Tauc plots shown in Fig.2. The energy gap is calculated by relation. $\alpha h\nu = A(h\nu - Eg)^n$ where n= ½ or 2 .For direct band gap materials it is 1/2 and for indirect gap materials it is 2 Here it is taken as 2. The band gaps of PPy and PPy- nanocomposites were determined by extrapolation of the plot of $(\alpha h\nu)^2$ v/s hν, as shown in Fig.2a,2b, 2c,2d,2e and 2f. Extrapolation of the line to the x-axis where the value of $(\alpha h\nu)^2$ is zero, gives a band gap value of 1.37 eV for PPy which was in good agreement with the results obtained (Nader Ghobadi, 2013; Eunah *et al*., 2000). The refractive index, n, can be calculated using the relation n = 3.3668 $(Eg)^{-0.32234}$ (Chakrabarty, 2013). The calculated values of energy gap and Refractive index are given in Table 1.

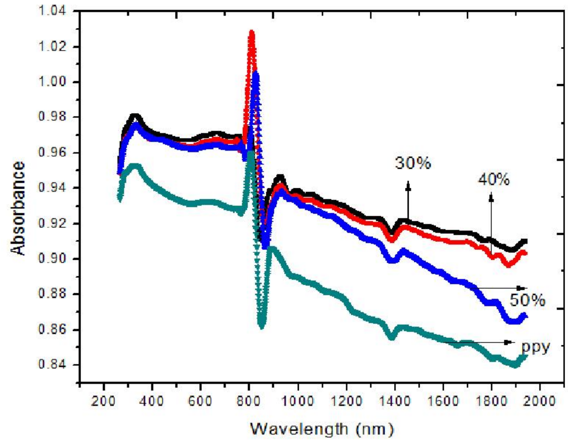

Fig.1. Absorption spectra of Ppy/$NizFe_2O_4$ nanocomposites

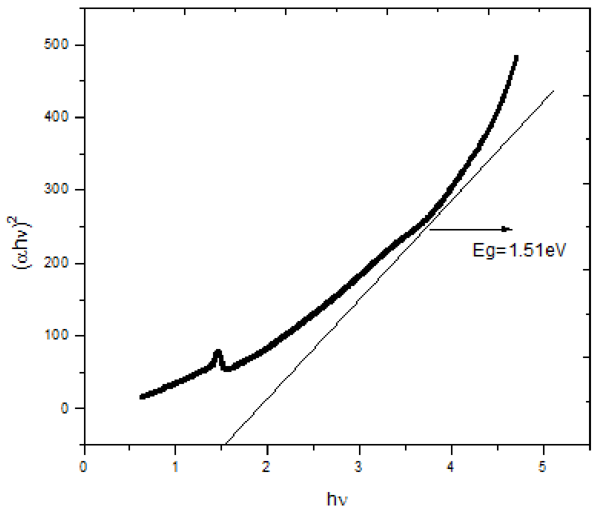

Fig.2a.Tauc's Plot for PPy/$NiznFe_2o_4$-10%

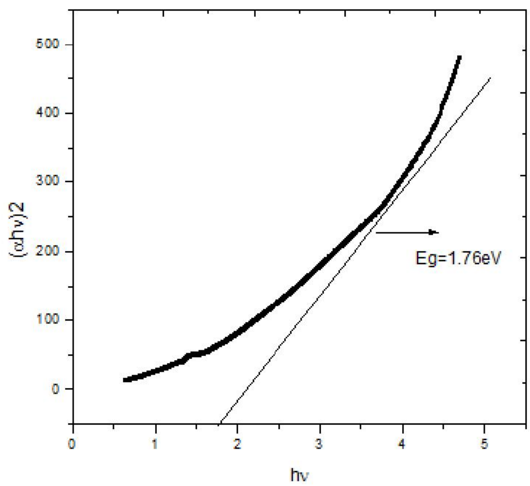

Fig.2b. Tauc's Plot for PPy/$NiznFe_2o_4$-20%

Fig.2a,2b, 2c,2d,2e and 2f . shows the plots of $(\alpha h\nu)^2$ v/s hν. Considering indirect transitions, the values obtained for E_g were 1.37 eV for PPy, 1.51ev for nanocomposites of 10%, 1.76eV for 20%, 1.61eV for 30%, 1.51eV for 40% and 1.49eV for 50%. (8).

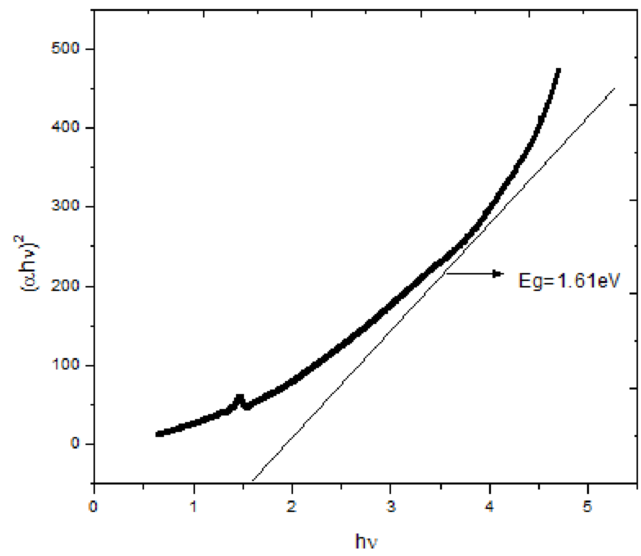

Fig.2c Tauc's Plot for PPy/NiznFe$_2$o$_4$-30%

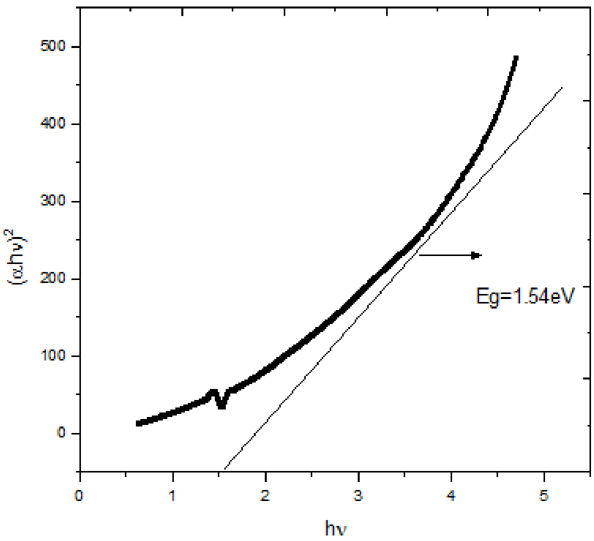

Fig.2d Tauc's Plot for PPy/NiznFe$_2$o$_4$-40%

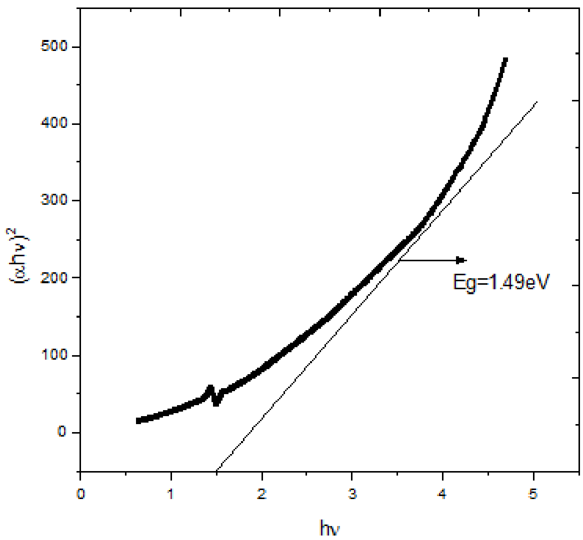

Fig.2e Tauc's Plot for PPy/NiznFe$_2$o$_4$-50%

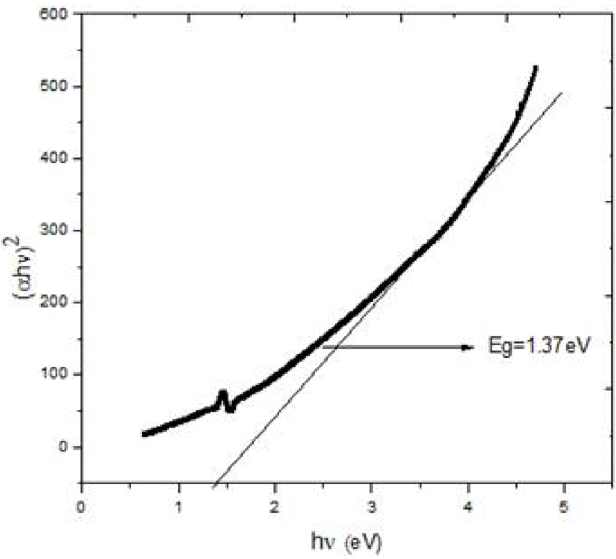

Fig.2f Tauc's Plot for PPy

Table 1. Band gap of PPy and PPy/ Nanocomposites

SL.No	Nanoparticles/ PPy %	Eg (eV)	R.I(n)
1	0%(pure PPy)	1.37eV	3.041
2	10%	1.51eV	2.947
3	20%	1.76eV	2.805
4	30%	1.61eV	2.887
5	40%	1.54eV	2.929
6	50%	1.49eV	2.960

Conclusion

The work highlights the determination of optical properties - band gap and Refractive index of nanocomposites using UV-VIS spectra. Characteristic peak around 846 nm was observed in all the nanocomposites confirming the formation of polypyrrole. The energy gap was determined using Tauc's plots. The results revealed that the band gap of the polypyrrole changes on doping with nanoparticles, The band gap of pure PPy was found to be 1.37eV. The nanocomposites of 20wt.% have highest band gap (1.76eV) and low refractive index (2.805) among all nanocomposites. The nanocomposites of 50wt.% have lowest band gap (1.49eV) and highest refractive index (2.960) among all nanocomposites. The optical properties of this polymer nanocomposites make them a suitable candidate for optoelectronic devices.

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