

Role of Batio3/Tio 2 Nanofillers on the Optical Characteristics of Biopolymer for Optics and Photonics Fields, and Future Application for Antibacterial Activity

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Abstract

In this work, the PVA/BaTiO₃/TiO₂ nanostructures were made by solution casting technique with various weight percentages of BaTiO₃/TiO₂ nanoparticles (0, 1, 1.5, 2, and 2.5) wt %. The structural and optical properties for films were studied. The optical microscope demonstrated that nanoparticles form a continuous system surrounded by polymers. This network is made up of pathways that lead indoors nanocomposites and allows absorbing carriers to move over them. Scan electron microscope revealed a strong dispersion of BaTiO₃ and TiO₂ on the polymeric matrix's surface. And the results revealed that as the concentration of BaTiO₃/TiO₂ nanoparticles rises, (the absorption- absorption coefficient- extinction coefficient- refractive index- real and imaginary dielectric constants- optical conductivity) increases. Optical energy gap for PVA was lessened from 4.5 eV of pure PVA to 3.25 eV for allowed indirect transition and from 4.25 eV to 3.4 eV for forbidden indirect transition while the BaTiO₃/TiO₂ nanoparticles concentration reached (2.5 wt.%), this conduct create it suitable of several optical approaches. With increasing concentrations for BaTiO₃/TiO₂ nanoparticles the transmittance is drop. The final results demonstrated that the PVA/BaTiO₃/TiO₂ nanostructures had good optical properties for use in optics and electronics devices.

Keywords: Polyvinyl Alcohol, Barium titanate, Titanium dioxide, Optical characteristics

1. Introduction

Nanotechnology has opened up a new field of study for processing and producing nanomaterials, which are materials with typical crystallite sizes of less than 100 nanometers. Nanocrystalline materials, nanocomposites, carbon nanotubes, and quantum dots are all examples of nanomaterials. Nanotechnology is a hot issue this year, with a wide range of applications ranging from new breakthroughs in method physics to exactly unique fields to developing innovative nanometer-scale materials. That is rapidly increasing and rising, with broad domains of study, improvement, and industrialized operations [1]. Nanofluids are liquid or solid compound materials made composed for nanofibers or solid nanoparticles floating in liquid. The active warm air conductivity of postponement has been discovered to be improved by nanoparticles with a higher thermal conductivity this surrounding fluid. Because of various advantages like as small weight, modest production processes, cheap price, high exhaustion strength, and strong corrosion resistance, polymer matrix nanocomposites are a popular and significant aspect of today's materials. The presence of nanoparticles in a polymer matrix significantly modifies physical material characteristics for example electrical, structural, thermal, and optical properties [2]. The PVA is regarded to be an excellent host medium for a wide range of nanoparticles. The prospect of generating ultra-transparent films with optimum optical characteristics motivates it. Because of their great dielectric properties, they have attracted a lot of attention flexibility is outstanding, and dielectric strength is rather robust. Because of its strong

dielectric characteristics, barium titanate (BaTiO₃) is a ferroelectric ceramic powder piezoelectric producing polymer nanocomposite films with ceramic fillers as transducers has garnered a lot of attention. Excellent thermal stability and adaptability .Titanium dioxide (TiO₂) is a redox-active material that is employed in water and air purification as well as photoelectron chemical cells because to its low cost, lack of toxicity, and strong photocatalytic activity. In this paper, fabrication and optical properties of PVA/BaTiO₃/TiO₂ nanocomposites are reconnoitered for optoelectronic applications [3, 4].

Experimental part

The films of PVA-BaTiO₃-TiO₂ nanocomposites were made by casting process with varied concentrations of (0, 1, 1.5, 2, and 2.5) wt%. This optical characteristic for nanocomposites films were studied by a double beam spectrophotometer (Shimadzu, UV-1800 A) at wavelengths ranging from 200 to 800 nm. The samples was tested in different concentrations using an Olympus type Nikon-73346 optical microscope which has a magnifying power of (10×). PVA-BaTiO₃-TiO₂ Nanocomposites films are examined by using (Bruker Nano GmbH, company German origin, type vertex 5600LV SEM).

The following formula defines absorbance (A) [5]

$$A = IA/I_0 \quad (1)$$

(IA) is the intensity for light absorbed through the material. (I₀) is the incident light intensity the following equation defines transmittance (T) [6]

$$T = IT/I_0 \quad (2)$$

(IT) is the intensity of light transmitted by the material and (I₀)

is the intensity of light incident. This absorption coefficient (α) is defined through the relative [7]

$$\alpha = 2.303A/t \quad (3)$$

T: is the thickness of the model.

The optical energy gap given by this relation $Ahu = B(hu - E_{gopt})^r \quad (4)$

B: is constant, hu : is the photon emerge, E g: is the optical energy band gap.

$r=2$ for allowed indirect transitions and $r=3$ for forbidden indirect transitions

This Refractive index (n) is known by resulting formula [8]

$$N = (1+R1/2) / (1+R1/2) \quad (5)$$

Reflectance (R). The extinction coefficient (k) calculated by [9]

$$k = \alpha\lambda / 4\pi \quad (6)$$

Dielectric constant is classified into two real (ϵ_1) and imaginary (ϵ_2) parts. Which are identified using the resulting formula [10]

$$\epsilon_1 = n^2 - k^2 \quad (7)$$

$$\epsilon_2 = 2nk \quad (8)$$

Optical conductivity (σ) is establish by way of by the relative [11]

$$\sigma = \alpha n c / 4 \quad (9)$$

Refractive index (n), velocity for light(c), and (α) absorption coefficient.

2. Results and Discussion

Fig. (1) Displays pictures of PVA/BaTiO3/TiO2 nanocomposites films that were collected at a magnification power of 10x for samples of various concentrations. However, as evidenced by the images, clearly differs from the samples (A, B, C, D and E). When BaTiO3 and TiO2 nanoparticle concentrations are rises in films to a level of (2.5) wt percent for PVA/BaTiO3/TiO2 nanocomposites, the nanoparticles begin to form an incessant network confidential the polymers. In the nanocomposites, this network has ways that lease charge carriers pass through [12].

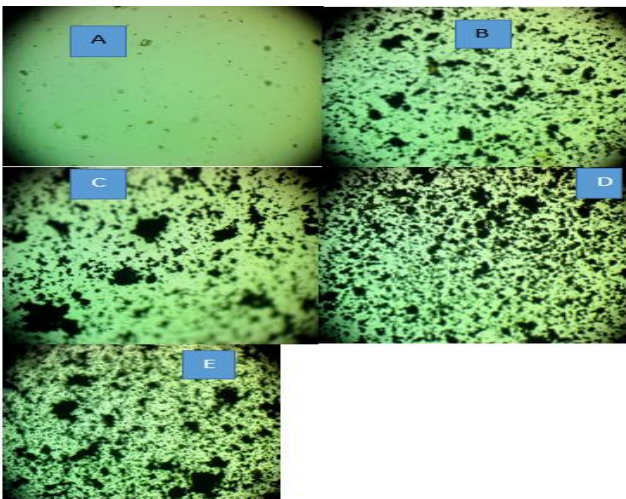


Fig. (1). The Photomicrographs of PVA/BaTiO3/TiO2 Nanocomposites : (A) of (PVA), (B) of 1wt% (C) of 1.5wt%, (D) of 2 wt% ,(E) of 2.5wt%.

Fig. (2) SEM images of PVA/BaTiO3/TiO2 nanocomposites. The compatibility of various polymer, PVA, and BaTiO3/TiO2 nanoparticle components was investigated using SEM. The films exhibit a uniform grain distribution across their surface morphologies PVA/BaTiO3/TiO2 nanoparticle aggregates or morphologies are randomly spread across the surface of the nanocomposites. The results reveal an rise in the number of

aggregations on the surface with growing [13].

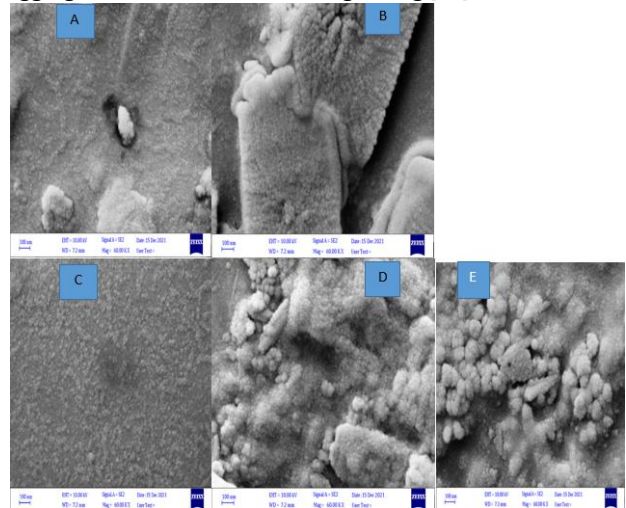


Fig. (2) The Photomicrographs of PVA/BaTiO3/TiO2 Nanocomposites : (A) of (PVA), (B) of 1wt% (C) of 1.5wt%, (D) of 2 wt% ,(E) of 2.5wt%

Fig. (3) Depicts the connection between PVA/BaTiO3/TiO2 nanocomposites' absorbance and wavelength. The figure shows that the absorbance of films is highest at a wavelength near the fundamental absorption edge (200 nm), then declines as the wavelength increases. In general, film absorbance is low in the visible and near-infrared areas. This is how this performance can be explained. While the wavelength of this incident photon lowers (near the fundamental absorption edge), it has enough energy to interact by way of atoms and is transmitted. While the wavelength of the input photon lowers (near the fundamental absorption edge), it interacts with the substance, causing absorbance to increase.

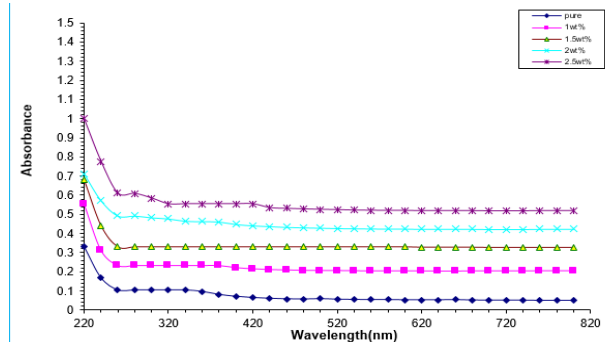


Fig.(3) Connection between absorption and wavelength of PVA/BaTiO3/ TiO2 nanocomposites.

Fig. (4) Depicts the connection between transmittance and wavelength for PVA/BaTiO3/TiO2 nanocomposites. According to this figure, the transmittance drops with the concentration of BaTiO3/TiO2 nanoparticles rises. This is due to the fact that the added (BaTiO3/TiO2) nanoparticles contain, because of the transported electron to higher level has occupied unoccupied locations of energy bands, this procedure does not result in emission of electrons in their external orbits, which can absorb electromagnetic energy. On this other small hand, pure (PVA) have high transmittance and absorbs some of the incident light, whereas docents flow through it. This is due to the necessity for a high-energy photon to break the electron connection and move it to the conduction band.

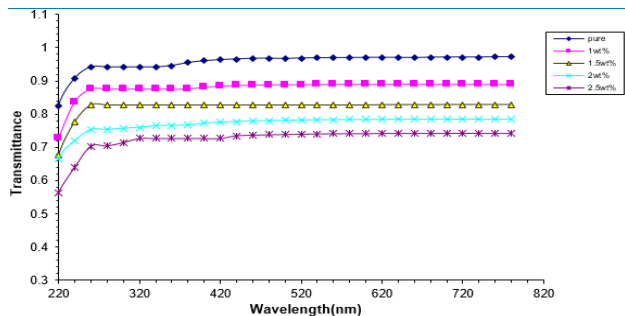


Fig. (4) Connection between transmittance and wavelength of PVA/BaTiO3/TiO2 nanocomposites.

Fig. (5) Depicts the relationship between absorbance coefficient and photon energy for (PVA/BaTiO3/TiO2) nanocomposites. We can see that by in height wavelength ,and ,small energy, this absorption coefficient is the least, meaning that the probability of electron change is negligible since this energy for the input photon is inadequate to passage that electron from the V.B to the C.B ($h\nu > E_g$) [14]. In higher energies, absorption is larger, indicating a high probability of electron transitions. As a result, the energy of the incident photon is necessary to transport the electron from the V.B to the C.B, indicating that incident photons, energy go above this forbidden energy difference. This demonstrates how the absorption coefficient can help limit the nature of an electron transmission, when the absorption coefficient is high ($>104 \text{ cm}^{-1}$) at high energies, a direct transition of an electron is expected to happen, and the energy and moment are retained by the (electrons and photons). However, because the absorption coefficients are ($>104 \text{ cm}^{-1}$) at small energies, it is probable that an electron would perform an indirect transition and that the electronic momentum will be conserved with the assistance of the phonon [14]. The coefficient of absorbance for PVA/BaTiO3/TiO2 nanocomposites is littler than (104 cm^{-1}), showing that the electron transition be there indirect, among other discoveries.

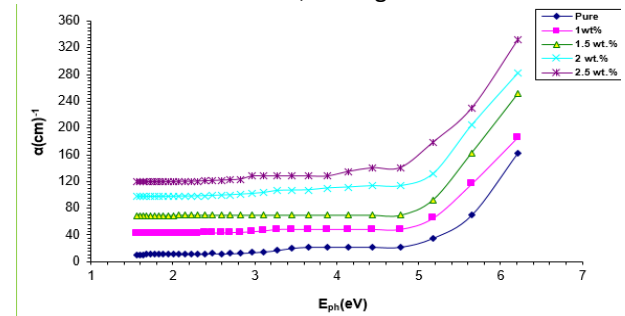


Fig.(5) Connection between absorption coefficient and photon energy of PVA/BaTiO3/TiO2 nanocomposites'

Fig. (6) Depicts the connection between absorption edge ($\alpha h\nu$) $1/2$ for PVA/BaTiO3/TiO2 nanocomposites and photon energy. We get that E_g of this allowed indirect transition. The E_g ideals drop as the weight percentages of barium titanate and titanium dioxide nanoparticles rise. This was ascribed formation for localized levels in this prohibited E_g . In this example, the electron passages as of V.B to this limited levels, and consequently to this C.B by way of weight percentage of barium titanate and titanium dioxide nanoparticles rises. Because of the heterogeneous character of nanocomposites (i.e.,

electronic conduction is dependent on the additional concentration), the density for this localized state increased as the concentration for BaTiO3/TiO2 nanoparticles rose [15].

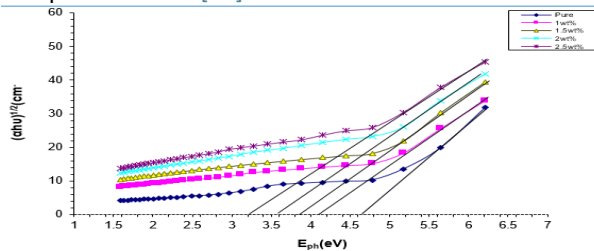


Fig. (6) Connection between absorption edge ($\alpha h\nu$) $1/2$ and photon energy for PVA/BaTiO3/TiO2 nanocomposites

This forbidden transition for this indirect energy gap is considered in this similar method, as shown in fig (7).

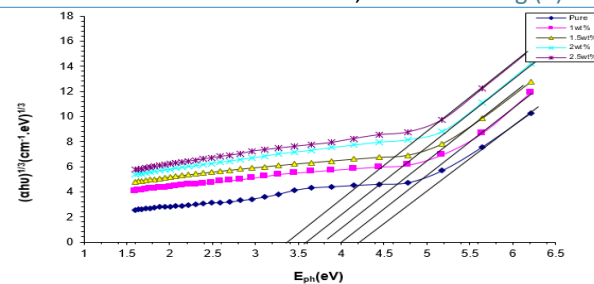


Fig. (7) Connection between ($\alpha h\nu$) $1\3$ (cm-1.ev) $1\3$ with photon energy for PVA/BaTiO3/TiO2 nanocomposites

Fig. (8) Depicts this connection between refractive index for PVA/BaTiO3/TiO2 nanocomposites' and wavelength. The figure clearly shows that refractive index rises with rising weight ratios for BaTiO3/TiO2 nanoparticle concentration to (PVA) nanocomposites as density rises. High refractive index values are obtained in the UV region due to its low transmittance, whereas low values are observed in the visible range because to its high transmittance [16].

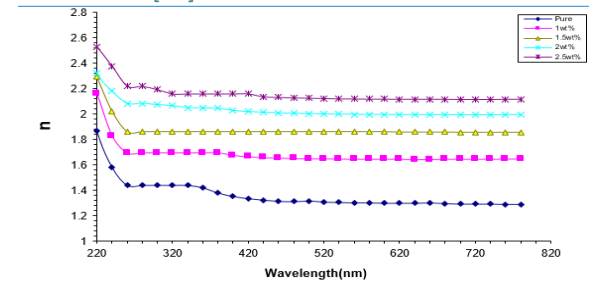


Fig.(8) Connection between refractive index with wavelength for PVA/BaTiO3/TiO2 nanocomposites

Fig. (9) Depicts this connection between extinction coefficient for (PVA/BaTiO3/TiO2) nanocomposite and wavelength. From the figure, we can note the extinction coefficient rises as the BaTiO3/TiO2 nanoparticles rise. The enhanced absorption coefficient is responsible for this. This is because of a rise in the absorption coefficient as percent of Barium titanate and titanium dioxide nanoparticles increase. This finding implies this atoms for BaTiO3/TiO2 nanoparticles will alter the structure for the add polymer [17].

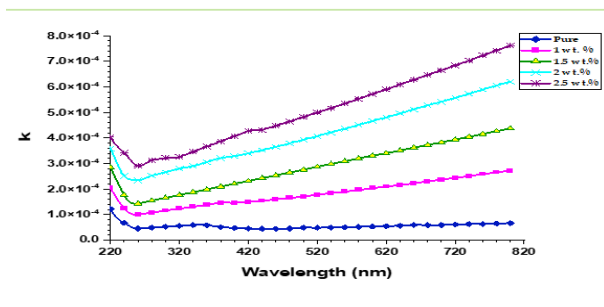


Fig. (9) Connection between extinction coefficient and wavelength for PVA/BaTiO₃/TiO₂ nanocomposites.

Fig.(10) depicts the connection between the real part of dielectric constant and wavelength of (PVA/BaTiO₃/TiO₂) nanocomposites .This figure displays the (ϵ_1) is extremely in essential of on (n_2) as a result of the low value of (k_2) in adding, when the concentrations of (BaTiO₃/TiO₂) nanoparticles raise, so does the actual dielectric constant [18].

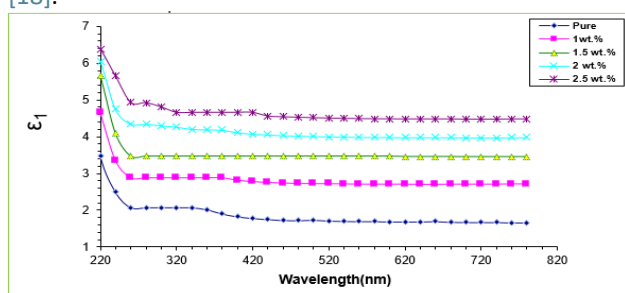


Fig. (10) Connection between real part of dielectric constant and wavelength for PVA/BaTiO₃/TiO₂ nanocomposites

Fig. (11) Depicts the connection between imaginary part of the dielectric constant for PVA/BaTiO₃/TiO₂ nanocomposites and wavelength. From this figure depicts this (ϵ_2) is reliant on (k) values that variation through the absorption coefficient because on the link between (ϵ_2) with (k) [19].

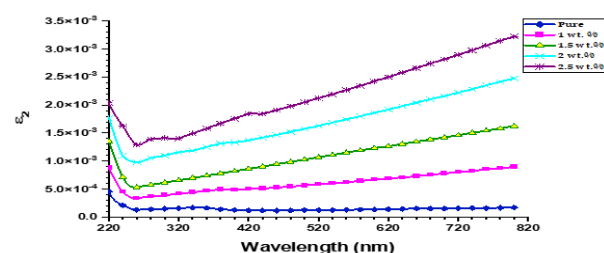


Fig. (11) Connection between imaginary part of dielectric constant and wavelength for PVA/BaTiO₃/TiO₂ nanocomposites.

Fig. (12) Depicts the connection between optical conductivity and wavelength in (PVA/BaTiO₃/TiO₂) nanocomposites. It was found that the optical conductivity of the (PVA) rises as the percentages of (BaTiO₃/TiO₂) in the (PVA) rise (2.5 wt. percent). These new levels in this band gap make it easier for electrons to move from the V.B to these local levels in the C.B. This results in a drop in the band gap and a rise in the conductivity [20-22].

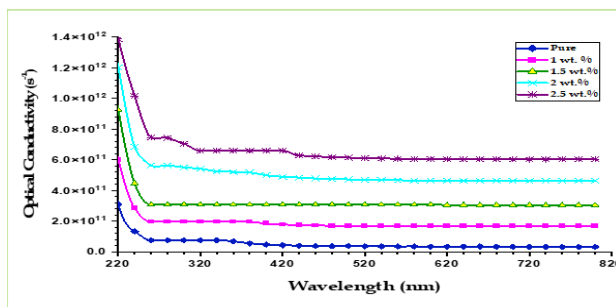


Fig. (12) Connection between optical conductivity and wavelength for PVA/BaTiO₃/TiO₂ nanocomposites.

3. Conclusion

The incorporation of BaTiO₃/TiO₂ nanoparticles into PVA were successfully occurred by solution-casting method. The optical microscope was that the nanoparticles in the polymers form a continuous network of particles. This network, which is built up of passage ways within nanocomposites from the, allows charging carriers to move across them as they pass through them. Scanning electron microscopy revealed several collections or pieces randomly scattered on this surface of PVA/BaTiO₃/TiO₂ nanocomposites films, which were homogenous and coherent. The optical characteristics revealed that when the concentration of BaTiO₃/TiO₂ nanoparticles increased, so did the (absorption, absorption coefficient, extinction coefficient, refractive index, real and imaginary dielectric constants and optical conductivity) are increases by rising of concentrations of BaTiO₃/TiO₂ nanoparticles, transmittance and optical energy gap decrease. The optical characteristics indicated that the PVA/BaTiO₃/TiO₂ nanostructures can be considered as promising materials for optoelectronics devices.

4. References

1. Obaid HN, Habeeb MA, Rashid FL, Hashim A. Thermal energy storage by nanofluids. journal of engineering and applied sciences. 2013;8(5):143-5.
2. Habeeb M, Hashim A, Hayder N. Fabrication of (PS-Cr₂O₃/ZnCoFe₂O₄) Nanocomposites and studying their dielectric and fluorescence properties for IR sensors. Egyptian Journal of Chemistry. 2019;62(Special Issue (Part 2) Innovation in Chemistry):709-17. <https://doi.org/10.21608/ejchem.2019.13333.1832>
3. Su J, Zhang J. Recent development on modification of synthesized barium titanate (BaTiO₃) and polymer/BaTiO₃ dielectric composites. Journal of Materials Science: Materials in Electronics. 2019;30(3):1957-75.
4. Mahsan M, Sheng CK, Isa MIN, Ali EGE, Razali MH, editors. Structural and physical properties of PVA/TiO₂ composite. Malaysia Polymer International Conference; 2009.
5. Jebur Q, Hashim A, Habeeb M. Structural, AC electrical and Optical properties of (Polyvinyl alcohol–Polyethylene Oxide–Aluminum Oxide) Nanocomposites for Piezoelectric Devices. Egyptian Journal of Chemistry. 2019;62(Special Issue (Part 2) Innovation in Chemistry):719-34. <https://doi.org/10.21608/ejchem.2019.14847.1900>

6. Choudhary S. Characterization of amorphous silica nanofiller effect on the structural, morphological, optical, thermal, dielectric and electrical properties of PVA–PVP blend based polymer nanocomposites for their flexible nanodielectric applications. *Journal of Materials Science: Materials in Electronics*. 2018;29(12):10517-34. <https://doi.org/10.1007/s10854-018-9116-y>
7. Siddaiah T, Ojha P, Kumar NO, Ramu C. Structural, optical and thermal characterizations of PVA/MAA: EA polyblend films. *Materials Research*. 2018;21. <https://doi.org/10.1590/1980-5373-MR-2017-0987>
8. Hashim A, Habeeb M, Jebur Q. Structural, Dielectric and Optical properties for (Polyvinyl Alcohol–Polyethylene Oxide–Manganese Oxide) Nanocomposites. *Egyptian Journal of Chemistry*. 2019;62(Special Issue (Part 2) Innovation in Chemistry):735-49. <https://doi.org/10.21608/ejchem.2019.14849.1901>
9. Strankowski M, Włodarczyk D, Piszczak Ł, Strankowska J. Polyurethane nanocomposites containing reduced graphene oxide, FTIR, Raman, and XRD studies. *Journal of Spectroscopy*. 2016;2016. <https://doi.org/10.1155/2016/7520741>
10. Habeeb M, Mahdi W. Characterization of (CMC–PVP–Fe₂O₃) nanocomposites for gamma shielding application. *IJETER*. 2019;7(9):247-55.
11. Habeeb MA, Kadhim WK. Study the optical properties of (PVA–PVAc–Ti) Nanocomposites. *Journal of Engineering and Applied Sciences*. 2014;9(4):109-13.
12. Habeeb M, Hamza RSA. Synthesis of (Polymer blend–MgO) nanocomposites and studying electrical properties for piezoelectric application. *Indonesian Journal of Electrical Engineering and Informatics (IJEEI)*. 2018;6(4):428-35. Available from: <http://section.iaesonline.com/index.php/IJEEI/article/view/511>
13. Habeeb MA. Dielectric and optical properties of (PVAc–PEG–Ber) biocomposites. *Journal of Engineering and Applied Sciences*. 2014;9(4):102-8.
14. Kramadhathi S, Thyagarajan K. Optical properties of pure and doped (KnO₃ & MgCl₂) polyvinyl alcohol polymer thin films. *International journal of engineering research and development*. 2013;6(8):15-8. <https://doi.org/10.1.1.415.6510&rep=rep1&type=pdf>
15. Jebur QM, Hashim A, Habeeb MA. Structural, electrical and optical properties for (polyvinyl alcohol–polyethylene oxide–magnesium oxide) nanocomposites for optoelectronics applications. *Transactions on Electrical and Electronic Materials*. 2019;20(4):334-43. <https://doi.org/10.1007/s42341-019-00121-x>
16. Habeeb M, Hashim A, Hayder N. Structural and Optical Properties of Novel (PS–Cr₂O₃/ZnCoFe₂O₄) Nanocomposites For UV and Microwave Shielding. *Egyptian Journal of Chemistry*. 2019;62(Special Issue (Part 2) Innovation in Chemistry):697-708. <https://doi.org/10.21608/ejchem.2019.12439.1774>
17. Hayder N, Habeeb MA, Hashim A. Structural, Optical and Dielectric Properties of (PS–In₂O₃/ZnCoFe₂O₄) Nanocomposites, *Egypt. J Chem*.63.
18. Habeeb MA, Hamza RSA. Novel of (biopolymer blend–MgO) nanocomposites: fabrication and characterization for humidity sensors. *Journal of Bionanoscience*. 2018;12(3):328-35. <https://doi.org/10.1166/jbns.2018.1535>
19. Abbas NK, Habeeb MA, Algidsawi AJK. Preparation of chloro penta amine cobalt (III) chloride and study of its influence on the structural and some optical properties of polyvinyl acetate. *International Journal of Polymer Science*. 2015;2015. <https://doi.org/10.1155/2015/926789>
20. Sugumaran S, Bellan C. Transparent nano composite PVA–TiO₂ and PMMA–TiO₂ thin films: Optical and dielectric properties. *Optik*. 2014;125(18):5128-33. <https://doi.org/10.1016/j.ijleo.2014.04.077>
21. Ghorbani V, Ghanipour M, Dorrnian D. Effect of TiO₂/Au nanocomposite on the optical properties of PVA film. *Optical and Quantum Electronics*. 2016;48(1):1-14. <https://doi.org/10.1007/s11082-015-0335-7>
22. Soliman T, Vshivkov S. Effect of Fe nanoparticles on the structure and optical properties of polyvinyl alcohol nanocomposite films. *Journal of Non-Crystalline Solids*. 2019;519:119452. <https://doi.org/10.1016/j.jnoncrysol.2019.05.028>