ISSN 2347 - 3983
Volume 7, No.8 August 2019
International Journal of Emerging Trends in Engineering Research
Available Online at http://www.warse.org/IJETER/static/pdf/file/ijeter01782019.pdf
https://doi.org/10.30534/ijeter/2019/01782019

Novel (PMMA-ZrO_2-Ag) Nanocomposites: Structural, Electronic, Optical Properties as Antibacterial for Dental Industries

[1]Angham Hazim [*2]Ahmed Hashim, [1]Hayder M. Abduljalil
[1]University of Babylon, College of Science, Department of Physics, Iraq
[2]University of Babylon, College of Education for Pure Sciences, Department of Physics, Iraq
ahmed_taay@yahoo.com

ABSTRACT

Poly-methylmethacrylate (PMMA)was widely accepted material in dental and medical fieldsbecause of the excellent biocompatibility and easy fabrication. In current paper, study the geometrical parameters, electronic and optical properties of the (PMMA-ZrO_2-Ag)nanostructures. The electronic properties include electrochemical hardness and electronic softness while the optical properties include absorbance**,** transmittance, absorption coefficient**,** extinction coefficient, refractive index, real and imaginary parts of dielectric constants and optical conductivity. The properties calculated by using Gaussian 0.9 program with Gaussian View 0.5 using density function theory (DFT) with local spin density approximation B3LYP level, 6-31G and STO-3D basis sets. The results showed that the addition of Ag nanoparticles lead to decrease the chemical hardness and increase in the softness. The optical properties for (PMMA-ZrO_2-Ag) nanocomposites showed that the absorbance**,** absorption coefficient**,** extinction coefficient, refractive index, real and imaginary parts of dielectric constants and optical conductivity of (PMMA-Al_2O_3) nanocomposites increase while the transmittance and energy band gap decrease with increase in Ag nanoparticles concentrations. The antibacterial results showed that the (PMMA-ZrO_2-Ag) nanocomposites have good antibacterial for positive and negative gram organisms.

Key words: PMMA, ZrO_2, silver, antibacterial,optical properties, nanocomposites.

1. INTRODUCTION

Polymers composites have an important role in dental field because their distinctive features allow a wide range of clinical implementations, which are impossible with the use of other types of materials. One of the commonly used polymers in dental filed is polymethylmethacrylate (PMMA), which uses either heat polymerized or self-polymerized acrylic resin. The popularity of acrylic resin is related mainly to its ease in manipulation, ease in finishing and polishing, as well as it needs inexpensive equipment [1,2]. Additionally, the acrylic resin (PMMA) has a good biocompatibility, reliability, dimensional stability, absence of taste, odor, tissue irritation and toxicity, teeth adhesion, insolubility in body fluids, relative ease of manipulation, good aesthetic appearance, and color stability [3-6],stability in the oral conditions and has high aesthetic quality. Unfortunately, until now the acrylic resin denture base material does not fulfill all the requirements of acceptable mechanical properties. Though, low mechanical properties against impact, bending, and fatigue are important issues to be addressed in order to improve acrylic polymers properties for removable orthodontic appliances and dentures. Many techniques have been used for improving mechanical properties such as chemical correction of polymeric structure by additives like polyethylene glycol dimethacrylate. The other useful method is to reinforce acrylic base composite by materials like fibers and particles[7-11].Because of an increasing interest in esthetics and concerns about toxic and allergic reactions to certain alloys, patients and dentists have been looking for metal-free tooth-colored restorations. Therefore, the development of new high strength dental ceramics, which appear to be less brittle, less limited in their tensile strength, and less subject to time dependent stress failure, has dominated in the later part of 20th century. These capabilities are highly attractive in prosthetic dentistry, where strength and esthetics are paramount. Zirconium oxide ZrO_2 has become a popular alternative to alumina as biomaterial and is used in dental applications for fabricating endodontic posts, crown and bridge restorations and implant abutments. It has also been applied for the fabrication of esthetic orthodontic brackets. Zirconium is the new and valuable material in the world of dentistry, which has been able to control the wonderful world of modern dentistry. This article has several characteristics distinguish them from the previous materials used in the manufacture of teeth such as transparency transparent zircon metal, which gives a great aesthetic dimension to the teeth, the complete neutrality for the mouth and gums, but more than that is active integration with the gums surrounding the dressing or crowns and thus conceal the problems that people suffer from inflammation of the gums and bad breath of the mouth, as well as zirconium has high resistance to breakage and does not cause discoloration of the gums[12-14]. Polymers have been used as insulators in early works because of their dielectric properties and high resistivity. Polymer-based insulators are used in electrical devices to separate conductors without passing current through themselves. The insulator applications of polymers include corrosion protective electronic devices, printed circuit boards and cable sheathing materials. Polymers have several advantages, such as low cost, easy processing, flexibility, good mechanical properties and high strength. In the microelectronic fabrication industry, it are used in the photolithography process. Polymeric nanocomposites consisting of inorganic nanoparticles and organic polymers represent a class of materials that have motivated considerable interest in recent years. The nanocomposites applications are quite promising in the fields of microelectronic packaging, medicine, injection molded products, sensors, membranes, aerospace, packaging materials, coatings, fire-retardants, adhesives, consumer goods, automobiles, optical integrated circuits, drug delivery [15-22].The aims of current study, the effect of additionzirconium oxide and silvernanoparticles on some electronic, optical properties and application antibacterial.

2. THEORETICAL PART

Density functional theory (DFT) is a quantum mechanical method used in physics and chemistry to investigate the electronic structure of many-electron systems, in particular molecules based up on a strategy of modeling electron correlation via general functional of the electron density. DFT is the most popular and useful methods available in computational physics and chemistry. DFT is today one of the most important tools for calculating the ground state properties of metals, semiconductors, and insulators[23].

The main concept of DFT depends on the ground state energy and all other ground state electronic properties are uniquely determined by the electron density. Also, the exact ground state of the system corresponds to the electronic density for minimal total energy.

Within the outline of the DFT, one of the global quantities is chemical hardness (H) it is a measurement of molecule resistance to the change or deformation and defined as the form [24]:

$$H=\frac{1}{2}\left(\frac{\partial\mu}{\partial N}\right)_{V(\vec{r})}\ldots\ldots\ldots\ldots(1)$$

In terms of I_E and E_A , the hardness is half of the energy gap between two frontier orbitals as in the following[24,25]:

$$H=\frac{I_E-E_A}{2}\ldots\ldots\ldots\ldots(2)$$

The soft molecule has a small energy gap and this means small excitation energies to the manifold of excited states, the electron density of soft molecule changes more easily than a hard molecule, and due to that, soft molecules will be more reactive than hard molecules. The global chemical softness S is a property of molecules that measures the extent of chemical reactivity. It is the inverse with hardness as below equation[24,26]:

$$S=\frac{1}{2H}=\left(\frac{\partial^2 N}{\partial E^2}\right)_{V(r)}=\left(\frac{\partial N}{\partial\mu}\right)_{V(r)}\ldots\ldots\ldots\ldots(3)$$

3. RESULT AND DISCUSSION

Figure 1 shows the optimize structures of pure polymethylmethacrylate (PMMA) and (PMMA-ZrO_2-Ag) studied in this research relax by employing the DFT with the B3LYP/6-31G and STO-3D level.

Table (1) shows the results of chemical hardness and chemical softness of the studied molecules. One can see, the hardness decreases and softness increases with increasing the nanoparticles addition of the pure polymethylmethacrylate PMMA.Figures 4 and 5 show the electrochemical hardness H and the electronic softness S of PMMA and (PMMA-ZrO_2-Ag) nanocomposites, respectively. These consequences are designate that, the band gaps in these structures anew more soft spatially the (PMMA-ZrO_2) has E_g equals to 2.3317eV. Now, comparing with the structures of PMMA, (PMMA-ZrO_2) and (PMMA-ZrO_2-Ag) have smaller values of H and greater values of S than the pure PMMA.

Figures (6-8)show the variation of absorbance for (PMMA-ZrO_2-Ag) nanocomposites with wavelength of the incident light. From the figures observed increase of the absorption for all nanocomposites after addition nano particles, this is due to theexcitations of HOMO level to the LUMO level[27].Figures(9-11) represents the absorption coefficient for (PMMA-ZrO_2-Ag)nano composites as a function of photon energy of the incident light. Advantage property of absorptioncoefficient succors to know the nature of electron transition. When the values of theabsorption coefficient ($\alpha < 10^4$) cm^{-1} of (PMMA-ZrO_2-Ag) nanocomposites are high, it is direct transition of electron. While, indirect transition of electron when the values of the absorption coefficient of nanocomposites($\alpha > 10^4$) cm^{-1}). The absorption coefficient of (PMMA-ZrO_2-Ag) nanocomposites is increased with the increase of the adding of Ag nanoparticle, this is property to the increase of number of charge carriers, hence,increase the absorbance of (PMMA-ZrO_2-Ag) and absorption coefficient[28-33].

Figures(12-14)indicate the energy gap for allowed indirect transition of nanocomposites. From the figures observed the energy gap of (PMMA-ZrO_2-Ag) nanocomposites is decreased with the increase of the addingAg nanoparticle, due tothe creation sub levels between valance and conduction bands; as a result of addition of the Ag nanoparticle[34-39].

Figures (15-17)showthe variation of real dielectric constant (ε_1) as a function of wavelength for (PMMA-ZrO_2-Ag) nanocomposites. Figures(18-20) show the effect of Ag nanoparticles on the imaginary part of dielectric constant (ε_2) for (PMMA-ZrO_2-Ag) nanocomposite.It is observed that their values increase with increasing of wavelength and real dielectric constant behave like refractive index.because the effect of extinction coefficient is very small increases in the high energies near the energy gap and the imaginary part of dielectric constant (ε_1) depends on extinction coefficient where the refractive index is approximately constantbehave like the extinction coefficient especially in the visible and near infrared regions of wavelength while extinction coefficient increases with the increase of the wavelength[40-44].

Figures (21-23) show the variation of optical conductivity with the wavelength for (PMMA-ZrO_2-Ag) nanocomposites., ascribed cause decreasedof the optical conductivity of all nanocomposites with increasing of the wavelengthto toughly on the wavelength of the radiation incident; the increase of optical conductivity at low wavelength of photon is owing to high absorbance of nanocomposites in this region, therefore, increase of the charge transfer excitations. The optical conductivity spectra represented to transmittance within the visible and near infrared regions. Also, the optical conductivity of nanocomposite is increased with the increase in the Ag nanoparticles , this attributed to the creation of new levels in the energy gap; the addition of Ag nanoparticles increase the density of localized stages in the band structure increase, therefore, the optical conductivity increases[45-50].

Figure 24shows the antibacterial activity of (PMMA-ZrO_2-Ag) nanocomposites against gram-negative (Escherichia coli) and gram positive (Staphylococcus aureus).The main mechanism that caused the antibacterial activity of (PMMA-ZrO_2-Ag) nanocomposites by the Ag nanoparticles might be through oxidative stress caused by ROS.it includes radicals like super oxide radicals (O^{-2}) hydroxyl radicals (–OH) and hydrogen peroxide (H_2O_2); and singlet oxygen ($^1O_2$)could be the reason damaging the proteinsand DNA in the bacteria. ROS could have been produced by the present (PMMA-ZrO_2-Ag) nanocomposites lead to the inhibition of most pathogenic bacteria like S. aureus, and E. coli.[51-56]. The inhibition zone increases with increase the concentrations of Ag nanoparticles, as shown in figure 30.

4. CONCLUTION

The samples of novel (PMMA-ZrO_2-Ag) nanocompositeswere fabricated for dental industries applications. The electronic and optical properties have been studied. The results showed that the chemical hardness decreases and the softness increases with increase in Ag nanoparticles concentrations. The optical properties for (PMMA-ZrO_2-Ag) nanocomposites showed that the absorbance**,** absorption coefficient**,** extinction coefficient, refractive index, real and imaginary parts of dielectric constants and optical conductivity of (PMMA-ZrO_2) nanocomposites increase while the transmittance and energy band gap decrease with increase in Ag nanoparticles concentrations. The results of antibacterial properties showed that the (PMMA-ZrO_2-Ag) nanocomposites have good antibacterial activity for positive and negative gram organisms bacteria.

REFERENCES

1. Elshereksi, N.W., Ghazali, M.J., Muchtar, A. and Azhari, C.H.,"Perspectives for Titanium-Derived Fillers Usageon Denture Base Composite Construction: A Review Article", Advances in Materials Science and Engineering, 2014, Article ID: 746252. http://dx.doi.org/10.1155/2014/746252, 2014.
2. Ahmed, M.A. and Ebrahim, M.I.,"Effect of Zirconium Oxide Nano-Fillers Addition on the Flexural Strength,Fracture Toughness, and Hardness of Heat-Polymerized Acrylic Resin",World Journal of Nano Science and Engineering,4, 50-57. http://dx.doi.org/10.4236/wjnse.2014.42008,2014.
3. Cooper S., Visser S., Hergenrother R., and Lamba N., "Polymers, in Biomaterials Science: An Introduction to Materials in Medicine", B. Ratner, A. Hoffman, and F. Schoen, Eds., 67–80, Elsevier Academic Press, San Diego, Calif, USA, 2nd edition, 2004.
4. Palitsch A., Hannig M., Ferger P., and Balkenhol M., "Bonding of acrylic denture teeth to MMA/PMMA and light-curing denture basematerials: the role of conditioning liquids", Journal of Dentistry, 40, 3, 210–221, 2012.
5. Anusavice J. K., Phillip's Science of Dental Materials,WB Saunders, Philadelphia, Pa, USA, 2003.
6. Bayindir F., Kurklu D., and Yanikoglu N. D., "The effect of staining solutions on the color stability of provisional prosthodontics materials", Journal of Dentistry, 40, 2, 41– 46, 2012.
7. Hamouda, I.M. and Beyari, M.M., "Addition of Glass Fibers and Titanium Dioxide Nanoparticles to the Acrylic Resin Denture Base Material: Comparative Study with the Conventional and High Impact Types", Oral Health and Dental Management, 13, 107-112, 2014.
8. Mowade, T.K., Dange, S.P., Thakre, M.B. and Kamble, V.D., " Effect of Fiber Reinforcement on Impact Strength of Heat Polymerized Polymethyl Methacrylate Denture Base Resin: In Vitro Study and SEM Analysis", Journal of Advanced Prosthodontics, 4, 30-36. http://dx.doi.org/10.4047/jap.2012.4.1.30, 2012.
9. Vallo, C.I., Abraham, G.A., Cuadrado, T.R. and Román, J.S.,"Influence of Cross-Linked PMMA Beads on the Mechanical Behavior of Self-Curing Acrylic Cements", Journal of Biomedical Materials Research Part B: Applied Biomaterials, 70, 407-416, http://dx.doi.org/10.1002/jbm.b.30054, 2004.
10. Sasaki, H., Hamanaka, I., Takahashi, Y. and Kawaguchi, T.,"Effect of Reinforcement on the Flexural Properties of Injection-Molded Thermoplastic Denture Base Resins", Journal of Prosthodontics, http://dx.doi.org/10.1111/jopr.12419, 2015.
11. Shirkavand, S. and Moslehifard, E.,"Effect of TiO2 Nanoparticles on Tensile Strength of Dental Acrylic Resins",Journal of Dental Research, Dental Clinics, Dental Prospects, 8, 197-203, 2014.
12. Coelho PG, Silva NR, Bonfante EA, Guess PC, Rekow ED, Thompson VP.,"Fatigue testing of two porcelain–zirconia all-ceramic crown systems",22–1127, Dent Mater 2009;25:11.
13. Manicone PF, Iommetti PR, RaffaelliL.,"An overview of zirconia ceramics: Basic properties and clinical applications", 19–826, J Dent 2007;35:8.
14. Chevalier J, Gremillard L, Deville S.,"Low-temperature degradation of zirconia and implications for biomedical implants",Annu Rev Mater Res 2007;37:1–32.

15. HayderAbduljalil, Ahmed Hashim, AlaaJewad, The Effect of Addition Titanium Dioxide on Electrical Properties of Poly-Methyl Methacrylate, European Journal of Scientific Research, Vol.63, No.2, pp.231-235, (2011).

16. Z.Al-Ramadhan, Ahmed Hashim and Alaa J. Kadham Algidsawi, The D.C electrical properties of (PVC-Al_2O_3) composites , AIP Conference Proceedings, Vol. 1400, No.1, https://doi.org/10.1063/1.3663109 , (2011).

17. Ahmed Hashimand AseelHadi, A Novel Piezoelectric Materials Prepared from (Carboxymethyl Cellulose-Starch) Blend-Metal Oxide Nanocomposites, Sensor Letters, Vol. 15, doi:10.1166/sl.2017.3910 , (2017).

18. Hashim A andHadi A., Novel Pressure Sensors Made From Nanocomposites (Biodegradable Polymers–Metal Oxide Nanoparticles): Fabrication and Characterization. UkrainianJournalofPhysics, 63(8), DOI:https://doi.org/10.15407/ujpe63.8.754 (2018).

19. Ahmed Hashimand QassimHadi, Novel of (Niobium Carbide/Polymer Blend) Nanocomposites: Fabrication and Characterization for Pressure Sensor, Sensor Letters, Vol.15, doi:10.1166/sl.2017.3892 , (2017).

20. Majeed Ali Habbeb, Ahmed Hashim, Abdul-Raheem K. AbidAli, The dielectric properties for (PMMA-LiF) composites , European Journal of Scientific Research, Vol. 61, No.3, pp.367-371, (2011).

21. Ahmed Hashim, Majeed Ali Habeeb, AseelHadi, Qayssar M. Jebur, and WaledHadi, Fabrication of Novel (PVA-PEG-CMC-Fe_3O_4) Magnetic Nanocomposites for Piezoelectric Applications, Sensor Letters, Vol. 15, doi:10.1166/sl.2018.3935 , (2017).

22. Ahmed Hashim and ZinahSattarHamad, Fabrication and Characterization of Polymer Blend Doped with Metal Carbide Nanoparticles for Humidity Sensors, J. Nanostruct., Vol.9, No.2, pp.340-348, DOI: 10.22052/JNS.2019.02.016 , (2019).

23. Abel Kolawole O. and Banjo S., “Theoretical Studies of Anti-corrosion Properties of Triphenylimidazole Derivatives in Corrosion Inhibition of Carbon Steel in Acidic Media via DFT Approach”, Analytical &\ Bioanalytical Electrochemistry, 10, 1, 136-146, 2018.

24. Oftadeh M., Naseh S. and Hamadanian M., "Electronic properties and dipole polarizaplility of thiophenol derivative via density functional theory", Computational and Theoretical Chemistry, 966, 20-25, 2011.

25. Proft F. De and Geerlings P., "Calculation of ionization energies, electron affinities, electronegativities, and hardnesses using density functional methods", the Journal of Chemical Physics, 106, 3270-3279, 1997.

26. Sadasivam K. and Kumareaan R., "Theoretical Investigation on the Antioxidant Behavior of chrysoeriol and HispidulinFavonoid Compounds-ADFT study", Computational and Theoretical Chemistry, 963, 227-235, 2011.

27. 10. Pal Indolia A, "Gaur MS Optical properties of solution grown PVDF-ZnOnanocomposite thin films", J Polym Res, 20(43), 1–8, 2013.

28. 12. Salman S, Bakr Nand Mahmood MH,"Preparation and study of some optical properties of (PVA Ni(CH3COO)2) composites", Intern J Curr Res 6(11):9638–9643, 2014.

29. Falah Ali Jasim, Ahmed. Hashim, Angham. G. Hadi, FarhanLafta, Saba R. Salman and Hind Ahmed, Preparation of (pomegranate peel-polystyrene) composites and study their optical properties, Research Journal of Applied Sciences, Vol.8, Issue. 9, PP. 439-441, 2013.

30. Falah Ali Jasim, FarhanLafta, Ahmed. Hashim, Majeed Ali, Angham. G. Hadi, Characterization of palm fronds-polystyrene composites, Journal of Engineering and Applied Sciences, Vol.8 , No.5, PP. 140-142, 2013..

31. Ahmed Hashim andAseelHadi, Synthesis and Characterization of (MgO-Y_2O_3-CuO) Nanocomposites for Novel Humidity Sensor Application, Sensor Letters, Vol.15, doi:10.1166/sl.2017.3900 , (2017).

32. ShaymaaHadi, Ahmed Hashim and AlaaJewad, Optical properties of (PVA-LiF) composites, Australian Journal of Basic and Applied Sciences, Vol.5, No.9, pp. 2192-2195, (2011).

33. Ahmed Hashimand ZinahSattarHamad, Synthesis, Characterization and Nanobiological Application of (Biodegradable Polymers-Titanium Nitride) Nanocomposites, Journal of Bionanoscience, Vol. 12, No.4, doi:10.1166/jbns.2018.1561 , (2018).

34. Abdelghany AM, Abdelrazek EM and RashadD,"Impact of in situ preparation of CdS filled PVPnano-composite", J SpectrochimicaActa Part A MolBiomolSpectr 130:302–308, 2014.

35. Ahmed Hashimand Noor Hamid, Fabrication and Properties of Biopolymer-Ceramics Nanocomposites as UV-Shielding for Bionanoscience Application, Journal of Bionanoscience, Vol. 12, No.6, doi:10.1166/jbns.2018.1591 , (2018).

36. Ahmed Hashimand ZinahSattarHamad, Novel of (Niobium Carbide-Biopolymer Blend) Nanocomposites: Characterization for Bioenvironmental Applications, Journal of Bionanoscience, Vol. 12, No.4, doi:10.1166/jbns.2018.1551 , (2018).

37. A. Hashim and Q. Hadi, Synthesis of Novel (Polymer Blend-Ceramics) Nanocomposites: Structural, Optical and Electrical Properties for Humidity Sensors, Journal of Inorganic and Organometallic Polymers and Materials, Vol.28, Issue 4, pp 1394–1401, https://doi.org/10.1007/s10904-018-0837-4 , (2018).

38. Hind Ahmed, Hayder M. Abduljalil, Ahmed Hashim, Structural, Optical and Electronic Properties of Novel (PVA–MgO)/SiCNanocomposites Films for Humidity Sensors, Transactions on Electrical and Electronic Materials, https://doi.org/10.1007/s42341-019-00111-z, (2019).

39. Hind Ahmed, Hayder M. Abduljalil, Ahmed Hashim, Analysis of Structural, Optical and Electronic Properties of Polymeric Nanocomposites/Silicon Carbide for Humidity Sensors, Transactions on Electrical and Electronic Materials, https://doi.org/10.1007/s42341-019-00100-2, (2019).

40. Mathai C.J. et al., "Effect of iodine doping on the band gap of plasma polymerized aniline thin films", J. Phys. D Appl. Phys, 35(17), 2206, 2002.

41. Hashim A. and Jassim A., Novel of Biodegradable Polymers-Inorganic Nanoparticles: Structural, Optical and Electrical Properties as Humidity Sensors and Gamma Radiation Shielding for Biological Applications, Journal of Bionanoscience, Vol. 12, (2018), doi:10.1166/jbns.2018.1518.

42. A. Hashim and Q. Hadi, Structural, electrical and optical properties of (biopolymer blend/ titanium carbide) nanocomposites for low cost humidity sensors, Journal of Materials Science: Materials in Electronics,Vol.29, pp.11598–11604, https://doi.org/10.1007/s10854-018-9257-z , (2018).

43. Alaa J. Kadham, Dalal Hassan, Najlaa Mohammad, Ahmed Hashim, Fabrication of (Polymer Blend-magnesium Oxide) Nanoparticle and Studying their Optical Properties for Optoelectronic Applications, Bulletin of Electrical Engineering and Informatics, Vol.7, No.1, (2018), DOI: 10.11591/eei.v7i1.839.

44. Ibrahim R. Agool, Firas S. Mohammed and Ahmed Hashim, The Effect of Magnesium Oxide Nanoparticles on the Optical and Dielectric Properties of (PVA-PAA-PVP) Blend, Advances in Environmental Biology, Vol.9, No.11, (2015) : 1-10.

45. Ahmed Hashimand Ali Jassim, Novel of (PVA-ST-PbO_2) Bio Nanocomposites: Preparation and Properties for Humidity Sensors and Radiation Shielding Applications, Sensor Letters, Vol. 15, No.12, doi:10.1166/sl.2018.3915 , (2017).

46. A. Hashim, I. R. Agool and K. J. Kadhim, Novel of (Polymer Blend-Fe_3O_4) Magnetic Nanocomposites: Preparation and Characterization For Thermal Energy Storage and Release, Gamma Ray Shielding, Antibacterial Activity and Humidity Sensors Applications, Journal of Materials Science: Materials in Electronics, Vol. 29, Issue 12, pp. 10369–10394, DOI: https://doi.org/10.1007/s10854-018-9095-z , (2018).

47. A. Hashim,K.H.H. Al-Attiyah,S.F. Obaid, Fabrication of Novel (Biopolymer Blend-Lead Oxide Nanoparticles) Nanocomposites: Structural and Optical Properties for Low Cost Nuclear Radiation Shielding, Ukr. J. Phys.,Vol. 64, No. 2, (2019), https://doi.org/10.15407/ujpe64.2.157.

48. Bahaa H. Rabee, Ahmed Hashim, Synthesis and characterization of carbon nanotubes -polystyrene composites , European Journal of Scientific Research, Vol. 60, No. 2, pp. 247-254 , (2011).

49. D. Hassan, A. Hashim, Preparation and studying the structural and optical properties of (poly-methyl methacrylate-lead oxide) nanocomposites for bioenvironmental applications, Journal of Bionanoscience, Vol.12, Issue 3, doi:10.1166/jbns.2018.1537 , (2018).

50. D. Hassan, A. Hashim, Structural and optical properties of (polystyrene-copper oxide) nanocomposites for biological applications, Journal of Bionanoscience, Vol.12, Issue 3, doi:10.1166/jbns.2018.1533 , (2018).

51. Behera S.S., Patra J.K., Pramanik K., Panda N. and Thatoi H., "Characterization and evaluation of antibacterial activities of chemically synthesized iron oxide nanoparticles", World J. Nano Sci. Eng., 2, 196–200, 2012.

52. Hind Ahmed, Ahmed Hashim and Hayder M. Abduljalil, Analysis of Structural, Electrical and Electronic Properties of (Polymer Nanocomposites/ Silicon Carbide) for Antibacterial Application, Egypt. J. Chem. Vol. 62, No. 4. pp.1167– 1176, DOI: 10.21608/EJCHEM.2019.6241.1522 , (2019).

53. Ahmed Hashim, Ibrahim R. Agool, and Kadhim J. Kadhim, Modern Developments in Polymer Nanocomposites for Antibacterial and Antimicrobial Applications: A Review, Journal of Bionanoscience, Vol. 12, No.5, doi:10.1166/jbns.2018.1580 , (2018).

54. NahedaHumood Al-Garah, FarhanLafta Rashid, AseelHadi, and Ahmed Hashim, Synthesis and Characterization of Novel (Organic–Inorganic) Nanofluids for Antibacterial, Antifungal and Heat Transfer Applications, Journal of Bionanoscience, Vol. 12, doi:10.1166/jbns.2018.1538 , (2018).

55. Kadhim K J, Agool I R and Hashim A., Synthesis of (PVA-PEG-PVP-TiO2) Nanocomposites for Antibacterial Application. Materials Focus, Vol.5, No.5, DOI: https://doi.org/10.1166/mat.2016.1371, (2016).

56. Kadhim K J, Agool I R and Hashim A., Effect of Zirconium Oxide Nanoparticles on Dielectric Properties of (PVA-PEG-PVP) Blend for Medical Application. Journal of Advanced Physics, Vol.6, No.2, DOI: https://doi.org/10.1166/jap.2017.1313 , (2017).

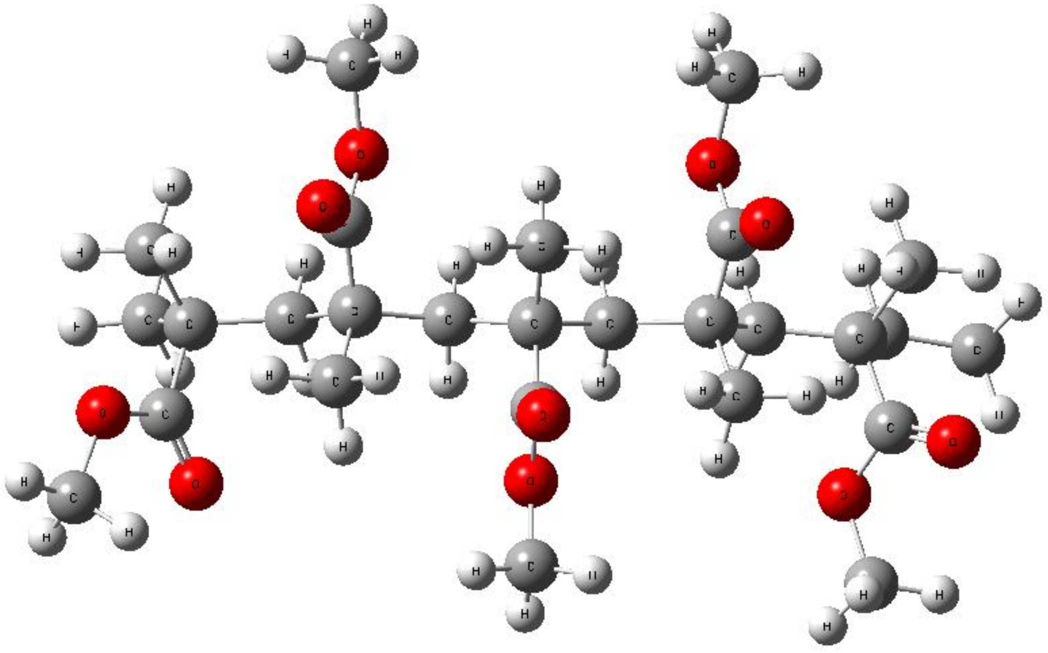

Figure 1: The optimization structures of the pure polymethlmethacrylate (PMMA).

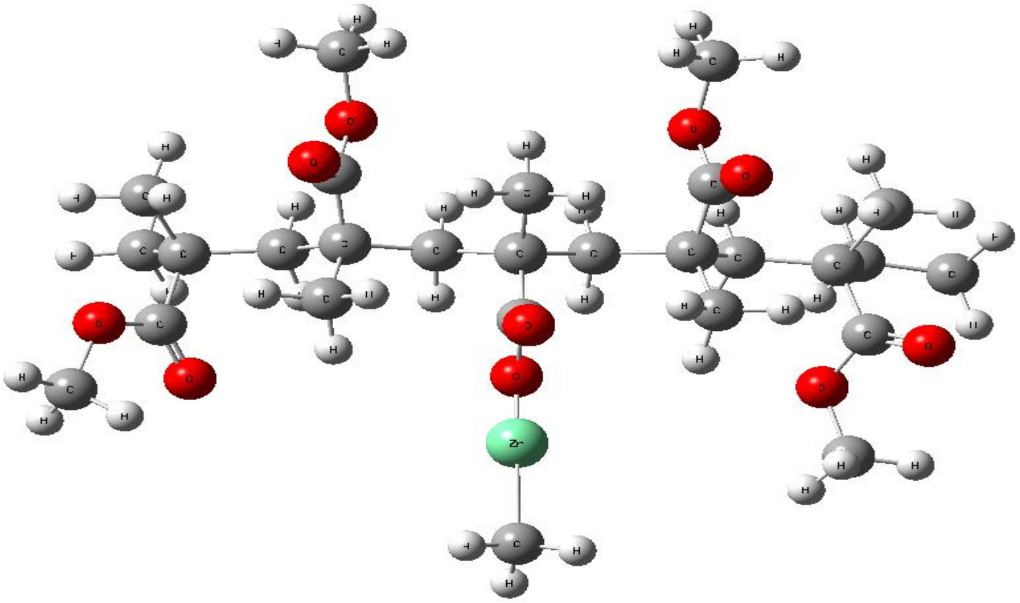

Figure 2: The optimization structures for (PMMA-ZrO_2) nanocomposites.

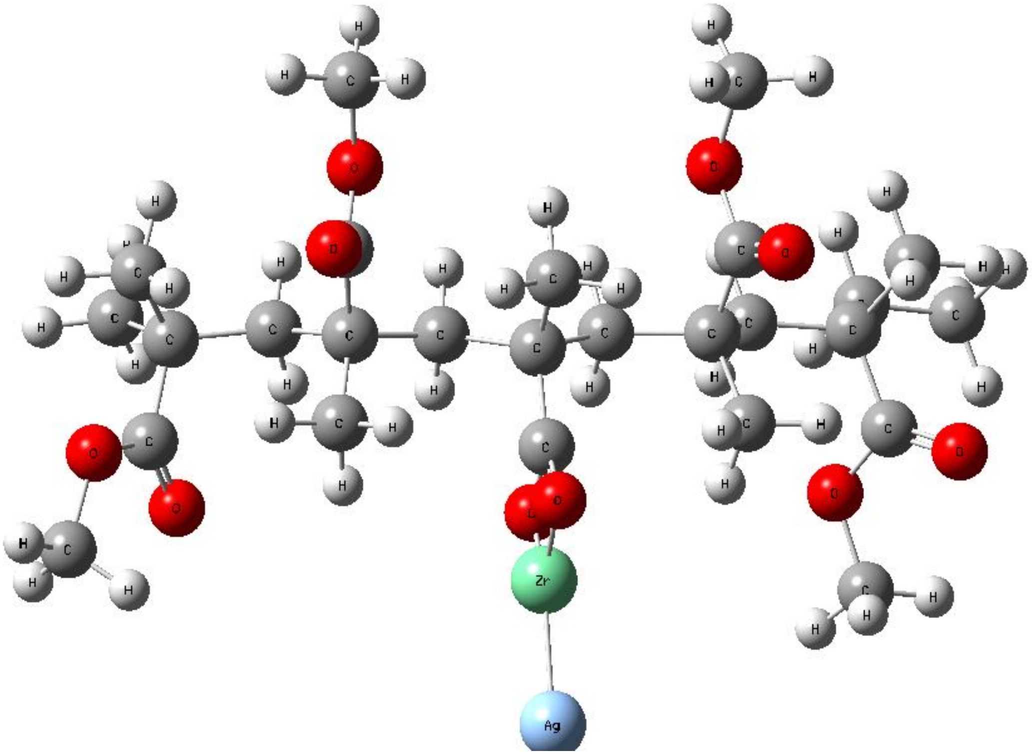

Figure 3: The optimization structures for (PMMA-ZrO_2-Ag) nanocomposites.

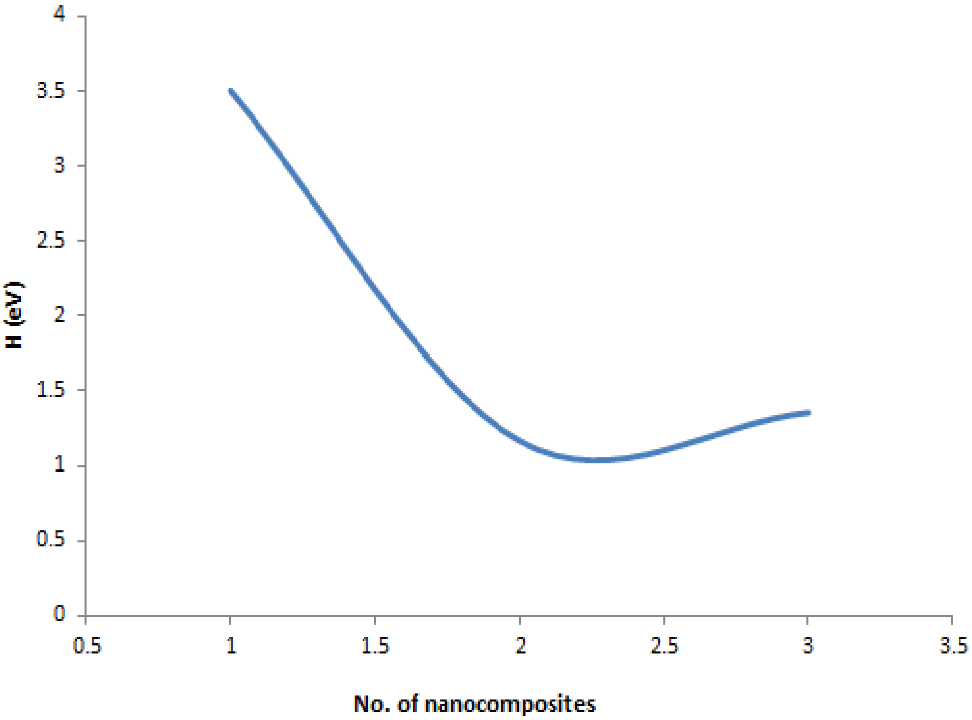

Figure 4: The electrochemical hardness for pure (PMMA) and nanocomposites.

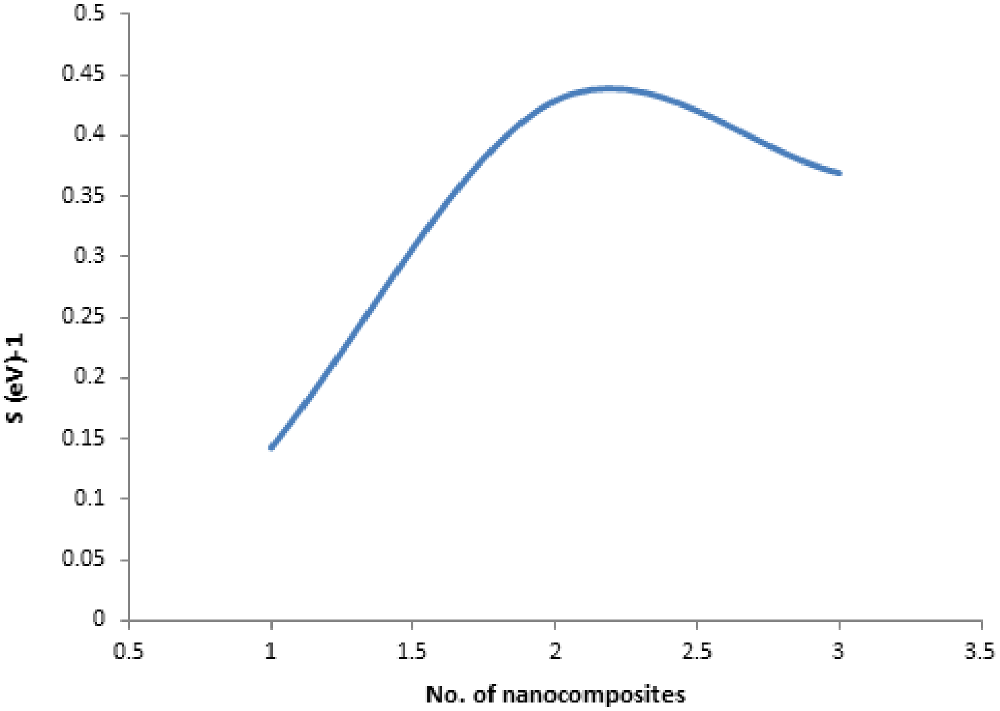

Figure 5: The electronic softnessfor pure (PMMA) and nanocomposites.

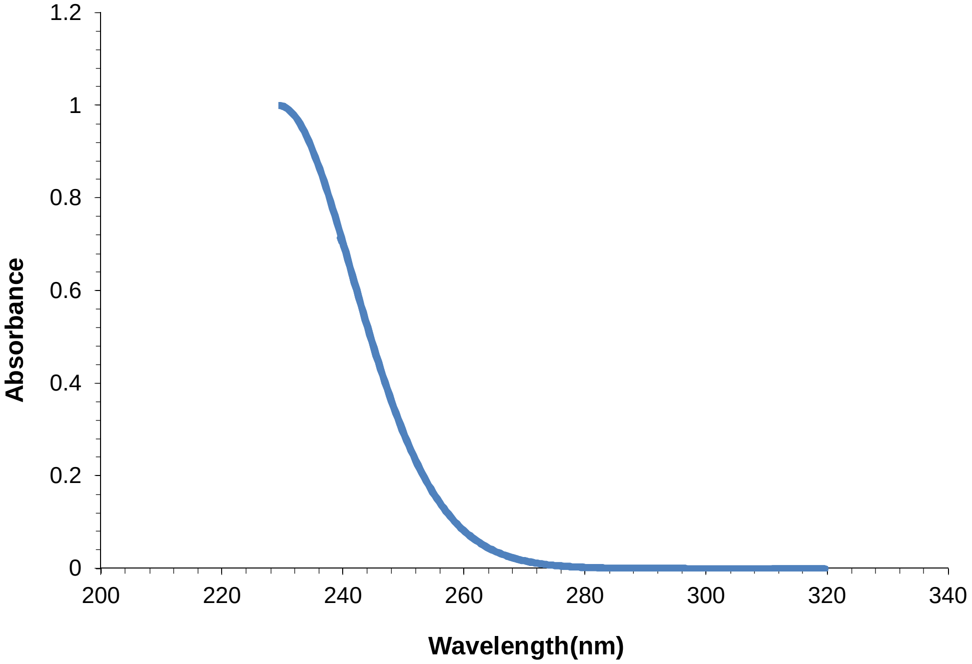

Figure 6: The absorbance as a function of wavelength for pure polymethylmethacrylate.

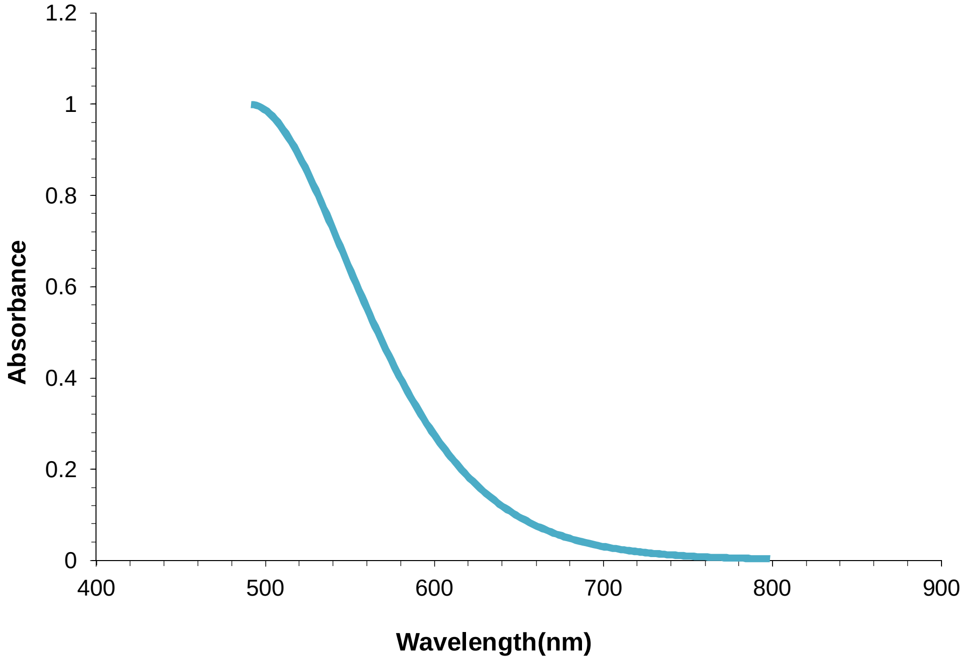

Figure 7: The absorbance as a function of wavelength for (PMMA-ZrO_2) nanocomposites.

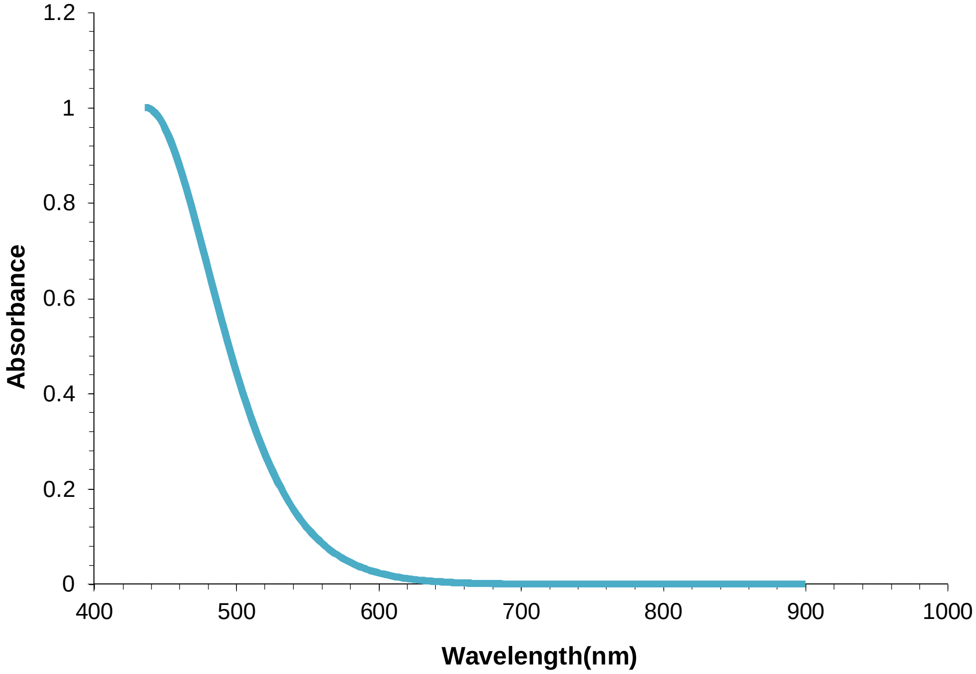

Figure 8: The absorbance as a function of wavelength for (PMMA-ZrO_2-Ag) nanocomposites

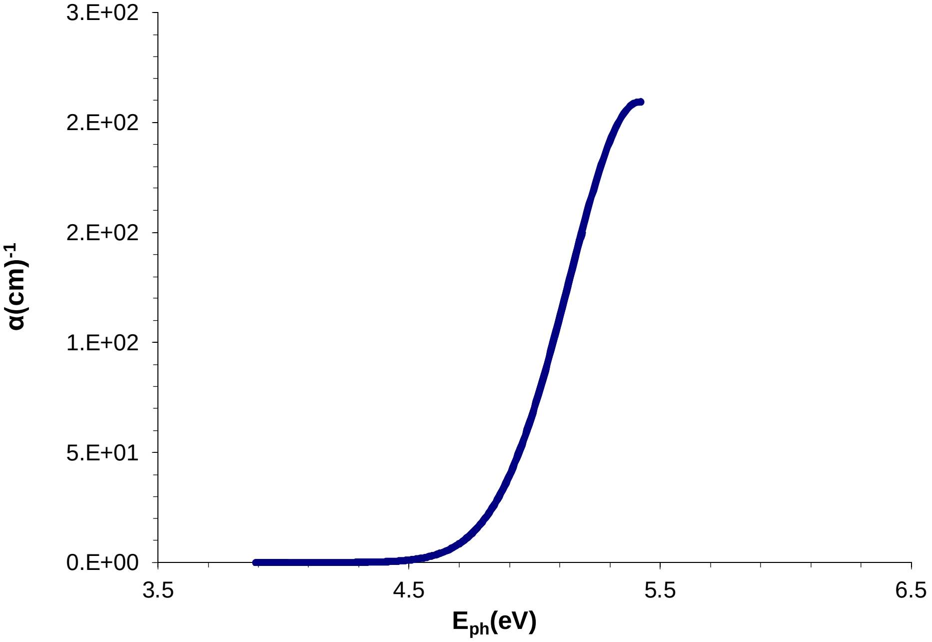

Figure 9: Variation of absorption coefficient (α) for polymethylmethacrylatewith photon energy.

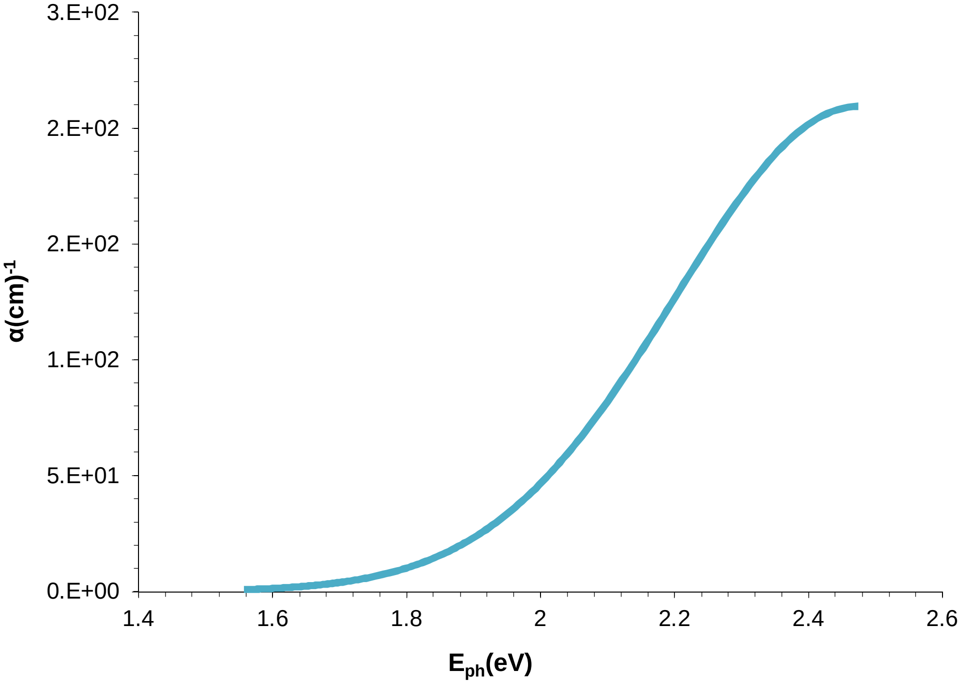

Figure 10: Variation of absorption coefficient (α) for (PMMA-ZrO_2)nanocomposites with photon energy**.**

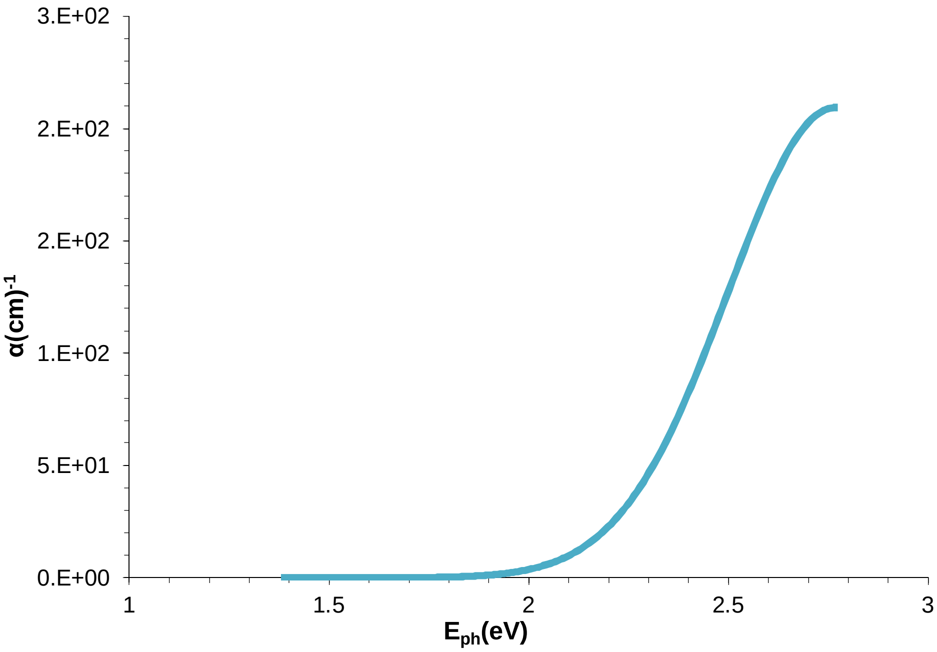

Figure 11: Variation of absorption coefficient (α) for (PMMA-ZrO_2-Ag) nanocomposites with photon energy.

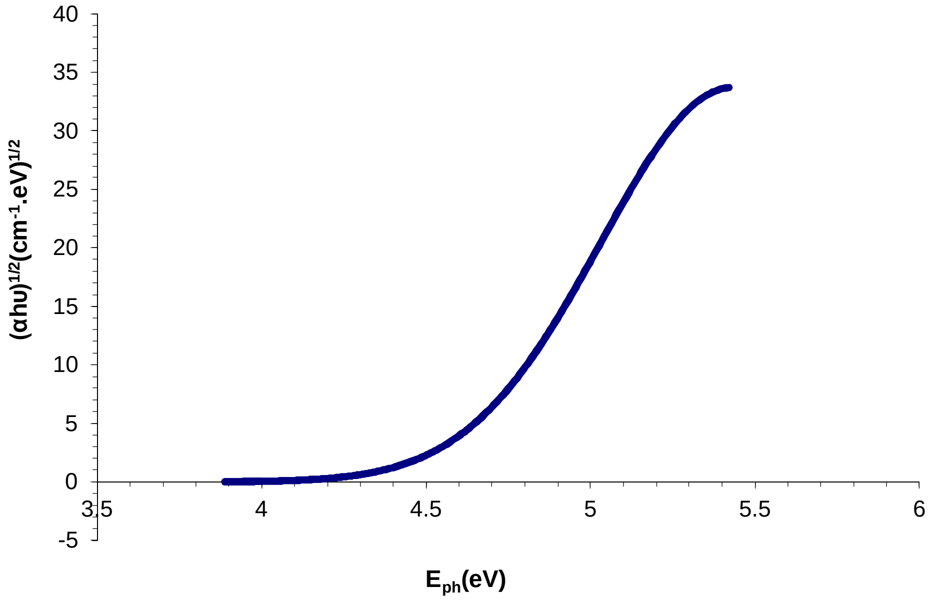

Figure 12: Variation of $(\alpha h\upsilon)^{1/2}$ for polymethylmethacrylate with photon energy.

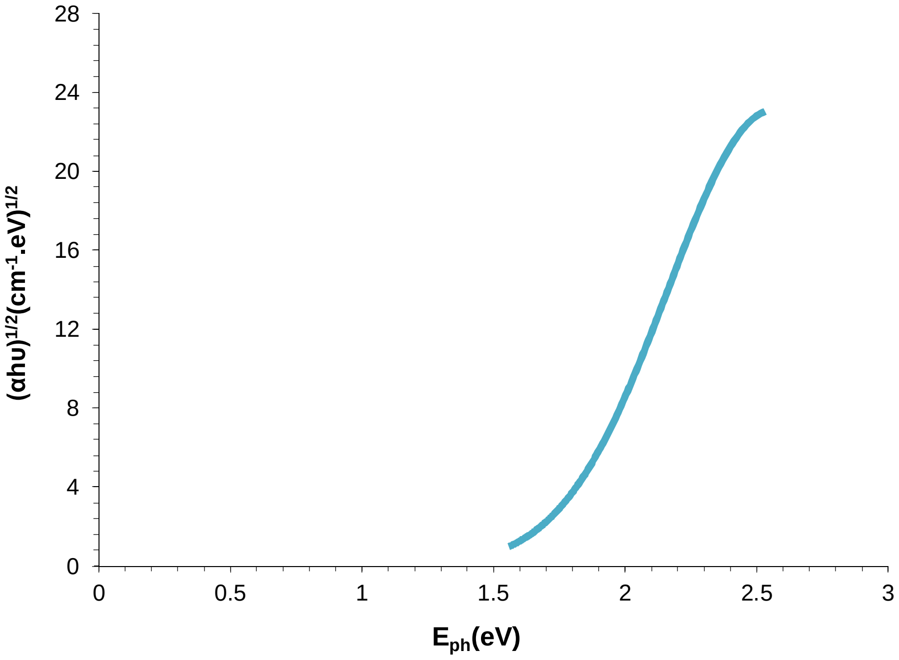

Figure 13: Variation of $(\alpha h\upsilon)^{1/2}$ for (PMMA-ZrO_2)nanocomposites with photon energy.

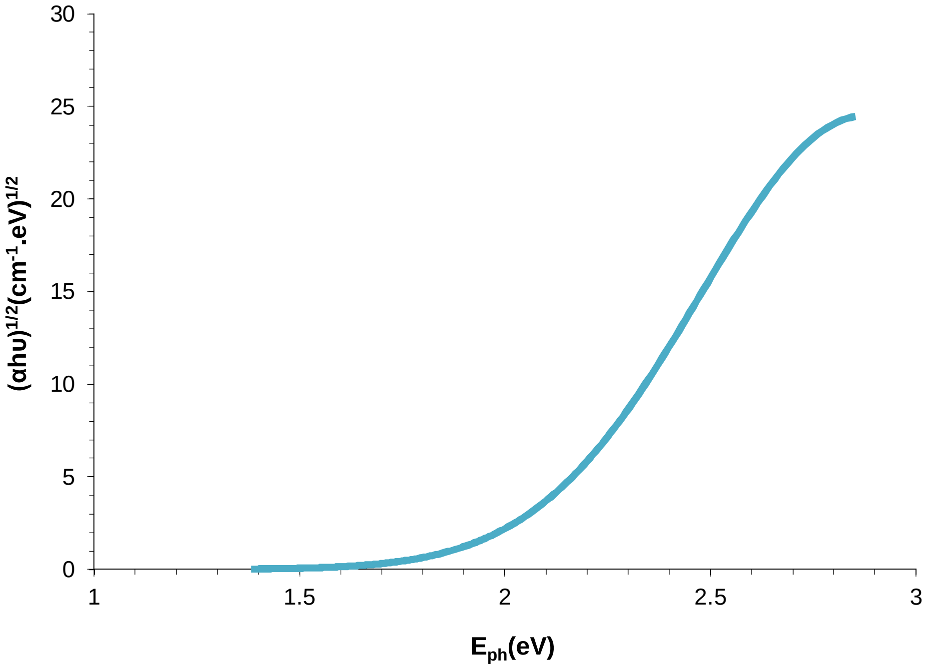

Figure 14: Variation of $(\alpha h\upsilon)^{1/2}$ for (PMMA- ZrO_2–Ag)nanocomposites with photon energy.

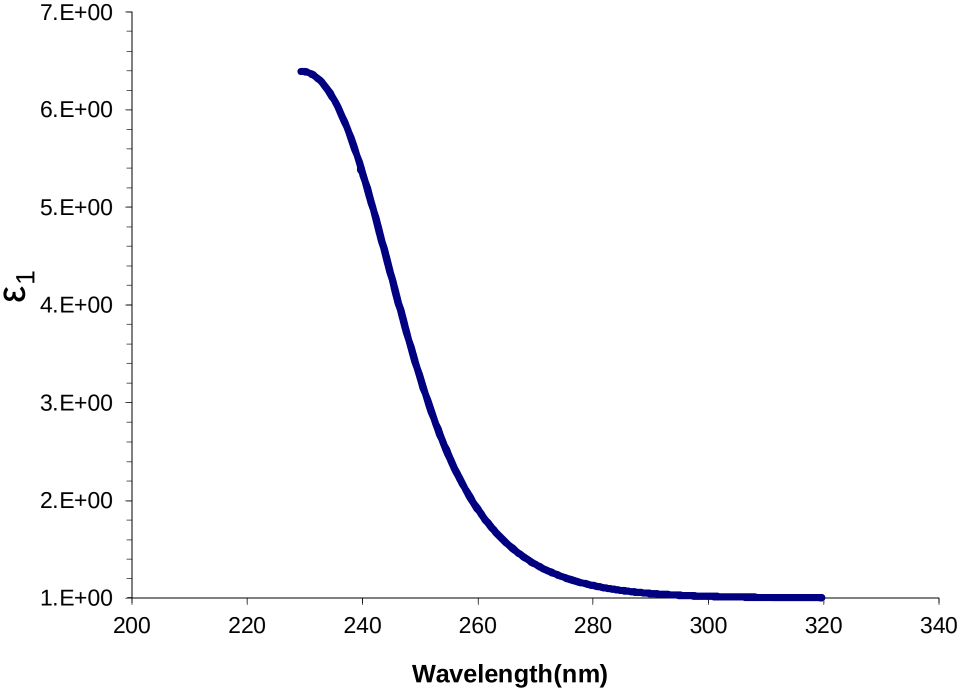

Figure 15: Real part of dielectric constant as a function of wavelength for pure PMMA.

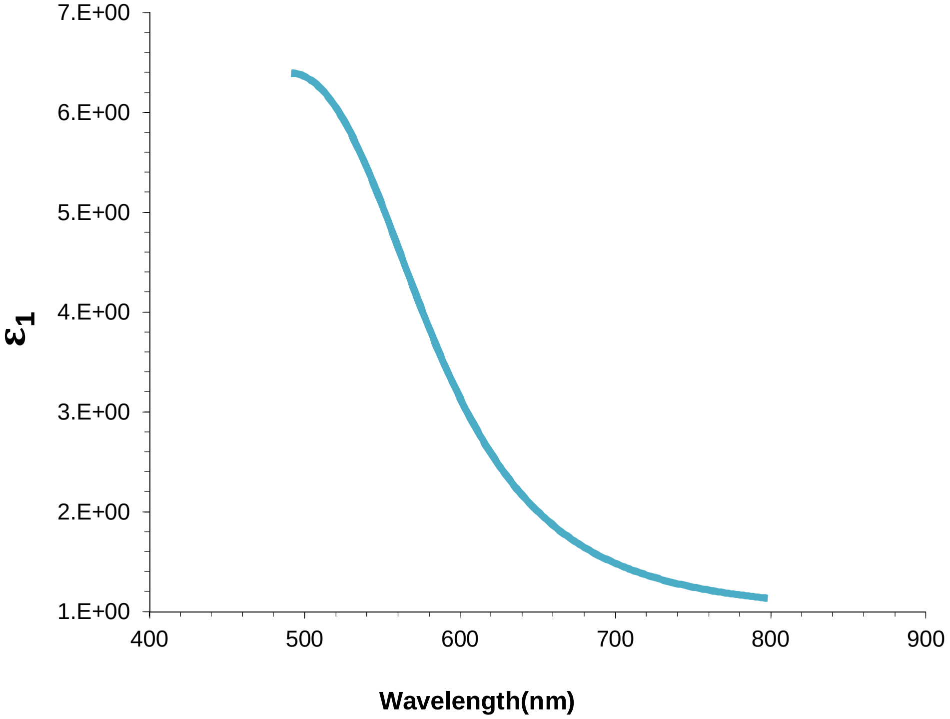

Figure 16: Real part of dielectric constant as a function of wavelength for (PMMA-ZrO2) nanocomposites.

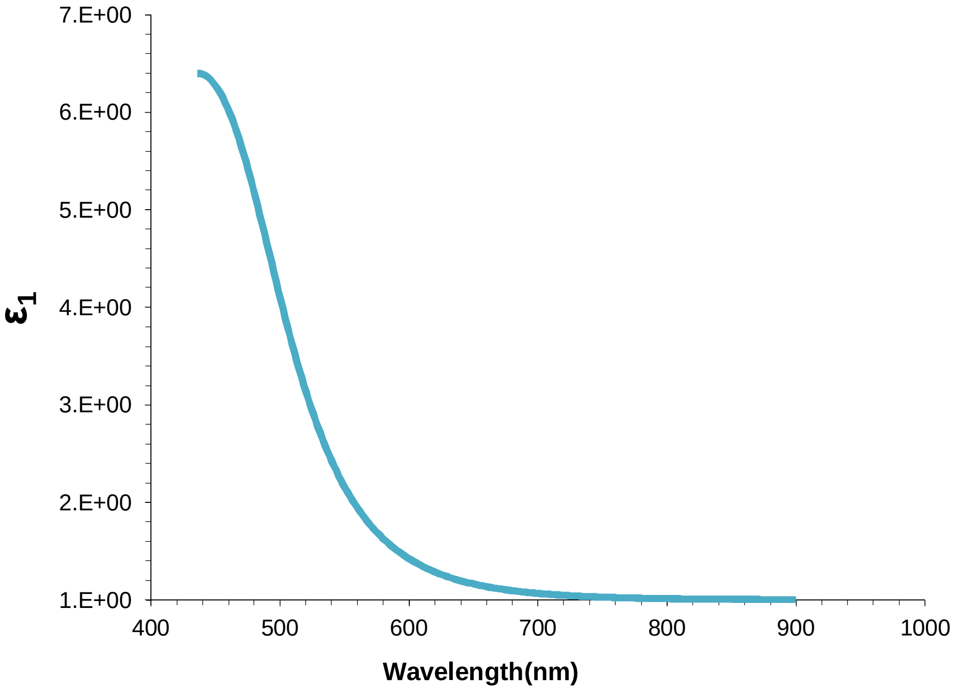

Figure 17: Real part of dielectric constant as a function of wavelength for (PMMA–ZrO_2-Ag) nanocomposites.

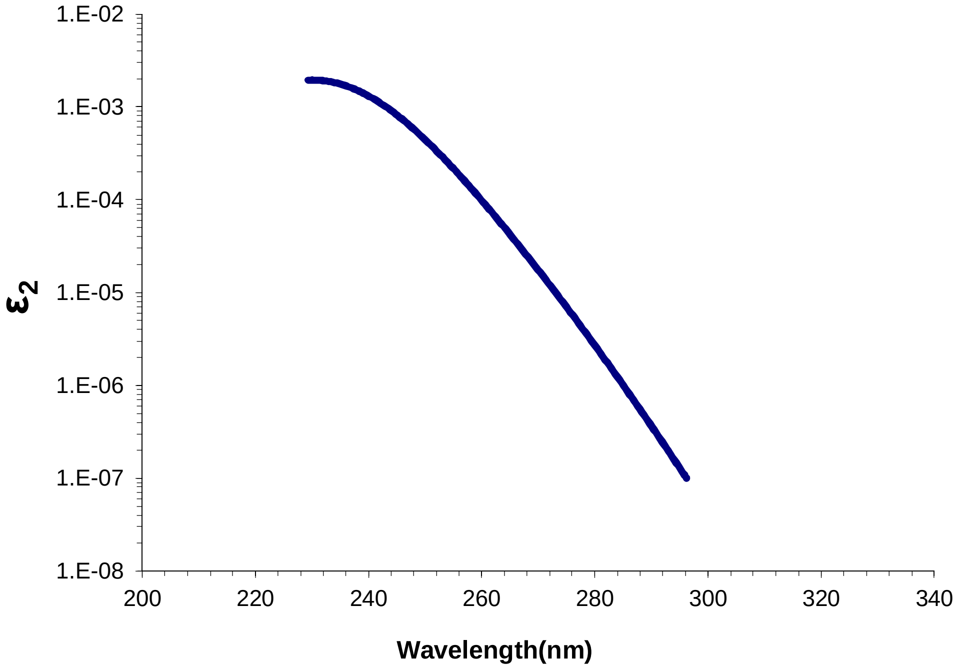

Figure 18: Imaginary part of dielectric constant as a function of wavelength for pure PMMA.

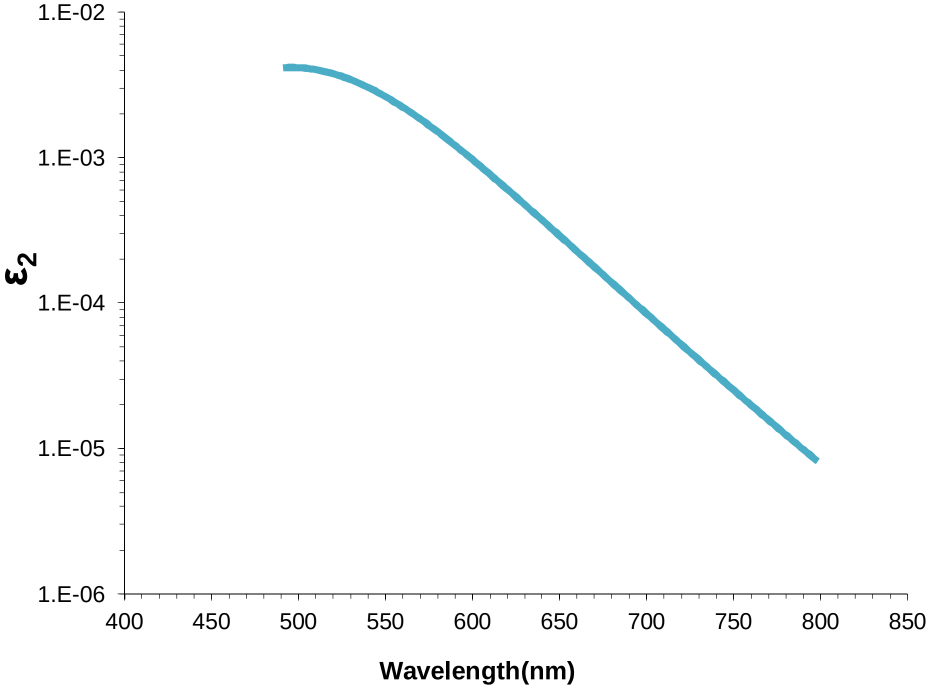

Figure 19: Imaginary part of dielectric constant as a function of wavelength for (PMMA-ZrO_2) nanocomposites.

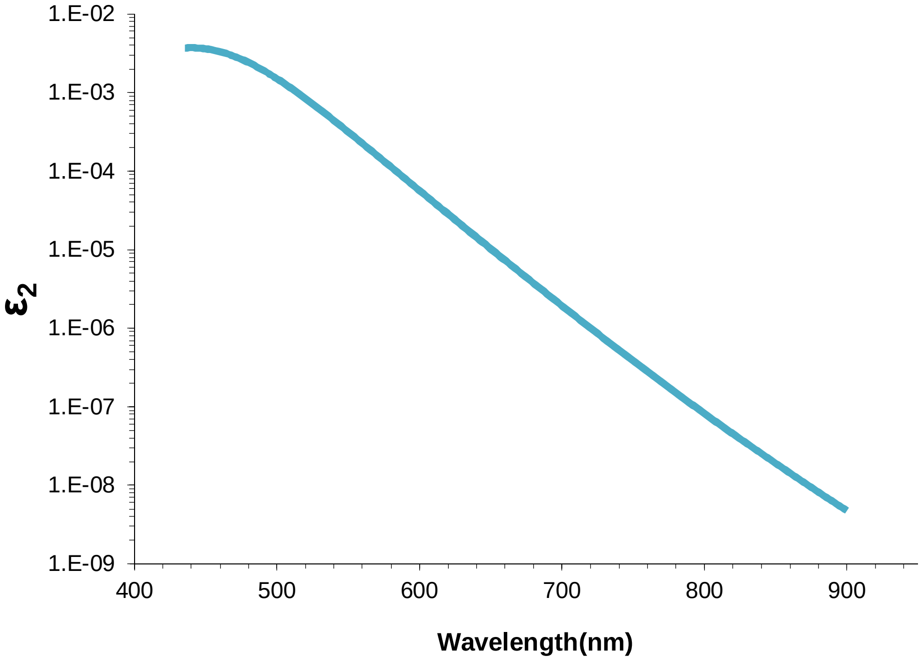

Figure 20: Imaginary part of dielectric constant as a function of wavelength for (PMMA-ZrO_2-Ag) nanocomposites.

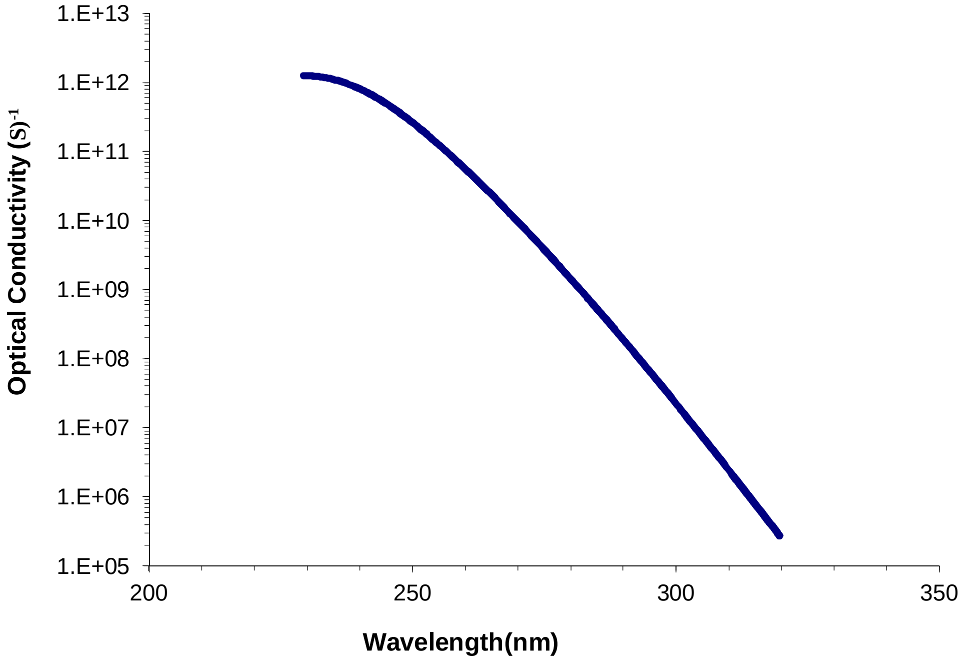

Figure 21: Variation of optical conductivity for pure (PMMA) with wavelength.

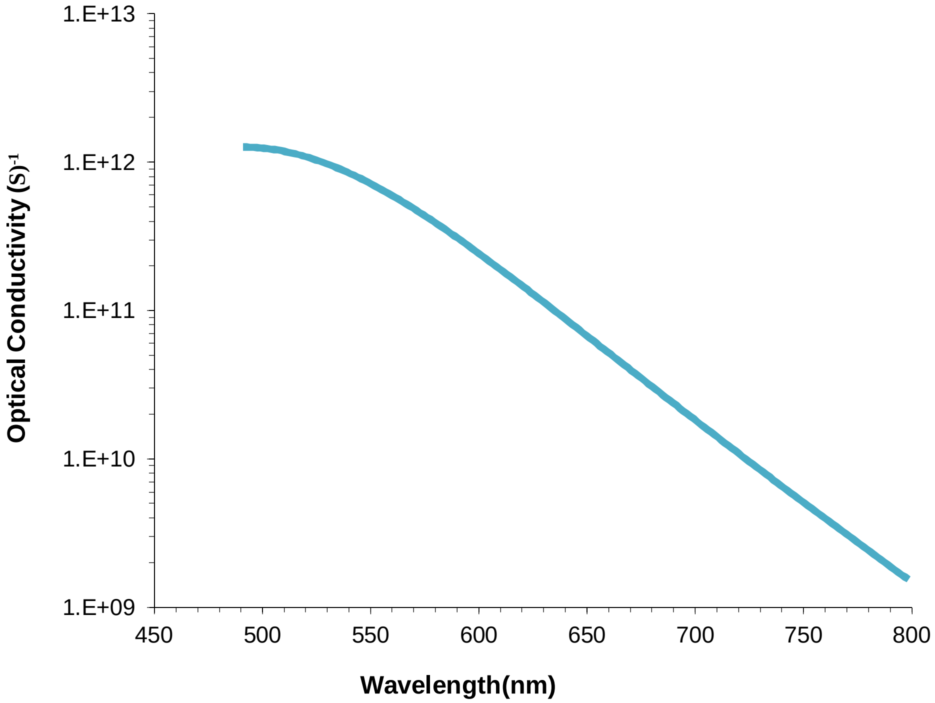

Figure 22: Variation of optical conductivity for (PMMA-ZrO2) nanocomposites with wavelength**.**

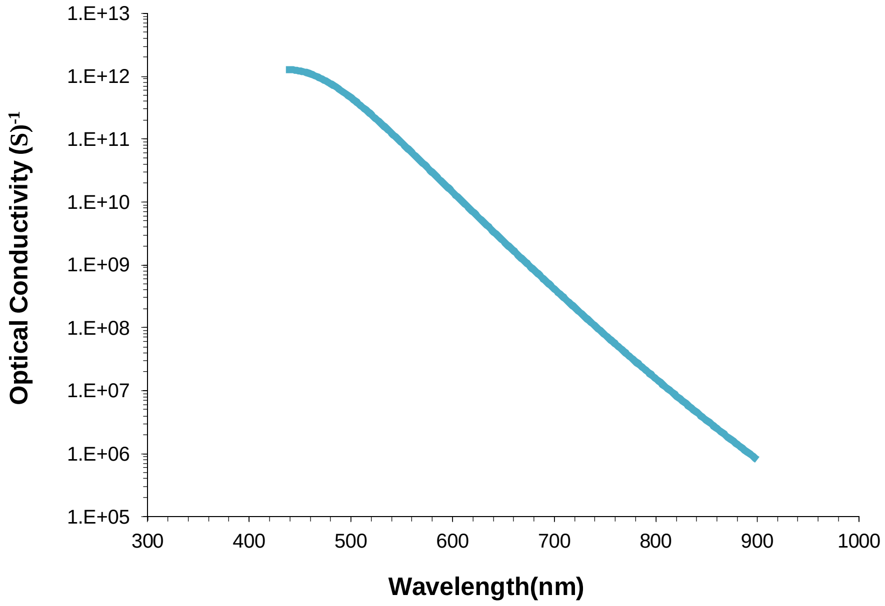

Figure 23: Variation of optical conductivity for (PMMA-ZrO_2-Ag) nanocomposites with wavelength.

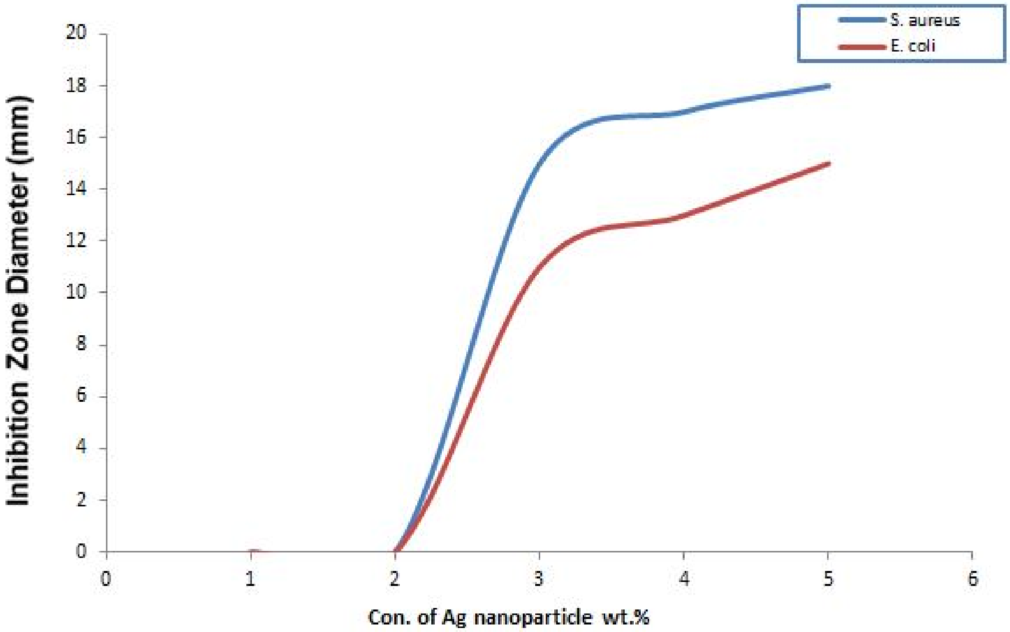

Figure 24: Antibacterial application of (PMMA-ZrO_2-Ag) as a function of Ag nanoparticles concentrations against E. coli and S. aureus.

Table 1: Shows some electronic variables of the pure PMMA and nanocomposites.

Materials	**H (eV)**	**S $(eV)^{-1}$**
PMMA	3.5049	0.1426
PMMA-ZrO_2	1.1658	0.4288
PMMA- ZrO_2-Ag	1.3555	0.3688