J Nanostruct 8(4): 359-365, Autumn 2018

RESEARCH PAPER

# Structural and Optical Properties of polyvinyl alcohol doped silver (PVA:Ag) film

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**ARTICLE INFO**

***Article History:***
*Received 18 July 2018*
*Accepted 16 September 2018*
*Published 01 October 2018*

***Keywords:***
*Density Functional Theory (DFT)*
*Optical Properties*
*Polyvinyl Alcohol*
*Silver*

**ABSTRACT**

The present paper investigates a detailed study on the optical properties of PVA/Ag nanocomposite films. In this interest, PVA/Ag nanocomposites with different ways of study, the first prepared film by reduction 0.2M of Ag+ ions in 2 gm of PVA and study the transmission absorption coefficient, refractive index, extinction coefficient, reflection, real & imaginary part of the dielectric constant and the energy gap. The results proved that the best values of the absorbency was within the range (350-500) nm, as well as for both we noticed an increase of the refractive index, the extinction coefficient and reflectivity with increasing energy, the second step of research was by using Density Functional Theory (DFT), It was calculate spectrum absorption, intensity and energy gap for the same compound PVA/Ag, The cooperation of polyvinyl alcohol (PVA) nanofibers with silver (Ag) nanoparticles (mean width 8nm) has been displayed utilizing thickness useful hypothesis (DFT) computations. The physical adsorption of PVA through the hydroxyl gathering, to the Ag, were calculated by using DFT theory.

**How to cite this article**
*Tahir KJ, Al-Yasari R. Structural and Optical Properties of polyvinyl alcohol doped silver (PVA:Ag) film. J Nanostruct, 2018; 8(4): 359-365. DOI: 10.22052/JNS.2018.04.005*

## INTRODUCTION

Polyvinyl alcohol (PVA) is a critical polymer, as a result of its one of a kind physical and concoction properties and it kept on pulling in numerous specialists, throughout the years [1]. This polymer can be made in powder, film and fiber shapes. It is a semi-crystalline polymer that emerges from the part of OH gathering and the hydrogen bonds [2-4]. It is likewise perceived as one of the not very many vinyl polymers solvent in water with a high straightforwardness and a decent adaptability. It is utilized modernly for emulsification, estimating and glues, in biomedical materials as medication conveyance framework and layers[5]. PVA can likewise be utilized as a part of therapeutic applications, for example, counterfeit veins, manufactured digestion systems, and contact lenses. It had been noted as a therapeutic material because of its similarity to the living body[6].

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Electrical properties of materials have for quite some time been of handy significance and hypothetical interest. It is surely understood that electric properties estimations are intense instruments to portray inorganic semiconductor doped on polymer nanocomposites which give data about electronic properties and demonstrate the relations amongst structure and electrical properties of nano composites[7]. In this worry, the polyvinyl liquor (PVA) polymer was picked as a host lattice because of the favorable position of its high mechanical quality, water dissolvability, great natural solidness and do pant [8]

subordinate electrical conductivity. Polyvinyl liquor (PVA) is a decent protecting material with low conductivity and low dielectric misfortune, and thus of significance to the microelectronics business, its electrical conductivity and charge stockpiling ability can be notably affected

by doping with Ag. The electrical and optical properties of polymers can be appropriately adjusted by the expansion of do gasp contingent upon their reactivity withthe host network[9]. Since Ag+ is a quick directing particle in a number of crystalline and shapeless materials, its fuse inside a polymeric framework will improve its electrical execution[10].

**PREPARATION**

In the study, PVA/Ag nanocomposite films were prepared. In this concern, 2.0 g of PVA is dissolved in 100 ml of de-ionized water with stirring at 80°C. The freshly prepared Ag solution 0.1 M was added drop wise in aqueous PVA with constantly blending for around 1 h to assurance the homogeneity of the arrangement. To balance out the PVA/Ag. The solution was discard to slide glass and left to dry at room temperature for 24 hours to dry film finally, the film is ready to test the necessary measurements, thickness of the film 1µm

**RESULT AND DISCUSSION**

The Optical properties of nanomaterials were investigated by using two methods: They are

*Optical properties by using spectrophotometer*

The absorption spectra in ultraviolet and visible regions (UV-Vis) emerge from electronic moves in the particles. The electronic absorption spectra of the explored tests have been recorded in the district from 190 to 1000 nm for PVA –Ag films. Fig. 1 exhibits UV- visible absorption spectra of film. From which, plainly a very nearly zero retention in the wavelength range 300 nm–1000 nm took after by an endless augmentation in the assimilation in the wavelength range 300 nm–450 nm with vicinity of absorption shoulder at 450nm. It is known that PVA-Ag films are clear and contains just single bond, thus, these lines it is required to retain.

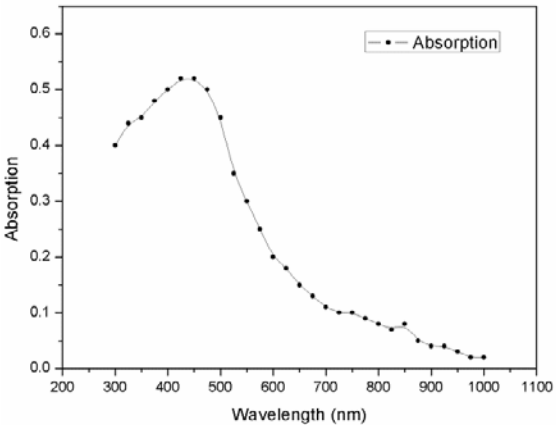


Fig. 1. Absorption spectrum of PVA-Ag film

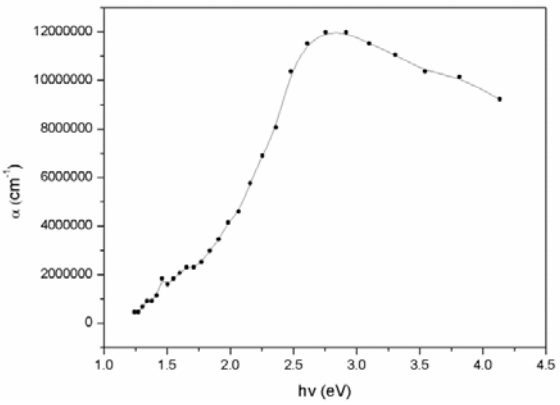


Fig. 2. Changed with the absorption coefficient and energy of the film

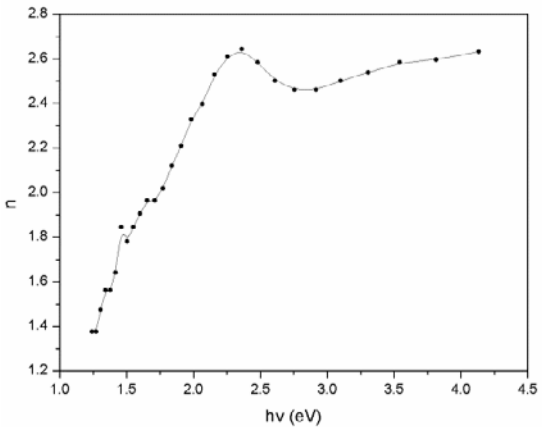


Fig. 3. Shows the changed refractive index as a function of photon energy incident of film

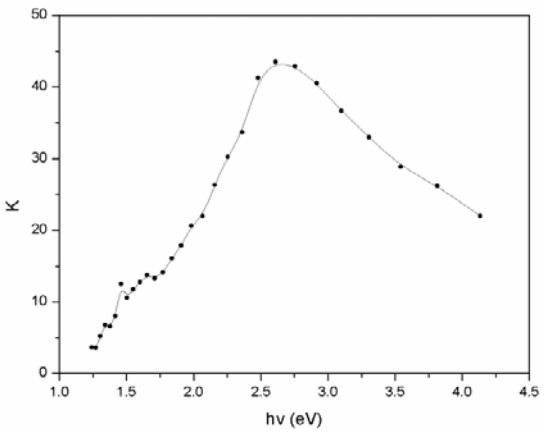


Fig. 4. Explains changed extinction coefficient as a function of photon energy of film

which is described as the relative rate of decreasing in light power. The ingestion coefficient α was processed from the equation[11]

$$\acute{a} = 2.303 * \frac{A}{t} \quad (1)$$

Where t is the thickness and A is absorption

Furthermore, the energy (hv) is calculated as well. Fig. 2 shows the relation between the absorption coefficient and energy.

The refractive index can characterized as a proportion between speed of light in vacuum (C), and speed inside the material. The estimation of refractive index (n) ascertained by equation [12].

$$n = \frac{\left(1 + R^{1/2}\right)}{\left(1 - R^{1/2}\right)} \quad (2)$$

Estimation of the extinction coefficient was done utilizing by means of equation [12]

$$K = \alpha\lambda / 4\pi \quad (3)$$

The relationship between the refractive index and the occurrence photon vitality appeared in Fig. 3.

In addition, the relationship between the extinction coefficient and the release photon energy is shown in Fig. 4.

*Optical Energy Gap*

The optical band gap which is the another feature of thin film was calculated from absorption coefficient data as a component of wavelength as given by [13];

$$\alpha (h\nu) = B(h\nu - Eg)^r \quad (4)$$

Where (r) is the power factor that determines the kind of transition and it can get the quantities 1, 2, 3, 1/2 and 3/2, depending on the method of the

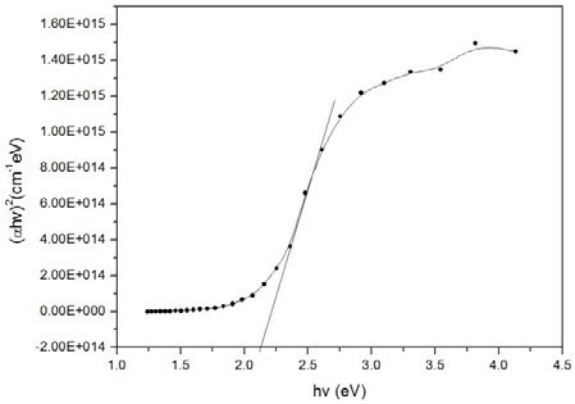


Fig. 5. $(\alpha h\nu)^2$ as a function of photon energy ($h\nu$) for films

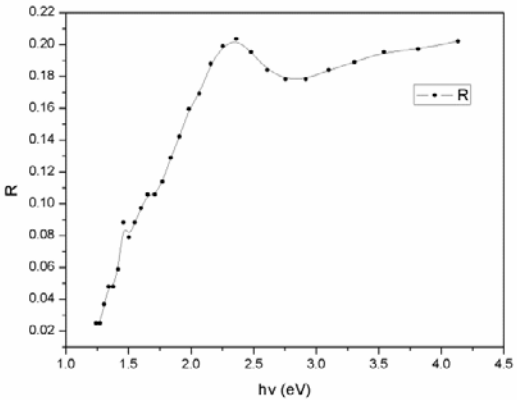


Fig. 6. explains changed of reflectivity as a function of photon energy to incident PVA-Ag film

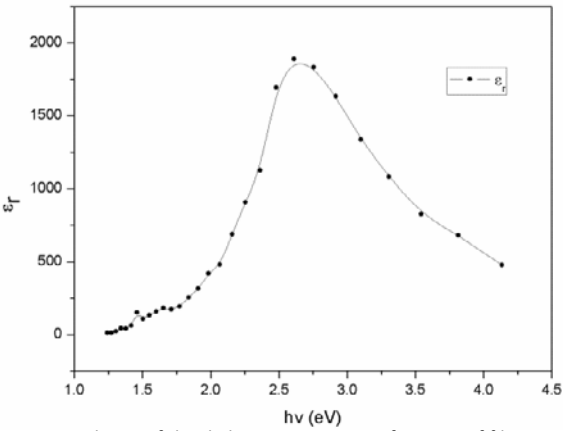


Fig. 7. real part of the dielectric constant as function of films.

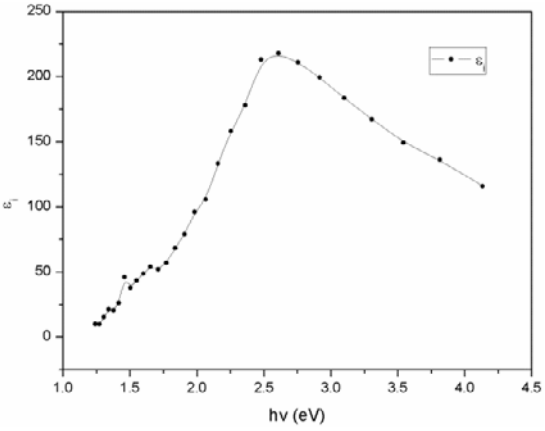


Fig. 8. Imaginary part of the dielectric constant as function of films.

electron moves that is responsible for the optical retention. It is necessary to understand that (r) can get the value of 1/2 in case of direct electronic transition transversely over direct energy gap in the k space. However, (r) takes the value 2, if there should be an occurrence of indirect electronic transition crosswise over roundabout energy gap. Both of the direct and indirect transtions happen and can be seen by plotting $(\alpha hv)^{2}$ and $(\alpha hv)^{1/2}$ versus photon vitality (hv).

Fig. 6 shows the plot of the $(\alpha hv)^2$ as a function of photon energy (hv), The energy gap was computed of the evaluating of the erect partition as show in figure below

The Fig. 5 shows energy gap around the range 2.1 eV. Also, The reflection spectrum of the films has been calculated by equation below [14].

$$R = 1 - A - T \quad (5)$$

Fig. 6 shows reflection curves against photon energy.

Additionally, dielectric constant was calculated from the real part by the equation (6) as following [15]

$$\dot{o}_r = n^2 - K^2, \quad \dot{o}_i = 2nK \quad (6)$$

Where (n) is the refractive index of the films and (k) is the extinction coefficient,

*Density Functional Theory (DFT)*

DFT is a computational quantum mechanical modeling method used in physics, chemistry and materials science to investigate the electronic structure and optical properties . It involves using the probability density functions of the electrons in a molecule to determine other properties of the molecule. Instead of solving problems with wave equations for each electron it uses the probabilities of electrons being at different locations. Ways applied in the Gaussian 09 group of agenda. The atomic properties of the mixes have been processed by DFT exploit the bench mark 6-31G (d,p) basic erect. The produced devoir B3LYP has appeared to be very fruitful for estimation the electronic properties, for example, ionization possibilities, electronic states and energy gab. The DFT allotment the electronic vitality as, where, and are the electronic active vitality, the electron vague fascination and electron-electron aversion headwords separately

The results of calculation gave energy gap of model which values are; Eg=5.157573 eV, 5.055804 eV, 7.247922 eV, and 7.25282 eV.

In this investigation, it can be seen that the solvent in water has a small effect on energy gap.

All these properties and calculations were figured by utilizing Gaussian 09 program, and Gaussian perspective 5.08 system is depending on (DFT) technique with premise set B3LYP/3-21G, while UV-VIS spectrum is computed by TD-DFT method.

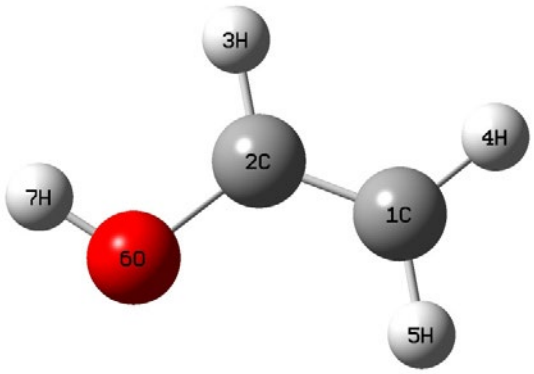


Fig. 9. Optimized structures of polyvinyl alcohol molecule using B3LYP/(6-31G)

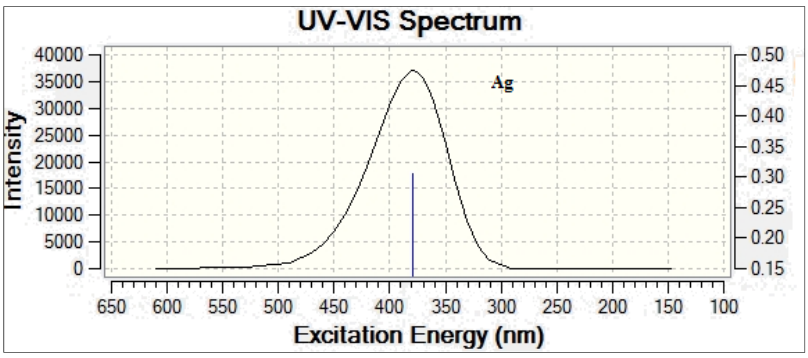


Fig. 10. UV-VIS spectra of Ag molecule using B3LYB /6-31G method

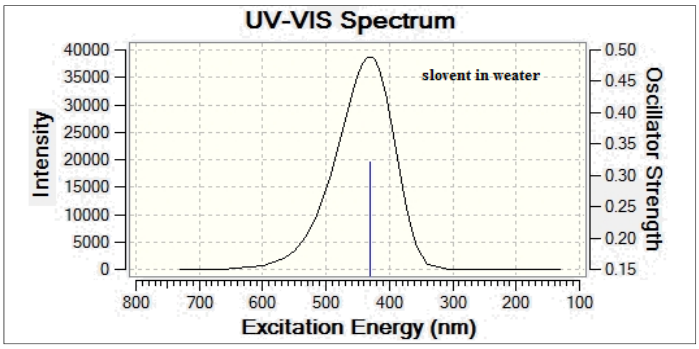


Fig. 11. UV-VIS spectra of Ag molecule solvent in water using B3LYB /6-31G method

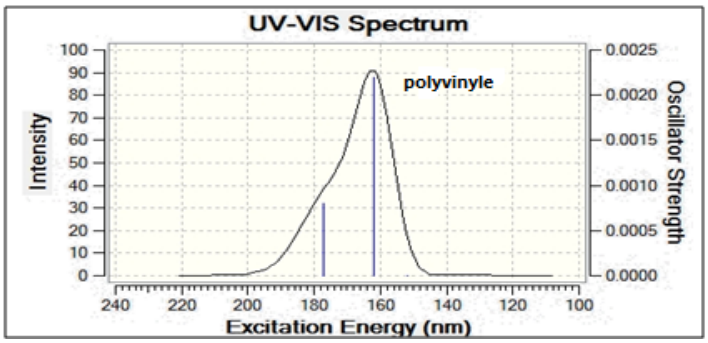


Fig. 12. UV-VIS spectra of polyvinyl molecule using B3LYB /6-31G method

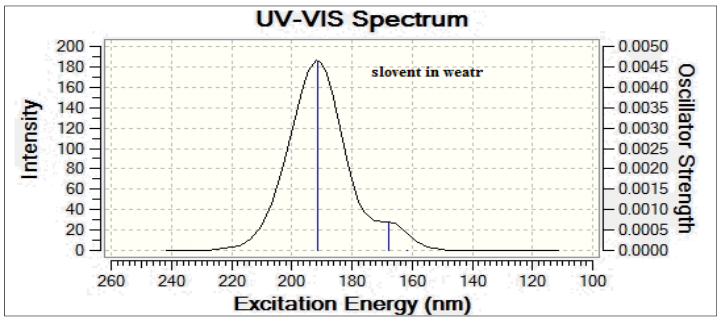


Fig. 13. UV-VIS spectra of polyvinyl molecule solvent in water using B3LYB /6-31G method

The UV-VIS spectra of silver molecule, silver molecule solvent in water, polyvinyl alcohol and polyvinyl alcohol solvent in water are shown in Figs. 9-12 respectively.

Figs. 9-12 show the harmonic vibrational frequencies and solvents effect for silver and polyvinyl alcohol, where they were calculated by using TD-DFT/ B3LYP level with 6-31G basis set. DFT theory has been used to determine the first three low-lying excited states of the UV-VIS absorption spectra of the silver and polyvinyl alcohol, as well as the effect of water on the these frequencies . For pure silver, it is found at band (378.86) nm, while for silver solvent in water is found to be at (430.76) nm respectively. On the other hand, polyvinyl alcohol it is found at range (177.23) nm and (162.05) nm respectively, while solvent in water is at wavelength (167.77) nm and (191.56) nm. Consequence, the water leads to increase the values of UV-VIS spectra for silver and polyvinyl alcohol comparing to the original models.

## COMPUTATIONAL DETAILS

All properties are computed by utilizing Gaussian 09 system, Gaussian perspective 5.08 project is utilizing (DFT) technique with premise set

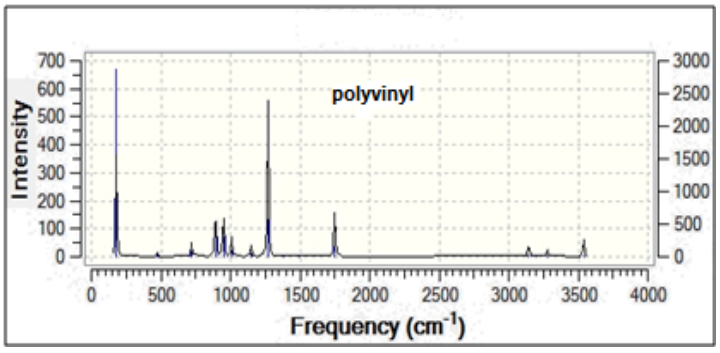


Fig. 14. Calculated IR spectra of polyvinyl molecule using B3LYB /6-31G method

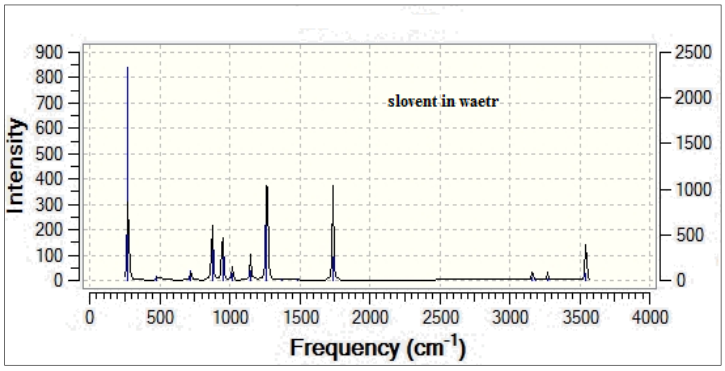


Fig. 15. Calculated IR spectra of polyphenel molecules solvent in water using B3LYB /6-31G method

B3LYP/3-21G, while UV-VIS spectrum is computed by TD-DFT method [16].

The produced devoir B3LYP was used to be very effective for computation the electronic properties, such ionization possibilities, electronic states and energy gaps [17].

## CONCLUSION

In synopsis, we have effectively incorporated silver nanoparticles-doped polyvinyl alcohol films. The silver particles are detached and exceptionally scattered from each other and the molecule bulk was effortlessly controlled. It has been observed that the concentration of sliver nanoparticles has greatly influenced the electrical and optical properties of PVA. The characterization of thin films (1µm thickness) was carried out by UV-VIS. Spectrophotometer and Density Functional Theory (DFT).

## CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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