

Optical Characteristics and Antibacterial Activity of PVA/ZnO Nanocomposites

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ABSTRACT

The process of solution casting was used to create nanocomposites with different amounts of Zinc Oxide nanoparticles (0.001, 0.002, 0.003, 0.004 and 0.005)g. The structural and optical properties of PVA/ZnO nanocomposites were examined. Scanning electron microscopy (SEM) of (PVA/ZnO) nanocomposite films at 0.003 g and 0.005 g shows ZnONPs appear to form groups and disperse well; for the quantity of ZnONPs to (PVA) polymer, it forms varied shapes in specific areas inside the polymer. UV-Visible spectroscopy was utilized to measure the optical properties in the (200-900) nm wavelength range. Experiments have shown that increasing the amount of ZnONPs in nanocomposites enhances the absorbance spectrum and absorption coefficient of PVA polymer. The energy band gap of PVA polymer decreased as the amount of ZnONPs grew. In a research of the antibacterial activity of these nanocomposites, pathogen microorganisms such as Staphylococcus aureus, Staphylococcus epidermidis, Escherichia coli, Klebsiella simlipneumoniae, and Candida albicans were utilized. According to the findings, the chemical nature and shape of the composites have a substantial impact on antibacterial activity, with antibacterial activity increasing as the amount of Zinc Oxide rise.

Keywords: Antibacterial Activity, Nanomaterials, Optical Properties, Zinc Oxide.

1. INTRODUCTION

Overuse of standard antibiotics has resulted in the creation of novel bacteria strains with increasing levels of resistance, posing a hazard to public health. Efforts from a range of scientific fields have been attempted to identify solutions that may help to reduce the problem. In this context, new bactericidal materials research has become a current and critical priority in materials science (1). Metal nanoparticles are combined with a polymer matrix to form nanocomposites. The potential benefits of these components can be combined to generate a material with enhanced optical, electrical, mechanical, and antibacterial properties. The two components of the composite have been associated to a significant increase in antibacterial activity. As a result, the polymer not only serves as a solid matrix for nanoparticles, but it also has the potential to boost antibacterial activity, there by increasing the material's applications in biomedicine, water purification, and agribusiness(2). Among the many polymer materials, Poly (vinyl alcohol) (PVA) are decomposable, biocompatible, non-toxic, synthetic polymers that are easy to deal with and offer biomedical, engineering, and technological applications. These polymers are soluble in water and form highly transparent films when solution-casting. PVA film has excellent properties such as high elasticity and flexibility, as well as good chemical resistance and thermal stability (3). Zinc Oxide is one of the most extensively used metal oxide nanomaterials due to its excellent chemical and

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physical properties. ZnO is frequently used in nanomedicine and daily products such as plasters and cosmetics due to its excellent adhesion and UV absorption properties. ZnO also possesses antibacterial and antimicrobial properties, making it a popular nanomedicine material (4). It is feasible to use nanocomposite to create new materials. To create antimicrobial nanocomposites, antibacterial nanoparticles can be combined with a polymeric matrix that already has antibacterial properties. It has been used safely in a wide range of therapeutic applications, including medications, body creams, and pharmaceuticals (5-7)

According to P. M. Narayanan *et al.* (8), one of the most important areas of nanotechnology nowadays is the development of reliable techniques for the production of Zinc Oxide nanoparticles. Zinc Oxide nanoparticles are widely known for their inhibitory and antibacterial activities. Antimicrobial resistance and *Candida albicans* among pathogenic microorganisms has recently become a major public health concern. The current study is focused on the synthesis, characterization, and application of zinc oxide nanoparticles as an antibacterial agent.

S. Gautam *et al.* (9), Antibiotic resistance is a major public health and food security issue. Because of the rising frequency and spread of antibiotic-resistant harmful microorganisms, antimicrobial packaging has emerged as a feasible solution. PVA, a synthetic polymer that is soluble in water, is being investigated as a potential biocompatible, biodegradable, low-substance cytotoxic material for a number of medicinal, industrial, and commercial applications. To widen its applications, graphene oxide (GO) was doped into polymer material and silver nanoparticles (Ag).

B. Abebe *et al.* (10), Metal oxide nanoparticles are one of the most popular active antibacterial materials. ZnO is a new antibacterial active material with a unique electrical arrangement and appropriate characteristics. Researchers are now working hard to increase ZnO antibacterial properties by building a composite using the same or other bandgap semiconductor materials and ion doping.

The goal of this study was to determine how incorporating Zinc Oxide nanoparticles into PVA/ZnO nanocomposites altered their structural, optical, and antibacterial properties.

2. THEORETICAL PART

The term "absorbance" refers to the ratio of the materials intensity of absorbed light (I_A) to the intensity of incident light (11).

$$A = \frac{I_A}{I_0} \quad (1)$$

The following equation gives the absorption coefficient (12).

$$\alpha = 2.303 \frac{A}{d} \quad (2)$$

where A denotes absorbance, the sample thickness is denoted by d.

The following equation was used to get the energy band gap(13).

$$\alpha h\nu = B(h\nu - E_g)^r \quad (3)$$

B is the constant in this equation, $h\nu$ is the photon energy, E_g is the optical energy gap amongst the valence band and the conduction band, r is the power that characterizes the transition process. r for the designated transitions as

direct allowed, direct forbidden, indirect allowed and indirect forbidden respectively, numbers 1/2, 3/2, 2 or 3 can be used.

3. EXPERIMENTAL WORK

Poly (vinyl alcohol) (PVA) is a powder, light-white solid polymer when it is pure. Figure(1) depicts the structure of PVA(14). Molecular weight $M_w=14000\text{g/mole}$, a melting point of 230°C and glass transition 100°C . The cast technique was used to generate films of pure PVA and PVA containing ZnO nanoparticles. By dissolving 0.5 g of PVA with (0.001, 0.002, 0.003, 0.004, 0.005)g of Zinc Oxide nanoparticle (particle size 80nm provided from China) in 15ml of water that's been distilled at room temperature, stirred for 3–4 hours with a magnetic stirrer (hot plate) in a temperature range of $(25\text{-}35)^\circ\text{C}$ to ensure that the PVA/ZnO films were dissolved completely. To get homogenous films, pour the solution into a glass plate with a diameter of 3 cm, allow gently for 3 to 4 days for the liquid to evaporate at room temperature. The absorption spectra were examined using a UV-Visible spectrophotometer (T70/T80 series UV/Vis spectrometer) in the wavelength range (200-900)nm. The films thickness was measured using a digital micrometer type (Tesda) (0.001mm) measuring precision of the (0-150) mm measurement range manufactured in Japan. Pure PVA and PVA/ZnO nanocomposite films studied using high-resolution scanning electron microscopy (ZEISS SIGMA VP Field Emission Scanning Electro). The microbiology lab at Mustansiriyah University Department of Biology, College of Science, contributed gram-positive (*Staphylococcus aureus*, *Staphylococcus epidermidis*) and gram-negative (*Escherichia coli* and *Klebsiella sp.*) bacterial cultures, as well as *Candida albicans*. Using diffusion methods in agar wells, this experiment was conducted in sterile petri- dishes with a diameter of 90 mm and sterile nutritional agar material. For bacteria and fungi, the diameter of the inhibitory zone (mm) was measured after 24 hours of incubation at 25°C .

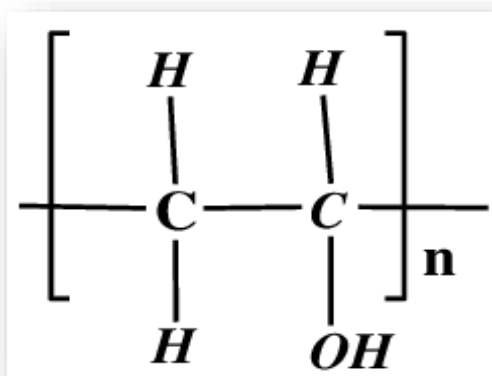


Figure1. Polyvinyl alcohol chemical structure(14).

4. RESULTS AND DISCUSSION

4.1 SEM Analysis

Figure(2) illustrates typical SEM images of (PVA, ZnONPs and PVA/ZnONPs). ImageA and B depicts pure PVA polymer and pure ZnONPs. ZnONPs the

particles are spherical and granular nature, with a step-by- step rise as a proportion of polymer nanoparticles as shown in Figure 2(C,D) resulting in surface morphological change. The white specks are ZnO nanoparticles, while the black backdrop is PVA film. The ZnO nanoparticles are observed to have varied forms in some locations that occur throughout the matrix, which are spread irregularly in the PVA matrix and occupy spaces between molecules.

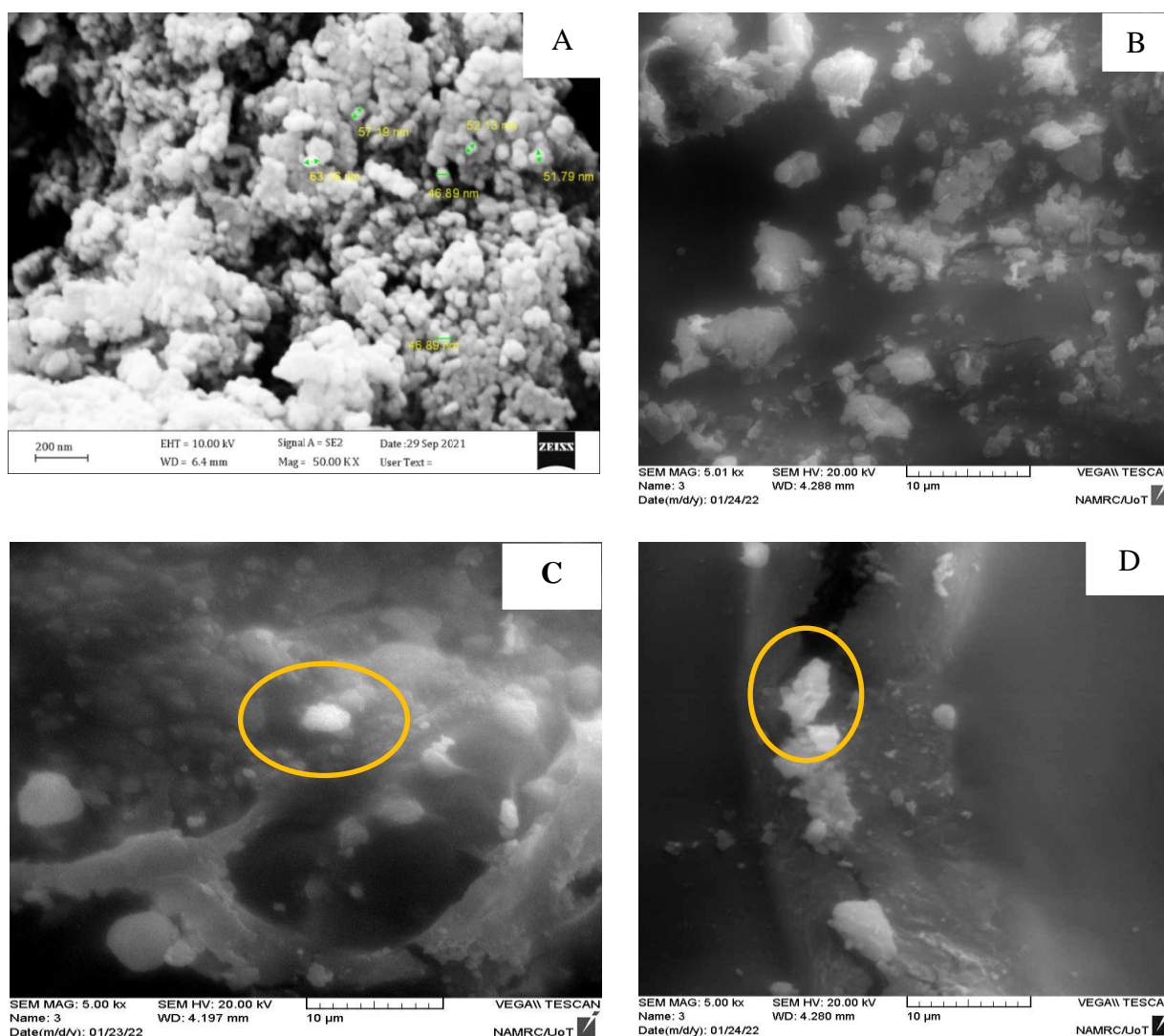


Figure 2. SEM images for (A) pure ZnONPs, (B) pure PVA polymer, (C) PVA/ZnONPs 0.003g (D) PVA/ZnONPs 0.005g

4.2 Optical Properties

The optical characteristics of polymer and nanocomposite films were investigated using the UV-Vis absorption spectroscopy method. The absorption spectra of pure PVA and PVA/ZnO nanocomposite films are shown in Figure (3). Pure PVA peak of absorption was measured at a wavelength of 250 nm a broad absorption band. This band was formed because of semicrystalline structure of PVA. Another explanation the existence of un-hydrolyzed acetate group and carbonyl structure containing which was associated with polymer matrix of

PVA. These bands were in accordance with electronic transitions $n-\pi^*$, $\pi-\pi^*$, respectively(15). Optical absorption spectrum of PVA/ZnO nanocomposite films display two bands at 280 nm and at 370nm with a reduced intensity which corresponded to the ZnO is present in the film. These bands were referred to as PVA absorption and ZnO nanoparticle excitons. The UV absorption spectrum demonstrates this, the greater the amount of ZnO in the matrix of PVA, the greater the absorbance of PVA host in the ultraviolet-visible range. Consequently, the absorption edge shifted across the lower energy or longer wavelength associated with the blue-green range of the visible spectral region with rising amount of the nanosize ZnO particle(16).

Table 1 Show highest peak in the absorption spectrum PVA/ZnO

Samples	Wavelength(nm)	Absorbance
pure PVA	280	0.128
PVA/ZnONPs (0.001g)	280	0.475
	370	0.437
PVA/ZnONPs(0.002g)	280	0.528
	370	0.437
PVA/ZnONPs(0.003g)	280	0.67
	370	0.617
PVA/ZnONPs(0.004g)	280	0.736
	370	0.784
PVA/ZnONPs(0.005g)	280	0.829
	370	0.855

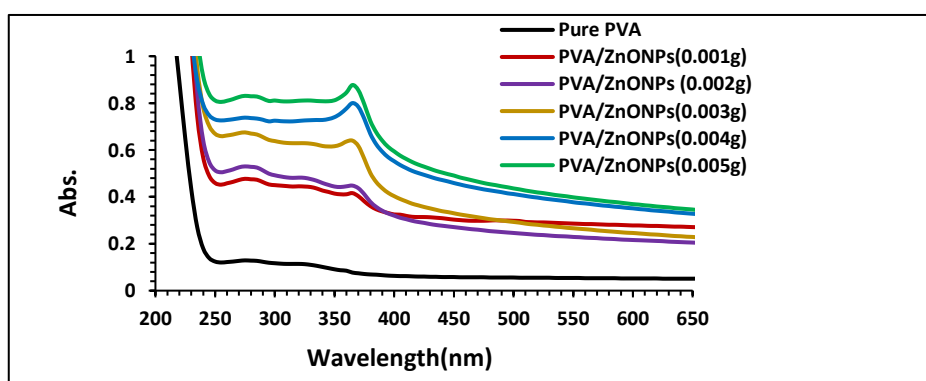


Figure3. Absorption spectrum of pure PVA and PVA/ZnO nanocomposite films

Absorption coefficient (α) is a distinctive attribute of every absorber molecule ion. It is a term that describes a substances ability to absorb light with a specific wavelength per

unit length. The absorption coefficient may be calculated using equation (2)(17). Figure (4) demonstrates the plot absorption coefficient vs incident photon energy PVA polymer with various amounts of ZnONPs. It shows that the energy absorption is low, implying that electron transitions are low. At high energies, absorption increases dramatically, indicating that electron transitions are likely. Increased additive ZnONPs increases the absorption coefficient of PVA/ZnO nanocomposites. The absorption coefficient has the benefit of concluding the type of the value of transition electrons the absorption coefficient is large direct electrons transitions are expected at greater energies. Before photons and electrons, it is possible to achieve momentum and energy conservation, if the expected indirect transition of electrons is reduced and the absorption coefficient is reduced. It is only through phonons that momentum is conserved. The measurements show that the absorption coefficient for PVA/ZnO nanocomposites is lower than (10^4cm^{-1}), suggesting that it contains an indirect energy band(18).

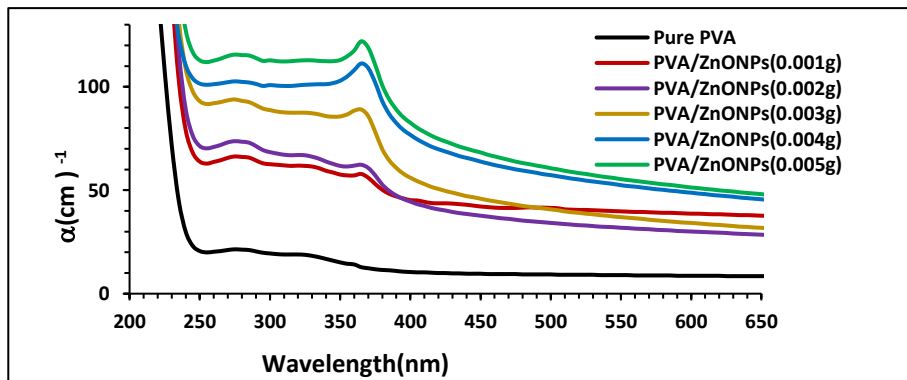


Figure4. Absorption coefficient for PVA/ZnO nanocomposite films

The optical energy band gap is the measure optical energy band gap required to improve the electronic band structure a material for film. Figure (5) shows amount of ZnONPs in the nanocomposites affects the energy band difference. Differences in energy band gap decreases as nanoparticle concentration indicated in Table(2) rises. An increases in localized levels of forbidden energy band gap cause in reduces energy gap value (18). PVA has an energy band gap of 4.92eV and when the amount of ZnO nanomaterial increases the energy band gap gradually decreases until it reaches 4.47ev.

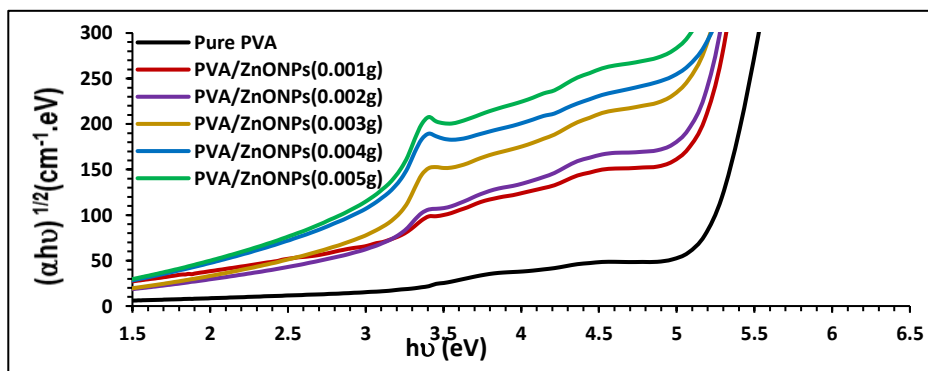


Figure5. Optical energy gap for PVA/ZnO nanocomposite film

Table2 Energy gap (E_g) for PVA/ZnO nanocomposite films

Sample	Energy gap(eV)
Pure PVA	4.92

PVA/ZnONPs(0.001g)	4.83
PVA/ZnONPs(0.002g)	4.74
PVA/ZnONPs(0.003g)	4.65
PVA/ZnONPs(0.004g)	4.56
PVA/ZnONPs(0.005g)	4.47

4.3 Antibacterial Activity

Pure PVA polymer and PVA/ZnO nanocomposites solutions have antibacterial properties. During the agar plate method, researchers test against positive bacteria (*Staphylococcus aureus*, *Staphylococcus epidermidis*), negative bacteria (*Escherichia coli*, *Klebsiella sp.*) and fungus (*Candida albicans*). The outcomes are given in Table (3). In most samples, positive bacteria (*Staphylococcus aureus* and *Staphylococcus epidermidis*) demonstrated stronger antibacterial activity than negative bacteria (*Escherichia coli* and *Klebsiella sp.*) and fungi (*Candida albicans*). The samples (pure PVA and PVA/ZnO 0.001g) do not show an effect on (*Staphylococcus aureus*, *Staphylococcus epidermidis*), respectively. Also, the sample (PVA/ZnO 0.002g) exhibit an effect of (11, 16mm) on *Staphylococcus aureus*, *Staphylococcus epidermidis*, respectively. From the samples (PVA/ZnO 0.003g) revelation an effect of (11,18mm) on *Staphylococcus aureus*, *Staphylococcus epidermidis*). The sample (PVA/ZnO 0.004g) demonstration an effect of (11,19mm) on *Staphylococcus aureus*, *Staphylococcus epidermidis*). The sample (PVA/ZnO 0.005g) show an effect of (11,21mm) on (*Staphylococcus aureus*, *Staphylococcus epidermidis*). All samples; pure PVA, PVA/ZnO (0.001, 0.002, 0.003, 0.004, 0.005)g do not illustrate an effect on *Escherichia coli*, *Klebsiella sp.*, *Candida albicans*) respectively. The capability of nanoparticles to prevent the growth of microbes is not fully known, although it is believed that DNA damages cellular proteins and loses its ability to reproduce(19). Figure 6 the antibacterial activity of the PVA and PVA/ZnO nanocomposite

Table3 Antibacterial activity of PVA polymer and PVA/ZnO nanocomposite against various pathogenic bacterial strains

Samples	Clear zone of inhibition (mm)				
	<i>Staphylococcus aureus</i>	<i>Staphylococcus epidermidis</i>	<i>Escherichia coli</i>	<i>Klebsiella sp.</i>	<i>Candida albicans</i>
pure PVA
PVA/ZnO (0.001g)
PVA/ZnO (0.002g)	11	16
PVA/ZnO(0.003g)	11	18
PVA/ZnO (0.004g)	11	19

PVA/ZnO (0.005g)	11	21
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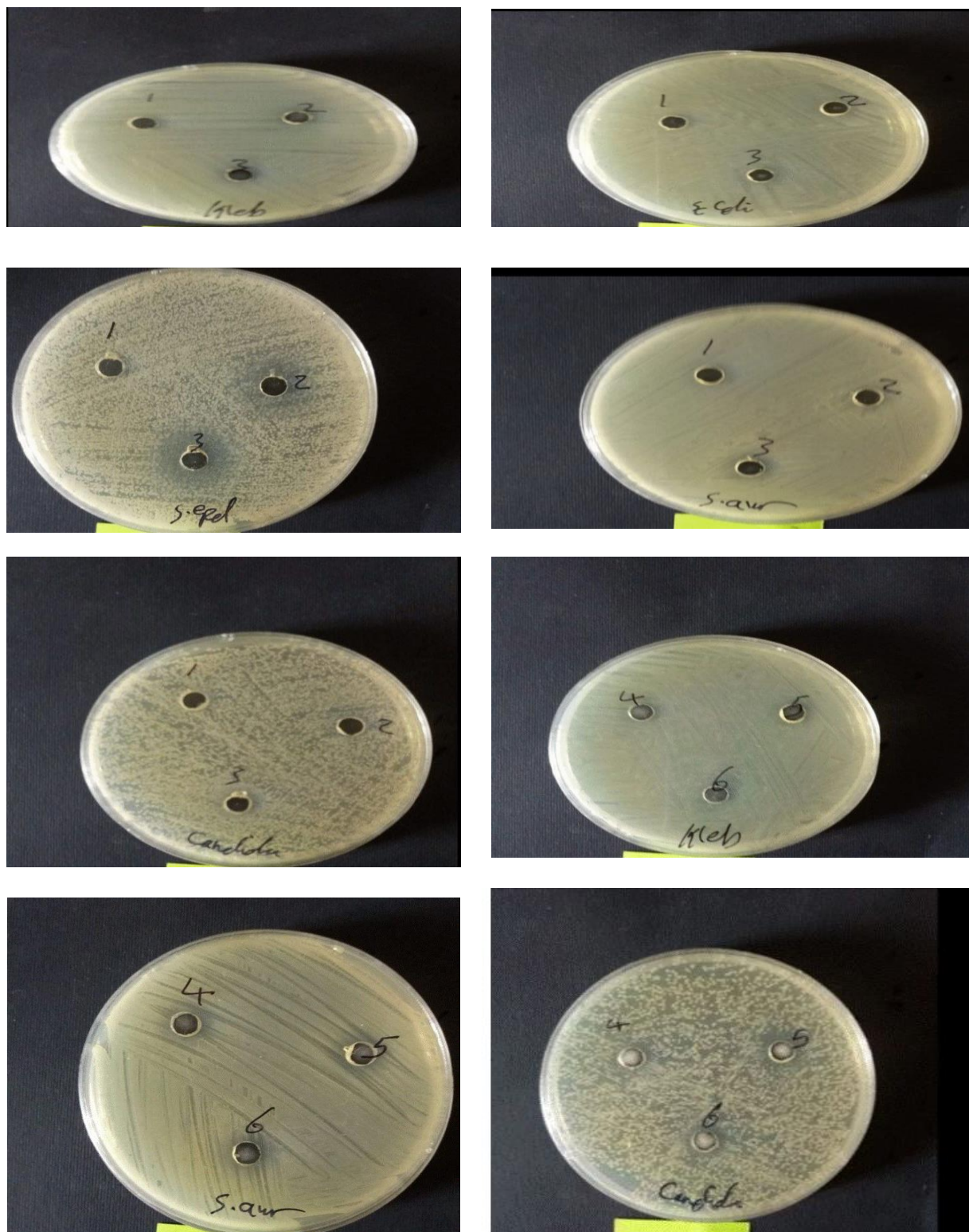


Figure 6. Antibacterial activity of PVA polymer and PVA/ZnO nanocomposite against various pathogenic bacterial strains

5. CONCLUSION

The films were made from pure PVA polymer and PVA/ZnO nanocomposites using a solution casting method. ZnO NPs appears to cluster and scatter well in (PVA/ZnO) nanocomposite films, according to scanning electron microscopy (SEM). It has been discovered that the ZnO nanoparticles have varied shapes in different parts of the matrix. When the ZnO ratio in nanocomposites rises, the absorbance and absorption coefficient of the PVA polymer improves optical characteristics. The energy gap to PVA polymer is decreased as the concentrations of ZnO nanocomposites raise. The findings revealed that ZnONPs had superior bacteriostatic efficacy against bacteria. The antibacterial activity increased when the concentration of ZnONPs was increased. ZnONPs may be promising antibacterial agents based on the inhibitory zone reported against Gram-positive, Gram-negative bacteria and *fung*.

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