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Elaboration of Optical and Some Morphological Characterization of (PEG/ZnO) Blend Doped by MWCNTs (0.1-0.3%) for Optoelectronics Applications

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ABSTRACT

The main objective of the present research is to compact PEG+ZnO blend/MWCNTs and to investigate their optical features for use in several optical instruments. The PEG+ZnO blend/MWCNTs were elaborated through the utilization of a casting technique with PEG+ZnO (9:1) modified with different concentrations of MWCNTs. The ratio of MWCNTs was 0.1-0.3%. The optical features have been tested at a range of wavelengths starting from 190 nm up to 1100nm. The dissection explained that with the increasing of MWCNTs ratio from 0.1-0.3%, the absorption's value of PEG+ZnOblend/MWCNTs was boosted with the increasing ratio of MWCNTs. Whenever the MWCNTs ratio was increased, the values of the band gap was drop down from 5.3-2. Ev for allowed transition and from 5.4-2.9 eV for forbidden transition. With increment of MWCNTs ratio, the other optical characteristics of PEG+ZnO/MWCNTs were boosted. That is to say, the result of optical characteristics findings illustrate that the PEG+ZnO/MWCNTs are being useful to be used in a versatile of optoelectronics devices.

1. INTRODUCTION

Researchers have recently shown great interest in nanostructured materials due to their potential use in the development of new nanoscale products. The growing interest in organic–inorganic composite polymeric materials has stimulated extensive research and development into new materials and systems [1-3]. Polymer composites are among the most widely used materials in various applications due to their unique properties, including enhanced mechanical strength and antimicrobial activity [4].

Polymer nanocomposites represent an important class of polymer nanomaterials that have been developed and engineered to exhibit specific physicochemical properties [5, 6]. Strong interactions and excellent dispersion of nanofillers within the polymeric matrix are considered key factors that significantly enhance the properties of nanocomposites [7-9]. Once this is achieved, numerous applications can benefit from the enhanced performance of polymers reinforced with nanostructured materials [10, 11].

They incorporate nanometer-sized fillers that provide unique advantages in enhancing polymer properties-such as mechanical [5], thermal, electrical, and magnetic characteristics-without sacrificing optical transparency [6], in comparison to their conventional counterparts. The properties of polymers that contain nanostructures depend not only on their internal architecture and the features of their individual components, but also on their interfacial characteristics [10, 11].

Polyethylene glycol (PEG) is a versatile polymer with a wide range of applications and is available in various molecular weights (MWs). PEG together with a high molecular weight is referred to as poly (ethylene oxide) (PEO) [9, 12]. PEG possesses essential features for example high water solubility, low toxicity, biocompatibility, and rapid biodegradability in aqueous environments [13]. It typically includes functional groups such as terminal hydroxyl groups, which can enhance its chemical reactivity [14]. These groups enhance the compatibility of PEG with a wide range of polymers and fillers, including their nanostructured forms, thereby improving material properties and enabling the development of advanced functional materials [15, 16]. These polymers have been extensively studied for a variety of applications, including photovoltaic cells, optics, optoelectronics, antimicrobial systems, and electronic devices [17, 18].

Their diacritical features are directly regarding to their internal structure, which varies depending on the composition of the polymer network [19, 20]. Although both pure and blended polymers exhibit various functional properties, they often suffer from limited optical performance due to structural defects within their internal architecture [21, 22].

As reported, the chemical composition, surface state, structural form, and microstructure of the materials play a critical role in determining their effectiveness in gas sensing and antimicrobial applications. Such applications often involve the synthesis and incorporation of various metal oxides, such as zinc oxide, aluminum oxide, and magnesium

oxide, among others [23]. Zinc oxide (ZnO) possesses a binding energy of 60 meV and a wide band gap of 3.3 eV, making it one of the most prominent semiconductor materials in recent years [24-26]. ZnO thin films have recently attracted significant research interest due to their promising electrical and optical properties. These include a high exciton binding energy, strong thermal conductivity, high electron mobility, excellent transparency, and other desirable features that make them suitable for room-temperature applications [27]. Nanocomposites are considered among the most advanced materials due to their unique characteristics, such as a high surface-to-volume ratio and enhanced antimicrobial activity, which result from their extensive contact with organic cells compared to micrometer-sized particles. Nanoparticles have also been reported to be beneficial in various disciplines, particularly in biomaterials [28, 29].

Among such nanostructures, three-dimensional bulk materials have gradually evolved into one-dimensional structures, such as multi-walled carbon nanotubes (MWCNTs), due to their superior physical and chemical properties compared to their bulk counterparts. Owing to their high specific surface area and exceptional electronic conductivity, MWCNTs have gained considerable attention. They exhibit outstanding mechanical, electrical, and thermal properties, making them promising candidates for energy storage applications. Incorporating MWCNTs into composite systems can enhance energy storage capacity by improving compositional stability [30]. Moreover, the reactive oxygen species (ROS) released on the surface of MWCNTs are very reactive, translating the pollutants into non-toxic metabolites and causing bacterial death [31]. MWCNTs in professional manner pass on the created electrons and rapidly dissociate the recombination of photogenerated carriers, thus enhancing the photocatalytic action [32, 33]. Additionally, the large surface area of MWCNTs and their capability to create electron-electron interactions with pollutants significantly boost their possibility to adsorb these pollutants, and then enhancing their efficiency for removing pollutants, PEG/ZnO doped MWCNTs have a good optical properties comparing with other composites [34, 35]. The novelty of PEG/ZnO/MWCNTs composites lies in their synergistic properties from three distinct materials: PEG offers stability and biocompatibility, ZnO provides photocatalytic and antimicrobial activity, and MWCNTs enhance electrical conductivity and mechanical strength. The narrowed band gap due to MWCNTs boosts photocatalytic efficiency. Their improved charge separation and electronic properties make them ideal for energy storage and sensor applications. Additionally, their antibacterial and biocompatible characteristics make them suitable for biomedical and environmental applications.

The important goal of this research is to prepare of ZnO and study the effect of MWCNTs on some morphological, optical characteristics of (PEG/ZnO) blend for optoelectronics applications.

2. EXPERIMENT

The solution of ZnO with a concentration of 0.5M has been intended by resolve zinc acetate (Zn (CH3COO)2) into (20ml) of distilled water and stirring the solution for about15 min at room temperature, the substance became transparent after slowly adding 2mls of acetic acid and stirring the mixture for 10 minutes. Four drops have been added of hydrochloric acid and then stirring the blend for five minutes. The mixture began to take on a more transparent quality. The color change occurred because of the addition of 2mls of acetic acid CH3COOH which was added gradually with constant stirring for a duration of 10 minutes. And the blend was stirred at 60C for 24 hours. The quantity of zinc acetate that is to be liquefied is determined by the next relation [26]:

$$M = \left(\frac{w_t}{M_{wt}}\right)\left(\frac{1000}{v}\right) \quad (1)$$

where, *M* is the molar concentration, or 0-5 M; Wt is the amount of zinc acetate that needs to be broken down; Mwt is the molecular weight of zinc acetate, or 219-497gm/mol; and v is the volume amount of distilled water. Without further purification, the components and substances used in this investigation were obtained from Sigma-Aldrich.

A film of PEG/ZnO/MWCNTs with different MWCNTs and blend of polymer ratios. The blend of polymer has been ready through liquefying 1gm of the respective polymers in (30ml) distill water with ratio (90%PEG/10%ZnO). MWCNTs were incorporated in the mix with addition proportions (0.01%, 0.02% and 0.03%). the nanocomposites were made by the drop casting process. The optical characters of blend/MWCNTs were measured on UV-18000AShimadzu spectrophotometer. Using the relation given to obtain the coefficient of absorption (α) [36]:

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

d represents the value of width; A is the value of absorbance. The value of energy gap (Eg) stays given via [37]:

$$(\alpha h\upsilon) = B\left(h - E_g\right)^m \quad (3)$$

B is a constant, h υ represent the photon energy, Eg express about the band gap energy, m can take the values 2 or 3 for both allowable and forbidden alterations.

The coefficient of extinction (k) stays introduced via the next relationship [38]:

$$k = \frac{\alpha\lambda}{4\pi} \quad (4)$$

λ represents the wavelength. Dielectric constant of both real ε1 and imaginary ε2 is introduced by Amin et al. [39]:

$$\varepsilon 1 = n^2 - k^2 \quad (5)$$

$$\varepsilon 2 = 2nk \quad (6)$$

The value of the optical conductivity (σ op) explains [40]:

$$\sigma_{op} = \frac{\propto nc}{4\pi} \quad (7)$$

3. RESULT AND DISCUSSION

Characterization by XRD is essential for understanding the structure and composition of synthesized materials. This vital information about the studied samples includes their

crystographs and cutouts analyzed by XRD. XRD spectra of prepared ZnO NPs are presented in Figure 1, the XRD peaks at 2Θ values of 31.6°, 34.4°, 36.5° indicate the crystallographic planes (100), (002), (101). as reported in the study, and this deal with (JCPDS card no.01-079-005) [41]. This indicates that ZnO was successfully prepared.

MWCNTs (from Cheap Tube the outer diameter 20-40nm, length 10-30 microne,purity 90%).

Optical microscopy images (OM) of PEG+ZnO, PEG+ZnO/(1%MWCNTS), PEG+ZnO/(2%MWCNTS), PEG+ZnO/(3%MWCNTS can be founded in Figures 2(a)-(d). The morphologies of the PEG+ZnO film are illustrated in Figure 2(a), which demonstrate that its surface is so soft and uniform Figures 2(a)-(d) show up the optical microscopy images (OM) of PEG+ZnO films and PEG+ZnO composites with different MWCNTS hybridization proportions with magnification factor of 40 X. It apparently illustrates smooth identical matrix of the prepared samples, beside a pretty spread of MWCNTS through PEG+ZnO films. They illustrate that this procedure was totally effectively invented the mixed and MWCNTS. in addition, MWCNTs contribution led to presumed variations in these films deprived of accumulation or distressing the optical transparency of the ready samples under the study [19]. The absorbance of (PEG+ZnO) before and after modified with (MWCNTs) were plotted as a function of wavelengths as obvious from Figure 3, it has been noticed that the absorbance's value increasing versus the mounting of the ratio of (MWCNTs) and there is clearly absorption band at 370nm, is generally broadened and overlap so that the MWCNTS absorb light through these specific wavelengths [42]. The energy gap values for both allowable and forbidden transitions blend/MWCNTs films is clarify in Figures 4 and 5 respectively, As the ratio of MWCNTs increase, a both of Egi and Egd observed to be reduce. MWCNTs have high electrical conductivity and delocalized π-electrons, which can interact with the ZnO semiconductor. The charge transfer between the MWCNTs and the ZnO nanoparticles or the PEG matrix facilitates electron donation or acceptance at the interface, which alters the energy states of the system. The π-electrons in the MWCNTs can couple with the conduction band of ZnO, leading to the formation of new hybridized electronic states within the band gap. This interaction lowers the energy threshold required for electron excitation, resulting in a reduced band gap. For the mixture without MWCNTs, allowed and forbidden are 5.3 eV and 5.4 eV, respectively. when 1 wt% of MWCNTs added, the allowed drop to 4.9 eV, and the forbidden drop to 4.4 eV. This outcome signalizes boosting in electronic interactions and enhancement of transferring of charges among the matrix of polymer and MWCNTs. It could show in a new energy states within the structure of the band of the matrix of polymer, which making easier electronic transitions [43, 44].

Figure 6 gets the absorption coefficient of PEG+ZnO blend modified with MWCNTs. which given a clear data about on the transition and its nature. It is clearly that the value of α smaller than 104cm- 1, and for that the indirect transition happened. The blend/MWCNTs manifested a low value of absorption coefficient, this related to its poor crystal structure [45].

Figure 7 shows the performances of k of PEG+ZnO/MWCNTs. The k values mimize, and after that go up with the increasing of the wavelength of photon. It is clearly obvious that the k value of PEG+ZnO/MWCNTs reduce with increasing the MWNTs proportion, which regarding to the density increment of the prepared films and value of α [46].

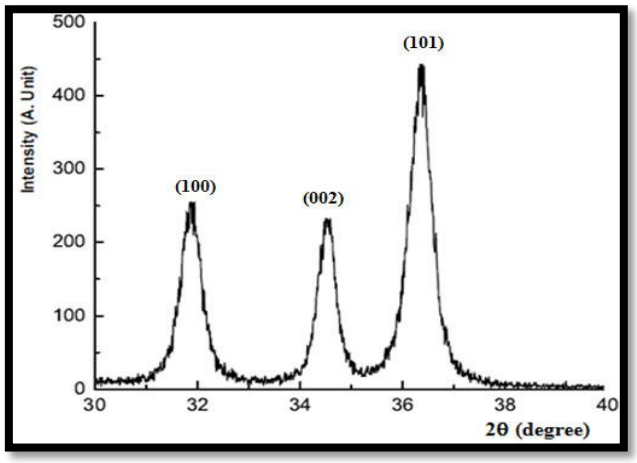
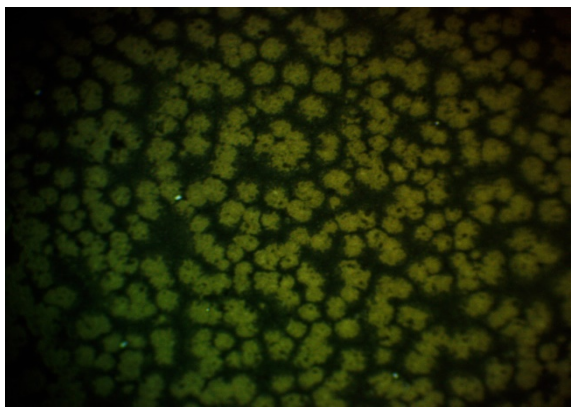
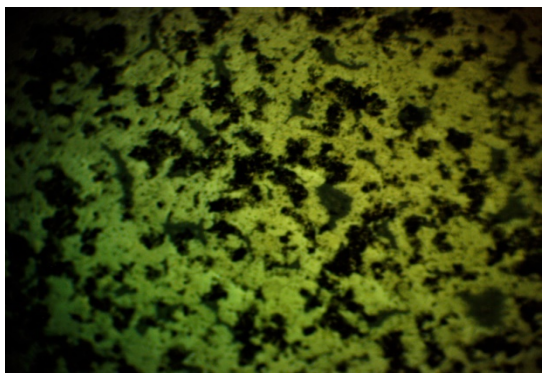


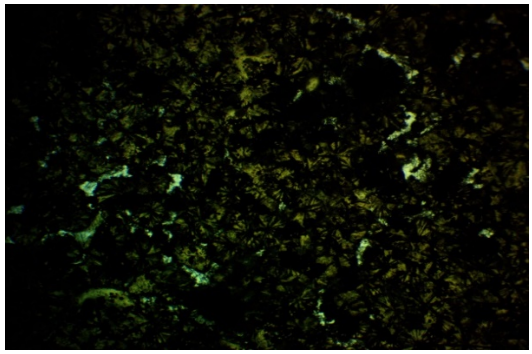
Figure 1. XRD Spectra of prepared samples of ZnO



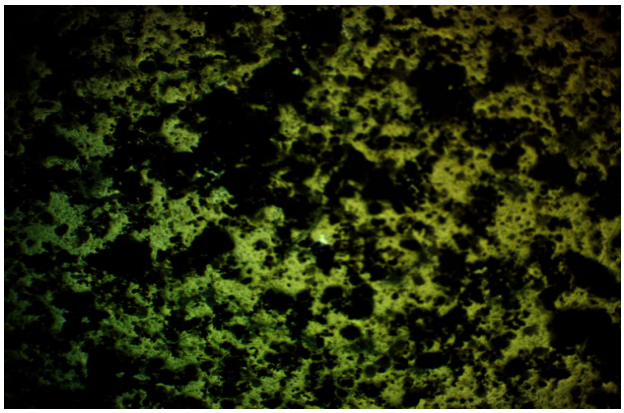
(a) PEG+ZnO



(b) PEG+ZnO/(1%MWCNTS)



(c) PEG+ZnO/(2%MWCNTS)



(d) PEG+ZnO/(3%MWCNTS)

Figure 2. Optical image of the surface of a thin film layer

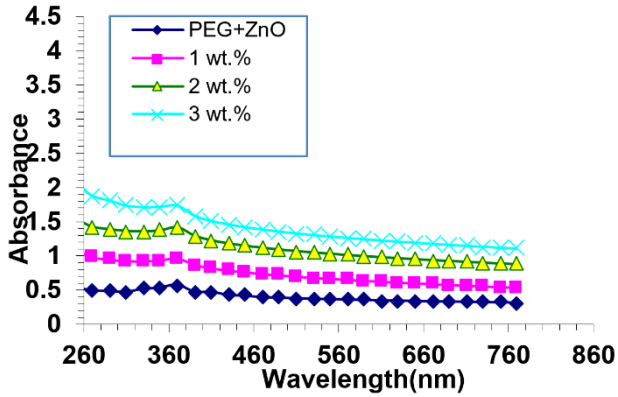


Figure 3. Absorption as a function of wavelengths for pure PEG+ZnO and, PEG+ZnO/(1%MWCNTS), PEG+ZnO/(2%MWCNTS) and PEG+ZnO/(3%MWNTS)

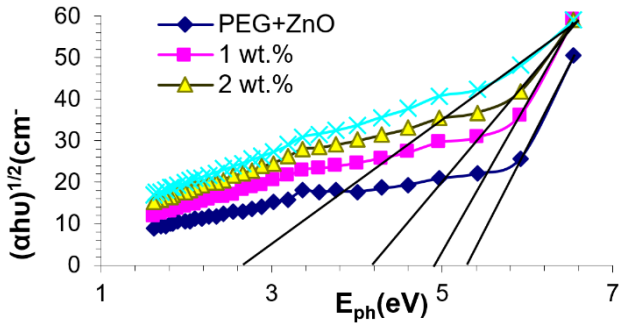


Figure 4. Eg value for PEG+ZnO/MWNTs for allowed transition

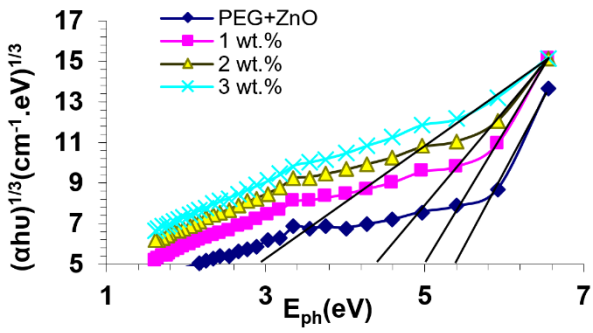


Figure 5. Eg value for PEG+ZnO/MWNTs for forbidden transition

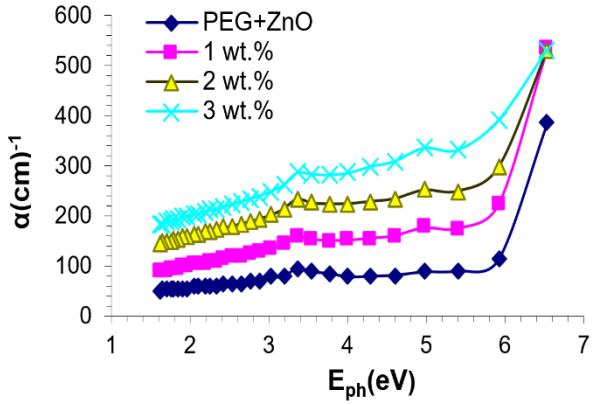


Figure 6. Absorption coefficient of PEG+ZnO/MWCNTs

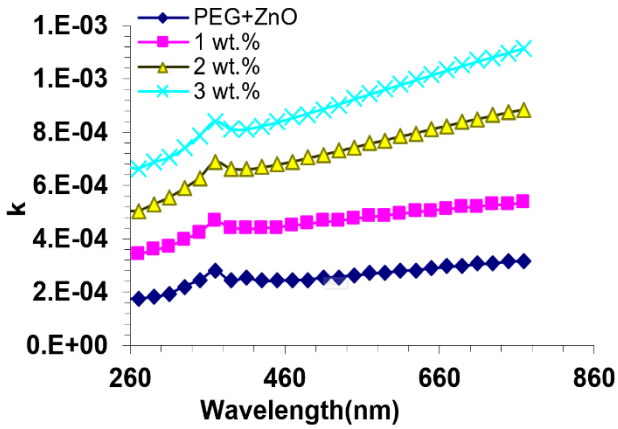


Figure 7. Extinction coefficient of PEG+Zn blend/MWCNTs

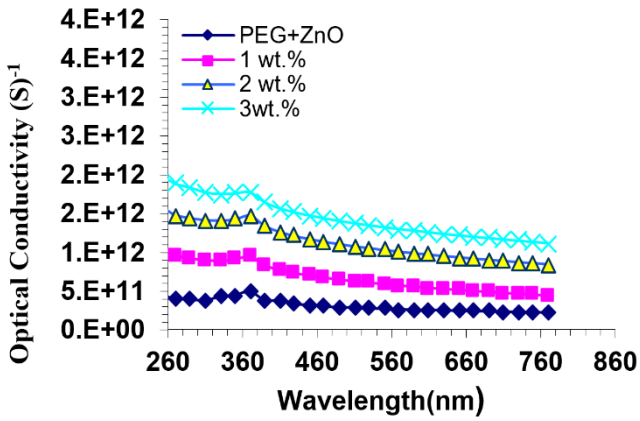


Figure 8. The optical conductivity versus wavelength of PEG+ZnO blend/MWCNTS

Figure 8 indicates the influence of MWCNTs on optical conductivity of prepared films. There is drop down in the value of optical conductivity with rising of the wavelength of photon. When the content of MWCNTs increase, the optical conductivity value will go up which is because of the increasing in absorbance and reduction of the energy gap [47].

The both of imaginary, real constants of dielectrics for PEG+ZnO/MWCNTs films are illustrated in Figures 9 and 10. The actual dielectric constant minimize according to the increment of photon wavelength.

The ε2 values go down, after that go up with the increment of the photon wavelength. It has been obtained from Figures 9 and 10 that the ε1 and ε2 drop down along with the increment

of MWCNTs ratio and that related to the increment of the value of k [46].

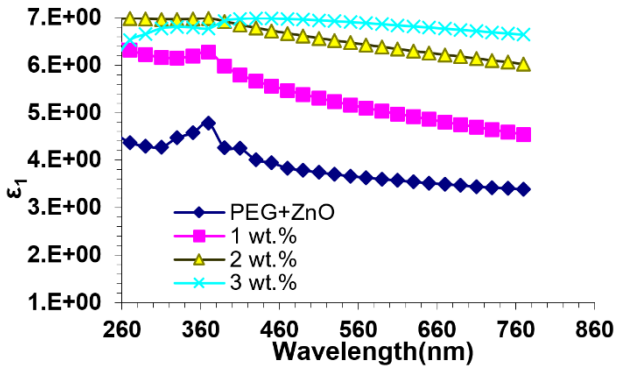


Figure 9. Real part of dielectric constant for PEG+ZnO blend/MWCNTs

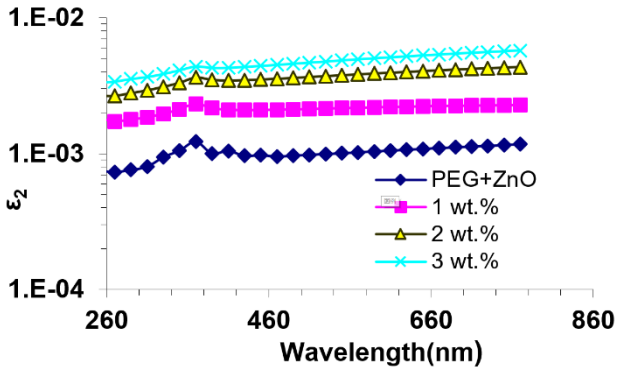


Figure 10. Imaginary part of dielectric constant for PEG+ZnO blend/MWCNTs

4. CONCLUSIONS

This work looks for the processing of PEG+ZnOblend/MWCNTs besides their optical features utilized in diverse optoelectronics applications. The optical features of PEG+ZnOblend/MWCNTs have been tested at a range of wavelengths from 190nm up to 1100nm. The dissection pointed that the incresing in the MWCNTs ratio led to boost in the value of absorption of PEG+ZnO while there is clearly reduction in the value of transmittance. The band gap decreases with an increase in MWCNTs content from 5.3 eV to 2.7 eV for allowed transition and from 5.4 eV to 2.9 for forbidden transition. PEG+ZnO/MWNTs show augmented optical properties with the incorporation of MWCNTs. The optical features exhibited that the mixture /MWCNTs films suitable to be utilized in diverse optoelectronics devices.

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