Experimental and Theoretical Approaches for Polyvinylchloride Enhanced with Metal Oxides/Graphene

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Abstract

Introducing graphene (G) into the polymer matrix is supposed to improve both the electrical and optical characteristics, especially in space applications. To study the effect of metal oxide and G on PVC, a matrix of PVC/ZnO/G nanocomposite was prepared and studied using different spectroscopic techniques. As a consequence, the Fourier Transform Infrared (FTIR) spectra for PVC/ZnO/G revealed two significant bands at 1596 cm^{-1} and 515 cm^{-1} , G and ZnO, respectively, confirming the composite synthesis. Also, X-ray Diffraction (XRD) and Field-emission Scanning Electron Microscopy (FESEM) result confirmed the interaction between PVC, ZnO, and G. Density functional theory (DFT) calculations were performed at B3LYPL/LAN2DZ on PVC nanocomposites with various metal oxides such as MgO, SiO_2 , TiO_2 , NiO, CuO, ZnO, and ZrO_2 and then reinforced with graphene quantum dots (GQDs). The findings of the HOMO/LUMO band gap energy, total dipole moment (TDM), and Molecular Electrostatic Potential (MESP) indicated that the effect of MgO in the presence of GQD gives a nanocomposite with high electronic characteristics with a TDM of 16.675 Debye ΔE 0.231 eV. The distinctive properties of such nanocomposite PVC/MgO/GQD ZTRI C46 enabling usage in optical and electrical components and systems, as well as anti-reflection coating applications for solar cells.

1- Introduction

Polymer nanocomposites have recently gained interest for their ability to enhance polymer characteristics with low nanoparticle concentrations [1, 2]. PVC is one of the most versatile polymers, and modification and functionalization of PVC increase and change the polymer characteristics [3, 4]. Studies polymer optical and electrical characteristics gained recently much interest owing to its functionality in optical devices [5, 6]. MOs, for example, are commonly used as nanofillers to improve the characteristics of polymers, lowering the cost of polymeric materials while enhancing their functionality [7–9]. The PVC/ZnO nanocomposite demonstrated that ZnO increased the dielectric properties and mechanical and thermal stability [10] of insulating polymers, allowing them to be used in electrical applications [11]. Furthermore, the PVC/ Fe_2O_3 nanocomposite demonstrated higher mechanical properties confirming that adding Fe_2O_3 nanoparticles increased resistivity of the PVC polymer matrix [12]. PVC with ZnO, SiO_2 , and Al_2O_3 enhance the refractive index materials appropriate to be used as solar cells anti-reflection cover and high refractive lenses applications, which could be adjusted by MOs type and content [13]. Moreover, increasing the number of NiO nanoparticles in the sample increases the impact nanoparticles on PVC matrix optical characteristics, suggesting these materials for electrical and photonic devices [14]. Moreover, theoretical calculations have recently been used to investigate chemical problems by studying molecular geometries [15, 16], molecule energies [17], infrared rays (IR) [18], and physical properties of structures [19]. There are several methods for investigating the materials chemical as well as physical properties that are often represent the organometallic interactions in addition to nanocomposites [20, 21]. DFT is currently regarded as the optimum method for molecular structure model simulation [22, 23]. Furthermore, DFT gives higher accuracy result approximate to the experimental result [24, 25]. Moreover, DFT:B3LYP/LanL2DZ calculations of a PVC/PEO/SiC nanocomposite were performed to study electronic

properties as well as spectroscopic features, revealed the ability of the new composite to utilized as optoelectronic material [26].

The objective of this study is to prepare a PVC/ZnO/G nanocomposite to investigate whether the molecular structure and morphology of the PVC surface are impacted. Furthermore, molecular modeling was used to investigate and evaluate the impact of MO nanoparticles on the electronic characteristics of PVC (MgO, Al₂O₃, SiO₂, TiO₂, Fe₃O₄, NiO, CuO, ZnO, and ZrO₂). To test the compatibility of the produced composites for optoelectronic applications, the TDM, band gap energy, and MESP were calculated. With the same parameters, the impact of doping GQDs on PVC/MOs nanocomposite was determined.

2- Material And Methods:

For composite preparation, high-molecular-weight PVC (Fluka #81392), zinc (II) acetate dihydrate (Fisher chemical, 99%), and sodium hydroxide (Fisher chemical, 97%) were utilized. During this experiment, deionized water (DI) was used. Furthermore, no purifications were performed on any of the materials.

2-1- Synthesis of ZnO Nanoparticles:

Precipitation method was used to ZnO nanoparticles synthetizations. Firstly, zinc (II) acetate dissolved in DI (100 mL) at 70°C. At that time 2 M sodium hydroxide in (100 mL) DI water was prepared and added drop wisely while stirring. The white precipitate then filtrated and washed. Prepared ZnO dried at 80°C for 24h. finally the ZnO sample calcined for 2 h at 500°C.

2-2- Preparation of PVC/ZnO/G Composite:

(70%) of PVC was dissolved in 100 ml of DI water then (0.01 gm) of ZnO and (0.02 gm) of G sheets were added to the solution after complete dissolve with stirring until a homogeneousness. Then putted at room temperature to dry.

2-3- Analytical Techniques:

All prepared samples were characterized using an Attenuated Total Reflection Fourier Transform Infrared (ATR-FTIR) with spectral range 4000–400 cm⁻¹ as well as resolution of 4 cm⁻¹ (Vertex 70, Bruker) spectrometer to study the intermolecular structure. Then, X-ray Diffraction (XRD) was used to study the nanofiller impact on crystal structure as well as phase composition via a Malvern Panalytical Empyrean 3 diffractometer to study the and crystal structure of prepared samples. Finally, Field-emission Scanning Electron Microscopy was used to study the morphology of the prepared samples using (FESEM, Quattro S, Thermo Scientific).

2-4- Calculation Details:

To investigate the influence of metal oxides on PVC electronic characteristics, a PVC model structure was interacted with MOs such as MgO, Al₂O₃, SiO₂, TiO₂, Fe₃O₄, NiO, CuO, ZnO, and ZrO₂. The GAUSSIAN09 [27] was used to compute all models at the Molecular Spectroscopy and Modeling Unit, National

Research Centre, Egypt. For structural computations, the DFT:B3LYP/LANL2DZ model was used [28–30]. For all model structures, the TDM, HOMO/LUMO band gap, in addition to MESP surface representing were computed in order to examine electrical characteristics.

3- Result And Discussion

3-1- PVC/ZnO/G Composite Experimental study:

a. FTIR Result:

The FTIR spectra of pure PVC, ZnO, G, and PVC/ZnO/G composite are shown in figure (1). The PVC characteristic bands were shown as follows: the stretching vibration of C-H occurred at 2914 cm^{-1} and 2970 cm^{-1} . Sharp bands at 1426 cm^{-1} and 1264 cm^{-1} can thus be attributed to the bending vibrations of CH_2 and C-H in CHCl , respectively. Finally, at 608 cm^{-1} , the band related to the stretching vibration of C-Cl was observed [31]. The ZnO nanoparticles are represented by the main band at 599 cm^{-1} according to the ZnO result [32]. The PVC/ZnO/G spectrum shows the characteristic bands of pure PVC with the appearance of two strong bands at 1596 cm^{-1} , representing the C-C of G and a ZnO band shifted to a lower wavenumber at 515 cm^{-1} which confirmed the composite formation.

b. XRD Result:

The XRD analysis, illustrated in figure (2), which reflect the structure and composition for producing nanoparticles and nanocomposite. The XRD pattern of pure PVC shows the characteristic peak at $2\theta = 17.00^\circ$ and 24.66° related to diffraction planes (001) and (201), respectively [33]. The hexagonal wurtzite structure of ZnO nanoparticles is illustrated in XRD pattern where the crystalline peaks are shown at around $2\theta = 31.77^\circ, 34.42^\circ, 36.26^\circ, 47.54^\circ, 56.58^\circ, 62.86^\circ, 66.37^\circ, 67.96^\circ, 69.10^\circ, 72.53^\circ, 76.94^\circ$ and 81.467° which related to the diffraction plans as (100), (002), (101), (102), (110), (103), (200), (112), (201), (202), and (104), respectively [34]. The G characteristic peak is illustrated at $2\theta = 25.01^\circ$ with respect to the (002) diffraction plane. Furthermore, PVC/CuO/G peaks at $2\theta = 18.07^\circ, 24.47^\circ, 31.69^\circ, 34.36^\circ, 36.19^\circ, 47.52^\circ, 56.57^\circ, 62.80^\circ, 67.89^\circ$, and 69.11° related to (110), (201), (301), (120), (101), (102), (110), (103), (112), and (201) diffraction plane containing PEO, CuO and G characteristic peaks indicated that the composite was successfully formed.

c. SEM Result:

Figure (3) represents surface morphological images of PVC, ZnO, G, and PVC/ZnO/G nanocomposite at various magnifications to analyse the changes on the PVC surface. The SEM image of pure PVC shows the fractured surfaces of pure PVC to be comparatively smooth. The interaction of PVC with both ZnO and G results in the presence of ZnO nanoparticles [35]. In addition to this, the G sheets on the surfaces of nanocomposite samples are in the form of agglomerated structures.

Based on the experimental findings, molecular modelling was used to investigate and evaluate the impact of (MgO, Al₂O₃, SiO₂, TiO₂, Fe₃O₄, NiO, CuO, ZnO, and ZrO₂) nanoparticles on the electronic properties of PVC in order to evaluate the atibility of the prepared composite for optoelectronic applications.

d. Building Model Molecule

Polymeric nanocomposite became essential owing to its wide variety of applications owing to the influence nanofillers have on the polymer matrix, which enhances the polymer matrix's essential features [36]. Therefore, four monomers of the PVC model structure are suggested to interact with a variety of MOs such as MgO, Al₂O₃, SiO₂, TiO₂, Fe₃O₄, NiO, CuO, ZnO, and ZrO₂. Change in HOMO/LUMO distribution as well as for MESP according to the interactions were studied, which is an important descriptor, to investigate the influence of MOs composition on the electronic properties of PVC.

e. Interactions of PVC/Metal Oxides

HOMO/LUMO Orbital Distribution

To represent the proposed study, four monomers of the PVC polymer chain interacted with different metal oxides such as MgO, Al₂O₃, SiO₂, TiO₂, Fe₃O₄, NiO, CuO, ZnO, and ZrO₂. The change in HOMO/LUMO distributions were studied, as shown in figure (4). The dispersion of HOMO/LUMO orbital in PVC is uniformly spread through the whole chain. However, HOMO/LUMO orbitals according to MOs interactions are redistributed and concentrated over MO atoms. Table (1) shows the computed TDM and band gap energy (E) values for model structures. The result of TDM showed that TDM increased for all PVC/MOs interactions from 7.302 Debye to 34.641, 18.634, 24.665, 08.842, 25.950, 34.179, 09.882, 23.417, 17.780, 26.714, 17.082, 31.949, 17.069 and 35.128 Debye for MgO, OMg, Al₂O₃, O₃Al₂, SiO₂, TiO₂, Fe₃O₄, NiO, ONi, CuO, OCu, ZnO, OZn and ZrO₂ respectively. Simultaneously, the band gap energy (ΔE) of PVC/MOs decreased from 5.479 eV to 0.448, 1.147, 1.419, 1.798, 0.922, 0.751, 1.063, 1.125, 0.883, 1.922, 1.449, 0.527, 1.512 and 0.767 for MgO, OMg, Al₂O₃, O₃Al₂, SiO₂, TiO₂, Fe₃O₄, NiO, ONi, CuO, OCu, ZnO, OZn and ZrO₂, respectively. As a result, the TDM rising in addition to reduce band gap energy (ΔE). As previously stated, increasing TDM with decreasing band gap energy (ΔE) enhanced the stability and electrical behavior of polymer matrix [37]. Consequently, PVC/MgO is the most electronically enhanced and stable structure.

Table 1. Calculated TDM (Debye) and ΔE (eV) using DFT:B3LYP/LANL2DZ of the PVC interaction with different metal oxides

Structure	TDM (Debye)	ΔE (eV)
PVC	07.302	5.479
PVC/MgO	34.641	0.448
PVC/OMg	18.634	1.147
PVC/Al ₂ O ₃	24.665	1.419
PVC/O ₃ Al ₂	08.842	1.798
PVC/OSiO	25.950	0.922
PVC/OTiO	34.179	0.751
PVC/Fe ₃ O ₄	09.882	1.063
PVC/NiO	23.417	1.125
PVC/ONi	17.780	0.883
PVC/CuO	26.714	1.922
PVC/OCu	17.082	1.449
PVC/ZnO	31.949	0.527
PVC/OZn	17.069	1.512
PVC/OZrO	35.128	0.767

Molecular Electrostatic Potential (MESP):

MESP stands as useful model representing the chemical structures electrostatic interactions with each other. The representation with reference to sequence of colors arranged as Red, Orange, Yellow, Green, and Blue, respectively. MESP colors mainly utilized to explore the structure sensitivity, reactivity besides stability. The importance of using MESP that it studies the influence of charge distribution changes on the structure's electronegativity, dipole moment, band gap, and chemical active sides [38]. Figure (5) shows the MESP of PVC and PVC reacted with several MOs, including MgO, Al₂O₃, SiO₂, TiO₂, Fe₃O₄, NiO, CuO, ZnO, and ZrO₂. On the MESP surface, the greatest charge region represented in red colour, the lowest charge region represented via blue colour, besides the zero electrostatic potential region defined by green denotes. The highest potential is often found in red locations, whereas the poorest potential is frequently seen in blue parts. The Cl atom was discovered to be the centre of active PVC reactivity. When PVC interacted with different MOs, the red colour diffused across the polymer chain's up and down terminals, showing that PVC reactivity increased, and MOs reinforced PVC's active sides. In PVC/ MOs interaction through the metal atom, the red colour of low potential located primarily around the MO oxygen atom, whereas in case of PVC/ MOs interaction through oxygen atom, red colon redistributed through polymer

chain besides expanded across the opposite side of PVC chain. Accordingly, PVC's electrical properties have increased, and it now could be used for numerous applications.

b. GQDs Interaction with PVC/MgO:

GQDs have a surface area for interaction, as well as having good edge atoms to interact other structures [39]. Furthermore, the bandgap adjusting feature and electron transport capacity of GQDs with varying sizes may be used in nanoelectronics devices and as optoelectronic materials [40]. As a result, PVC/MO/GQD, in its four forms: ATRI, AHEX, ZTRI, and ZHEX, was created to combine with the highest PVC/MO enhanced structure. For the suggested structures, HOMO/LUMO orbital distributions and MESP mapping were also investigated. As shown by investigation, PVC/MgO was the chemically stable and active structure. PVC/MgO suggested to study the effect of four GQD forms the interaction as shown in figure (6). The band gap of PVC/MgO in table (2) decreased from 0.448 eV to 0.382, 0.324, 0.231, and 0.344 eV for PVC/MgO/GQD ATRI C60, PVC/MgO/GQD AHEX C42, PVC/MgO/GQD ZTRI C46, and PVC/MgO/GQD ZHEX C54, respectively. As a result, PEO/CuO/GQD ZTRI C46 is the most effective, stable, and unique in electrical characteristics antireflection coating applicants

Table 2. Calculated TDM (Debye) and ΔE (eV) using B3LYP/LANL2DZ of the PVC/MgO interactions with GQDs

Structure	TDM (Debye)	ΔE (eV)
PVC/MgO/ GQD ATRI C60	25.445	0.382
PVC/MgO/ GQD AHEX C42	24.652	0.324
PVC/MgO/ GQD ZTRI C46	16.675	0.231
PVC/MgO/ GQD ZHEX C54	21.846	0.344

4- Conclusion

A PVC/ZnO/G composite was synthesized and investigated using ATR-FTIR, XRD, and FESEM. The presence of the two significant bands of G and ZnO in the spectrum verified the production of PVC/ZnO/G. Moreover, SEM images reflect the effect of ZnO and G on the PVC surface. The type and concentration of MOs in the PVC matrix might modify its electrical and optical properties and control the band gap. The TDM, HOMO/LUMO and MESP results could be used to predict the properties of such nanocomposites for use in optical components and devices. Furthermore, the PVC/MgO/GQDs composite improved PVC's electrical and optical properties. The composite PVC/MgO/ GQD ZTRI C46 effect on PVC characteristics to operate as an anti-reflection coating application for solar cell nanocomposites, which is important in space applications.

Declarations

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Figures

Figure 1

The ATR-FTIR transmittance result for PVC, ZnO, G and PVC/ZnO/G composite

Figure 2

XRD diffraction pattern for PVC, ZnO, graphene (G) and PVC/ZnO/G nanocomposite.

Figure 3

FESEM images with different magnifications for PVC, ZnO, G and PVC/ZnO/G composite

Figure 4

DFT:B3LYP/LANL2DZ of PVC and PVC interacted with different metal oxides HOMO-LUMO calculations and its optimized structure as

- (a) PVC (b) PVC/MgO (c) PVC/OMg (d) PVC/Al₂O₃ (e) PVC/O₃Al₂
(f)PVC/SiO₂ (g) PVC/TiO₂ (h)PVC/Fe₃O₄ (i)PVC/NiO (j)PVC/ONi

(k)PVC/CuO (l) PVC/OCu (m)PVC/ZnO (n)PVC/OZn (o)PVC/ZrO₂

Figure 5

DFT:B3LYP/LANL2DZ of PVC and PVC interacted with different metal oxides MESP mapping as

(a) PVC (b) PVC/MgO (c) PVC/OMg (d) PVC/Al₂O₃ (e) PVC/O₃Al₂

(f) PVC/SiO₂ (g) PVC /TiO₂ (h) PVC/ Fe₃O₄ (i) PVC/NiO (j) PVC/ONi
(k) PVC/CuO (l) PVC/OCu (m) PVC/ZnO (n) PVC/OZn (o) PVC/ZrO₂

Figure 6

DFT:B3LYP/LANL2DZ calculations for optimized structure and HOMO/LUMO orbital distribution and MESP as contour of the PV/MgO interactions with GQDs as

(a) PVC/MgO/GQD ATRI C60	(b) PVC/MgO/GQD AHEX C42
(c) PVC/ MgO/GQD ZTRI C46	(d) PVC/MgO/GQD ZHEX C54