



Kingdom of Saudi Arabia
Imam Mohammad Ibn Saud Islamic University (IMSIU)
Faculty of Sciences – Department of Physics



Effect of Nano Oxides Mixture on Optical Properties

**A graduation project submitted to the Department of Physics in partial fulfillment of the requirements
for the degree of Bachelor of Science in Applied Physics**

by

Alanoud Mohammed Almutairi & Dinah Radan Alotibi

Supervisor

Prof. Wafaa Morsi

IMSIU-Riyadh-KSA

February, 2025

Contents

List of Figures	iii
List of Tables	iv
Acknowledgements	v
Abstract	vi
الملخص	vii
1 Introduction	1
1.1 Polymer	1
1.1.1 Polyvinyl Chloride (PVC)	1
1.1.2 Electronic structure of Polyvinyl Chloride (PVC)	1
1.1.3 Properties of Polyvinyl Chloride (PVC)	2
1.2 Nanoparticales	2
1.2.1 Structure of Nanoparticles	2
1.2.2 Nano types and shapes	2
1.2.3 Nano Oxides	4
1.2.4 Properites of Nano Oxide	4
1.3 Optical Properties	4
1.3.1 Types of Optical Properties	5
1.4 spectrum	5
1.5 Nano applications	5
1.6 Nano composites with polymer	6
1.6.1 Types of nanofillers in polymer nanocomposites	6
1.7 Advantages of Polymer nanocomposites	6
1.8 Applications of Polymer Nanocomposites	7
1.8.1 Energy and Electrical Applications	7
1.8.2 Medical applications	8
1.8.3 Adsorption of pollutants	8
1.8.4 Sensing applications	8

1.9	UV-Visible Spectrometer-Absorption Theory	8
1.10	Beer-Lamber	8
1.11	Optical band gap	9
1.11.1	Types of band gap	10
1.12	Urbach Energy	11
1.13	Literature review	12
2	Experimental Methods	13
2.1	Preparation Methods	13
2.2	Sample	13
2.3	Spectrophotometer UV-VIS Device	14
3	Result and Discussion	15
3.1	Spectrophotometer UV-VIS Device Result	15
3.2	Energy gap	16
3.3	Urbach Energy	18
4	Reference	21

List of Figures

1.1	Polymer and a Monomer of Polyethylene	1
1.2	Nanomaterials classification by dimension	3
1.3	Nanomaterials classification by composition	3
1.4	Optical properties of materials	5
1.5	Spectrum	5
1.6	Nanoparticles applications	6
1.7	Different uses of polymer nanocomposites	7
1.8	Beer- Lambert diagram.	9
2.1	HR-TEM of Pbo nanoparticles	13
2.2	Spectrophotometer UV-VIS Device	14
3.1	Absorbance Peaks	16
3.2	band gap of PVC(pure)	17
3.3	band gap of PVC/1% Pbo	17
3.4	band gap of PVC/2% Pbo	18
3.5	Urbach Energy of PVC(pure)	19
3.6	Urbach Energy of PVC/1% Pbo	19
3.7	Urbach Energy of PVC/2% Pbo	19

List of Tables

3.1	Valued for direct band gap	17
3.2	Values for Urbch Energy of (Pbo)	18

Acknowledgements

(وَأَخِرُ دَعْوَاهُمْ أَنْ الْحَمْدُ لِلَّهِ رَبِّ الْعَالَمِينَ)

الحمد لله عند البدء والختام فما انتهى درب ولا خُتم جهد ولا تم سعي الا بفضل سبحانه
نُهدي هذا النجاح إلى كل من عائلتنا واصدقائنا وكل من سعي معنا لإتمام هذه المسيرة
وأيضاً نشكر البروفسورة وفاء مرسى لما عملته معنا بتوجيهنا وإرشادنا بخبراتها القيمة ومساعدتنا في إنهاء البحث.

Abstract

In this study, the effect of adding lead oxide (PbO) to PVC at different concentrations: PVC/1% PbO, PVC/2% PbO, and pure PVC, on the optical properties of the material was investigated. The object of this study is to measure and evaluate the impact of different PbO concentrations on the optical properties of PVC, through the analysis of absorption, band gap (E_g), and Urbach energy using the UV-Visible Spectrophotometer. The results showed that increasing the PbO concentration leads to higher absorption, while lower concentrations result in reduced absorption. It was also found that the band gap (E_g) decreases with increasing PbO concentration, in contrast to pure PVC, where the band gap was higher. Regarding Urbach energy, it was lower in pure PVC and gradually increased with higher PbO concentrations, indicating an increase in the disturbances in the material's structure. The decrease in the band gap indicates that the modifications to the material's composition have improved its optical properties, which may make it more efficient for optical applications .

الملخص

في بحثنا، قمنا بدراسة تأثير إضافة جزيئات أكسيد الرصاص النانوي (Pbo) إلى بوليمر بولي فينيل كلورايد (PVC). تم إضافة جزيئات Pbo بنسب 1%، 2%، و 0% إلى البوليمر على التوالي. كانت الخصائص البصرية هي الهدف الرئيسي في الدراسة، وتم إجراء قياسات الامتصاص باستخدام مطيافية الأشعة المرئية وفوق البنفسجية Ultraviolet-Visible spectrophotometer، وطاقة فجوة الروابط (Eg)، وطاقة أورباخ (Eu). أظهرت النتائج أن زيادة تركيز Pbo يؤدي إلى زيادة الامتصاص، في حين أن التركيزات الأقل تؤدي إلى تقليل الامتصاص. كما تبين أن فجوة الطاقة (Eg) تنخفض مع زيادة تركيز Pbo، على عكس PVC (pure)، حيث كانت فجوة الطاقة أعلى. فيما يتعلق بطاقة أورباخ، كانت أقل في PVC (pure) وزادت تدريجياً مع زيادة تركيزات Pbo، مما يشير إلى زيادة الاضطرابات في بنية المادة. يشير الانخفاض في فجوة الطاقة إلى أن التعديلات في تركيب المادة قد حسنت من خصائصها البصرية، مما قد يجعلها أكثر كفاءة في التطبيقات البصرية.

Chapter 1

Introduction

1.1 Polymer

Polymer is any of a class of natural or synthetic substances composed of very large molecules, called macromolecules, that are multiples of simpler chemical units called monomers, as illustrated in Figure 1.1. Polymers make up many of the materials in living organisms. [1]

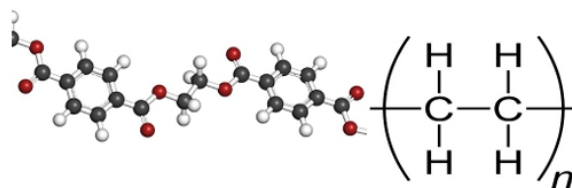


Figure 1.1: Polymer and a Monomer of Polyethylene.

1.1.1 Polyvinyl Chloride (PVC)

Polyvinyl Chloride (PVC) is a synthetic plastic polymer known for its durability, chemical resistance, and cost-effectiveness. It is a thermoplastic material produced through the polymerization of vinyl chloride monomer. PVC is widely used in various industries due to its versatility and ability to be molded into different shapes and sizes. It serves in multiple fields such as construction, packaging, electrical, automotive, and medical applications. [2]

1.1.2 Electronic structure of Polyvinyl Chloride (PVC)

PVC has a linear structure, consisting of repeating vinyl chloride units. Its chemical formula is $(C_2H_3Cl)_n$. The **monomer** of Polyvinyl Chloride (PVC) is vinyl chloride. PVC is created through the polymerization of vinyl chloride molecules. Vinyl chloride is a colorless gas with the chemical formula $CH_2=CHCl$. [3]

1.1.3 Properties of Polyvinyl Chloride (PVC)

- **High Mechanical Properties and Hardness:** PVC's mechanical strength improves with increasing molecular weight but decreases with rising temperatures.
- **Good Electrical Insulation:** Due to its polar nature, PVC is a good insulator, though its electrical insulation is less than non-polar polymers like polyethylene and polypropylene. It is suitable for low-voltage and low-frequency applications.
- **Resistance to Chemicals and Corrosion:** PVC resists acids, salts, fats, and alcohols, making it resistant to sewage corrosion and ideal for sewer pipe systems.
- **Water and Weather Resistance:** PVC fabric's water resistance makes it widely used for coats, skiing equipment, shoes, jackets, aprons, and sports bags. [4]

1.2 Nanoparticles

Nanoparticles are tiny materials with sizes ranging from 1 to 100nm [5]. Nanoparticles exist in the natural world and are also created as a result of human activities. Because of their submicroscopic size, they have unique material characteristics and are manufactured. Nanoparticles may find practical applications in various areas, including medical engineering, catalysis, and environmental remediation. [6]

1.2.1 Structure of Nanoparticles

The structure of a nanoparticle of a material is generally determined by the chemical composition of the material, the number of atoms in the particle, and the character of the chemical interaction between atoms. Nanoparticles can have a regular crystalline structure, can be amorphous, or can form a pseudoclose packing undescrivable by any of the crystallographic space groups. For each of these structural states of a nanoparticle, there is a certain set of numbers of the atoms involved in the particle that corresponds to optimum stable configurations.[7]

1.2.2 Nano types and shapes

Classifications of NMs are still based on four dimensions:

1. **Zero-dimensional nanomaterials (0-D):** this class's nanomaterials have all three dimensions in the nanoscale range. Examples are quantum dots, and nanoparticles.
2. **One-dimensional (1D):** the nanomaterials in this class have one dimension outside the nanoscale. Examples are nanotubes, nanorods, and nanowires.

3. Two-dimensional (2D): the nanomaterials in this class have two dimensions outside the nanoscale. Examples are nanosheets, nanofilms, and nanolayers.
4. Three-dimensional (3D) : in this class the materials are not confined to the nanoscale in any dimension Example :graphite sheets, fullerenes, quantum dots. [8]

The most common Nanoparticles , like nano ribbons, nanotubes, and carbon nano fibers, are shown in Figure 1.2 [9].

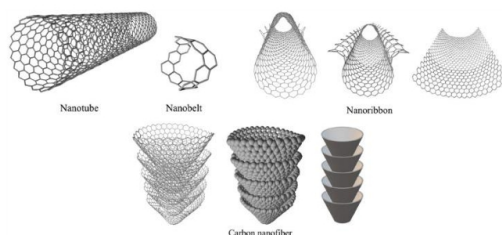


Figure 1.2: Nanomaterials classification by dimension

Nanomaterials can also be classified into three groups according to their composition or nature:

1. Organic nanomaterials, which include carbon-based nanomaterials such as fullerenes, carbon nanotubes (CNTs), single-wall carbon nanotubes (SWCNTs), multi-wall carbon nanotubes (MWCNTs), graphite, and nanofibers.
2. Inorganics nanomaterials consist of metal and oxide-based nanomaterials such as Ag, Au, Fe, Ti, Zn.
3. Hybrid nanomaterials, which are a combination of organic-organic nanomaterials, organic-inorganic nanomaterials, and inorganic-inorganic nanomaterials, also known as composites ,as indicated in Figure 1.3 [10]



Figure 1.3: Nanomaterials classification by composition

1.2.3 Nano Oxides

Nano oxide is a class of nanomaterials composed of metal. Because of their special qualities, nano oxides are useful in many different technologies, such as energy storage and nanomedicine .

1.2.4 Properites of Nano Oxide

- **High Surface Area:** The small size of metal oxide nanoparticles results in a high surface-to-volume ratio, which enhances their reactivity, adsorption capacity, and catalytic activity.
- **Optical Properties:** Many metal oxide nanoparticles exhibit interesting optical properties, such as absorption, emission, and scattering of light, which can be tuned by controlling their size, shape, and composition. This makes them useful for applications in photocatalysis, sensing, and imaging.
- **Magnetic Properties:** Some metal oxide nanoparticles, such as iron oxide and cobalt oxide, exhibit magnetic properties that can be exploited for applications in data storage, magnetic separation, and biomedicine.
- **Electronic Properties:** Metal oxide nanoparticles can exhibit unique electronic properties, such as semiconducting behavior, high dielectric constants, and resistive switching, which are useful for applications in electronics, energy storage, and sensing.[11]

1.3 Optical Properties

Optical properties of nanomaterial such as absorption, transmission, reflection, and light emission are dynamic and may differ significantly from properties exhibited by the same bulk material. A wide range of optical effects may be produced for a variety of applications by simply manipulating its shape, size, and surface functionality. This manipulation may be achieved via different means, depending on the composition, size, and orientation. The optical properties of nanomaterial are very important in a variety of ways. They are capable of confining their electrical properties to produce a quantum effect with the possibility of the variation in shape, size, or type having effect on the color they produce. [12]

1.3.1 Types of Optical Properties

- **Absorption:** a Participial Absorption Energy That is transferred from the wave into the particles of a substance.
- **Transmission:** A wave passes through a substance .
- **Reflection:** A wave hits a boundary between two media and does not pass through, but instead stays in the original medium, resulting in reflection. as depicted in Figure 1.4 . [13]

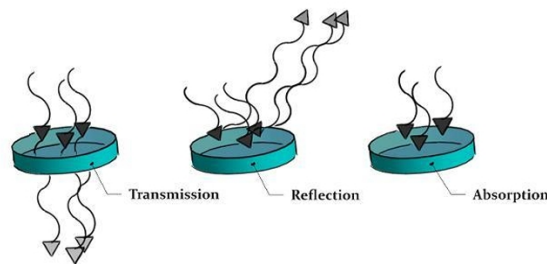


Figure 1.4: Optical properties of materials

1.4 spectrum

Spectrum is the distribution of electromagnetic radiation intensity (such as light) as a function of wavelength or frequency. It can be continuous, containing all wavelengths, or a line spectrum, consisting of discrete lines unique to each element. Another type is the band spectrum, which appears as closely spaced groups of lines and is associated with molecular radiation, as indicated in Figure 1.5 [14].

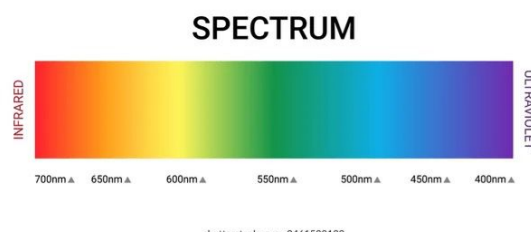


Figure 1.5: Spectrum

1.5 Nano applications

Nanoparticles, due to their unique or enhanced physicochemical properties, are used in a wide range of applications in across various fields. Here, we present some examples of these applications in Figure 1.6 .[15]



Figure 1.6: Nanoparticles applications .

1.6 Nano composites with polymer

Polymer matrices and tiny quantities (e.g. a few weight percent of the polymer matrix) of nanometer-sized additives make up polymer nanocomposites.

The goal of creating polymer nanocomposites is to enhance the mechanical, thermal, and electrical characteristics of polymers. The primary difference between polymer nanocomposites and conventional polymer composites, like carbon fiber-reinforced polymers, is the size of the interfacial region between polymer matrices and nanometer-sized fillers. The performance properties of polymer nanocomposites may surpass those of conventional polymer composites.[16]

1.6.1 Types of nanofillers in polymer nanocomposites

1. Nanoplatelets (One Nanoscale Dimension) : Nanofillers with one nanoscale dimension, such as thin sheets. Example: Graphene nanoplatelets.
2. Nanofibers (Two Nanoscale Dimensions): Nanofillers with two nanoscale dimensions, where the length is usually on the micron scale. Example: Nanocellulose fibers.
3. Nanoparticles (Three Nanoscale Dimensions): Nanofillers with all three dimensions in the nanoscale range, Example: Silica nanoparticles.

1.7 Advantages of Polymer nanocomposites

The important advantages of polymer nanocomposites include increased stiffness, increased resistance to fire, increased thermal and dimensional stability, good optical prop-

erties, and improved barrier effect. The polymer nanocomposites have certain advantages over conventional composites and neat polymers, such as:

1. Polymer nanocomposites are much lighter than the conventional composites.
2. Their thermal and mechanical properties are potentially superior.
3. The barrier properties of polymer nano-composite are much enhanced as compared to pristine polymer.
4. They exhibit increased biodegradability of biodegradable polymers and excellent flammability properties.

Some of the potential applications of polymer nanocomposites in renowned fields are discussed below. Figure 1.7 shows the different uses of polymer nanocomposites in various fields.[17]

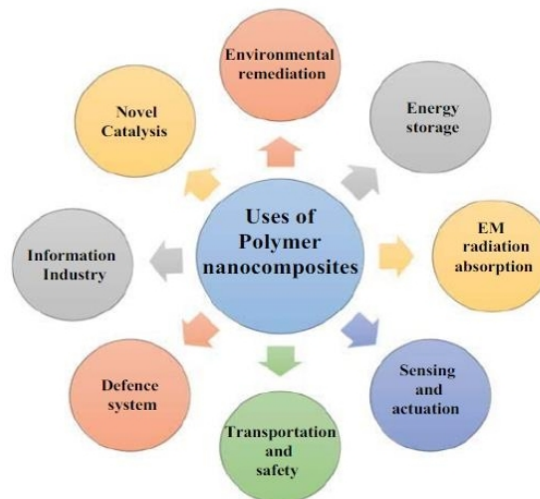


Figure 1.7: Different uses of polymer nanocomposites

1.8 Applications of Polymer Nanocomposites

Polymer Nanocomposites have unique properties and applied in many areas, including:

1.8.1 Energy and Electrical Applications

Owing to terrific energy storage capacity, polymer nanocomposites are potentially utilized in the field of electrical field and equipment, Polymer nano-composite having conductive NPs as fillers can synthesize conductive polymer nanocomposite offer applications in the electronic devices. Polymer nanocomposite-based electrode materials show greater stability and ability, and the synergetic effects are generated by the interaction between the

nanocomposite components. Nanocomposites containing high dielectric polymer can store energy electrostatically and are utilized widely in electric power systems and electronics due to their durability, capability to configure in different shapes and high breakdown strengths.

1.8.2 Medical applications

The fabrication of polymer nano-composites into the hierarchical nano-structure scan creates functional nano-materials having advanced properties for different bio-medical applications, Polymer nanocomposites were potentially utilized for antibacterial activity drug delivery, magnetic resonance imaging ,bone tissue engineering , and dental materials.

1.8.3 Adsorption of pollutants

Polymer nanocomposites have attracted technologists and scientists in water purification processes and systems due to high surface area, improved processability, stability, cost-effectiveness, and tunable properties. Polymer nanocomposites exhibit rapid decontamination efficacy with high selectivity in removing different pollutants. Polymer nanocomposites were extensively utilized for the adsorption of various dyes, metallic ions and microorganisms from wastewater.

1.8.4 Sensing applications

The electrochemical properties of the polymer nanocomposites as transducers can be utilized potentially for the manufacturing of biosensors and electro-chemical sensors, The impact of nano-fillers in the polymer nanocomposites plays a key role in the sensing, processing, and actuating capabilities of the nanocomposite electrodes in biosensing and electrochemical applications. Polymer nanocomposites are utilized for the sensing of gases, metal ions, and DNA.

1.9 UV-Visible Spectrometer-Absorption Theory

These electronic transitions are generally associated with changes in the energy levels of electrons within atoms, ions, or molecules. This results in absorption spectra that are characteristic of the atoms and molecules involved in the electronic transitions.

1.10 Beer-Lamber

Beer's Law is an equation that relates light's attenuation to a material's properties. The law states that a chemical's concentration is directly proportional to a solution's ab-

sorbance. You may use this relation to determine a chemical species' concentration in a solution using a colorimeter or spectrophotometer. The relation is most often used in UV-visible absorption spectroscopy. Note that Beer's Law is not valid at high solution concentrations, as indicated in Figure 1.8. [18]

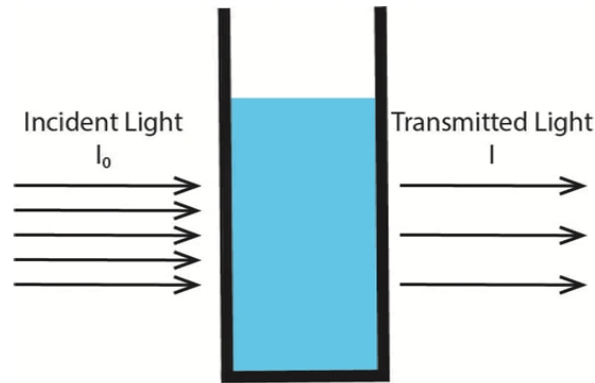


Figure 1.8: Beer- Lambert diagram.

When radiation passes through a solution, the amount of light absorbed or transmitted is an exponential function of the solute's molecular concentration and the length of the path the radiation

$$\frac{I}{I_0} = e^{-\alpha l} \quad (1.1)$$

travels through the sample. Therefore,

Where I_0 is the intensity of the incident light, I is the intensity of light transmitted through the sample, l is the thickness of the sample, and α is the absorption coefficient

$$\log_{10} \frac{I}{I_0} = \alpha l \log e \quad (1.2)$$

The ratio I / I_0 is known as transmittance T , and the logarithm of the inverse ratio I_0 / I is known as the absorbance A . Mathematically, absorbance is related to percentage transmittance T by the expression:

$$A = \log_{10} \frac{I_0}{I} = 0.4343 \alpha l \quad (1.3)$$

$$\alpha = \frac{A}{l \times 0.4343} = 2.303 \frac{A}{l} \quad (1.4)$$

1.11 Optical band gap

The calculation of the optical band gap is carried out using two methods:

- The first method is determined by:

$$E_g = hv = \frac{hc}{\lambda} = \frac{1240(ev.nm)}{\lambda(nm)} \quad (1.5)$$

Where v is the frequency, h is Planck's constant, and c is the speed of light

- The second method is the Tauc equation

The absorption in the UV and visible regions is attributed to direct allowed transitions of electrons from the valence band to the conduction band. The value of the band gap can be

$$(\alpha hv)^n = \beta(hv - E_g) \quad (1.6)$$

determined from the equation

here β is constant, $n=0.5, 2, 2/3$, and $1/3$, depending on the nature of the transition for indirect allowed, direct allowed, direct forbidden, and indirect forbidden transitions respectively. Plotting a graph of $(\alpha hv)^n$ versus the photon energy hv . Comparing the Tauc equation with the straight-line equation by putting the y-axis equal to zero, and fitting a straight line to the linear part of the graph to give the value of the optical band gap

$$y = mx + c \quad (1.7)$$

$$0 = \beta(hv - E_g) \quad (1.8)$$

$$hv = E_g \quad (1.9)$$

1.11.1 Types of band gap

- **Energy gap is direct:** In materials with a direct band gap, electrons can transition directly from the valence band to the conduction band without the need for a change in momentum. This means that the electronic transition occurs directly, allowing the material to absorb light efficiently at the specific wavelength, transitioning electrons directly from the valence band to the conduction band. Electrons move faster in this case, making direct band gap materials more efficient in light absorption. Examples of materials with a direct band gap include germanium and certain organic semiconductors.
- **Energy gap is indirect:** In materials with an indirect band gap, the transition from the valence band to the conduction band requires a change in momentum.

This means that the electrons do not transition directly but need to absorb or emit photons or phonons (vibrational states of the crystal lattice) to conserve momentum. Therefore, the transitions are less efficient in light absorption compared to direct band gap materials. Silicon is an example of a material with an indirect band gap [19].

1.12 Urbach Energy

Urbach Energy (Eu) represents the width of the exponential tail in the optical absorption spectrum near the band edge. It quantifies the degree of disorder in materials, including structural or thermal disorder. Lower Eu values indicate a more ordered structure, while higher values suggest significant disorder .[20]

The Urbach Energy is derived from the relationship between the absorption coefficient (α) and photon energy (E):

$$\alpha(E) = \alpha_0 \exp\left(\frac{E - E_0}{E_u}\right) \quad (1.10)$$

1.13 Literature review

The Polymer nanocomposites have received considerable interest during the past few years due to their enhanced properties. In particular, PVC/PbO composites demonstrated improved water uptake, swelling, and ion exchange capacity, while PVC/PbO/graphite composites exhibited higher porosity and ionic conductivity. Optimal performance was achieved at specific filler concentrations [21].

Moreover, increasing the PbO content in the composites has been shown to enhance radiation attenuation. The best shielding performance was observed with PVC nanocomposites, which provided optimal radiation protection for both gamma rays and X-rays [22].

PbO has also proven effective in de-halogenating mixed halogenated plastic wastes, highlighting its potential in waste treatment applications [23].

Further studies showed that the addition of PVA increased the transparency of the films, while the incorporation of CuO decreased it. Both the insulating and optical properties were modified as a result of these additions[24].

Additionally, increasing PbO concentration in PVC improved its density, refractive index, and radiation shielding properties, while reducing the optical band gap and neutron shielding efficiency [25].

Lastly, the enhancement of the optical and electrical properties of PVA through blending with PVP and incorporating MgO nanoparticles has been observed. The films, fabricated using solution casting, demonstrated improved properties with the inclusion of MgO [26].

The literature [27] reports the development of highly transparent PVC/ (Cd_{0.5}Zn_{0.5}O) nanocomposite films with excellent UV-shielding efficiency and enhanced thermal stability.

Olad and Nosrati [28] successfully synthesized a PVC/ZnO–polyaniline hybrid nanocomposite coating, significantly improving corrosion protection for iron.

Chapter 2

Experimental Methods

2.1 Preparation Methods

PbO nanoparticles were synthesized using the sol-gel method. Lead acetate and oxalic acid were dissolved in double-distilled water and magnetically stirred. The resulting sol was heated to facilitate gel formation, then cooled while stirring and allowed to age at room temperature. Finally, the gel was subjected to high-temperature treatment to obtain PbO nanoparticles.[29]

2.2 Sample

In this study, a pre-prepared samples are PVC (pure), PVC/1%Pbo and PVC/2%Pbo with of nano Lead oxide (PbO) ranges from 24 nm to 70 nm. The samples were measured and tested using UV - Vis spectrophotometer. The sample of Pbo nanoparticles is shown in Figure 2.1.[30]

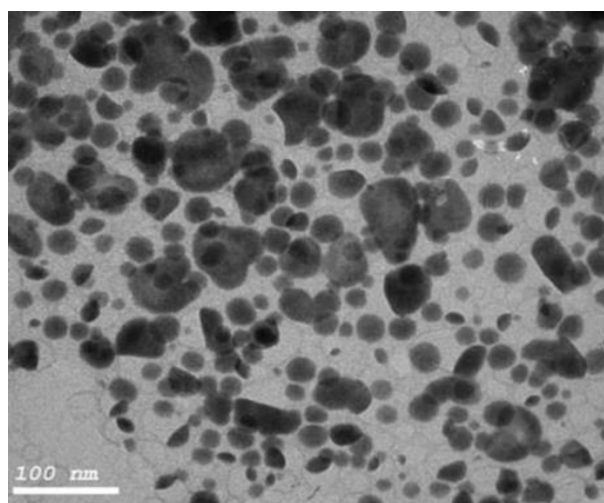


Figure 2.1: HR-TEM of Pbo nanoparticles

2.3 Spectrophotometer UV-VIS Device



Figure 2.2: Spectrophotometer UV-VIS Device

UV-Vis spectroscopy (SHIMADZU) was employed to analyze the sample, offering detailed information on its absorbance properties within the ultraviolet and visible regions. The measurements identified key absorption peaks, revealing the presence of specific chromophores or electronic transitions. To ensure precision, baseline corrections were applied, and appropriate solvents and cuvettes were chosen to minimize interference. This technique provided reliable data for accurately detecting the sample's optical properties, facilitating its identification and characterization. The measurement method in UV-visible spectroscopy involves several interconnected steps to ensure accurate results. Here are the basic steps:

1. Prepare The samples:

Prepare the samples without impurities and use appropriate tools to hold the sample to avoid fingerprints

2. Instrument Calibration:

Use the sample's solvent as the "blank" to measure the background and correct the readings. Set the instrument to the appropriate wavelength based on the expected absorption spectrum of the substance.

3. Measuring the Sample:

The instrument directs light at the selected wavelength through the sample. The intensities of the incident and transmitted light are recorded to obtain the absorption data.

4. Data Analysis:

The recorded data is used to analyze. The resulting spectrum can provide qualitative insights about the molecular structure and transitions within the substance.

These steps ensure an accurate and reliable absorption spectrum.

Chapter 3

Result and Discussion

3.1 Spectrophotometer UV-VIS Device Result

The UV-Vis spectrum for PbO is studied between 200 to 800 nm, encompassing the ultraviolet and visible regions, and The absorption Peaks of Pbo appear in two regions:

- 1. UV Region (200-400 nm):** Strong absorption is typically observed in this region due to electronic transitions in PbO. Peaks are often located between 250 and 300 nm, depending on factors like particle size and crystalline phase.
- 2. Visible Region (400-800nm):** Absorption in this range is weaker but may appear due to material-specific properties like aggregation or structural variations.

These results were obtained using a UV device, as shown in Figure 3.1, indicating that absorption increases at a PbO concentration of 2%, reaching its highest level within the 200 to 330 range and . In contrast, absorption decreases at a PbO concentration of 1% between 200 and 310. For pure PVC, the absorption rate was lower. It is evident that as the PbO concentration increases, absorption increases , with pure PVC exhibiting the lowest absorption 1 .

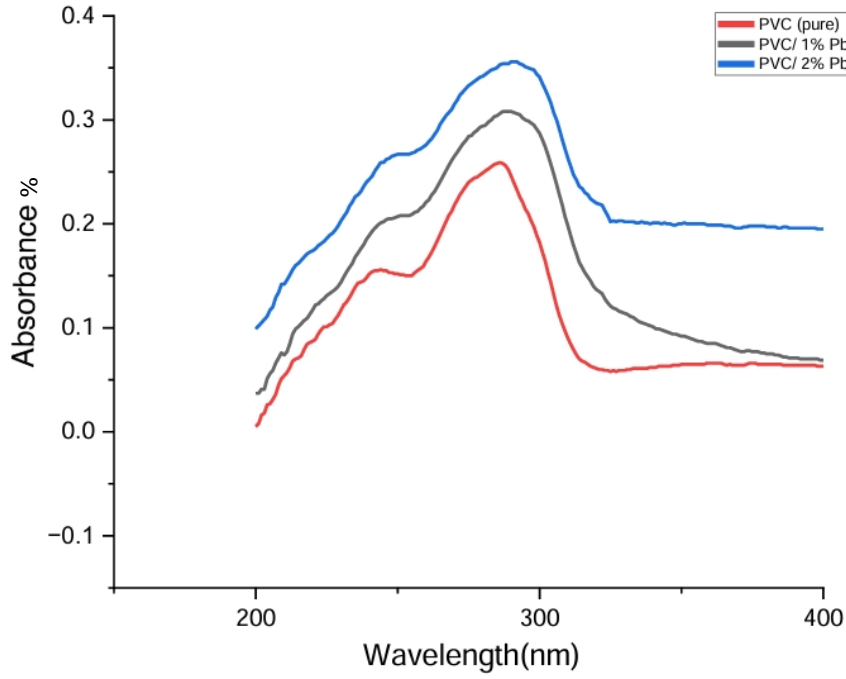


Figure 3.1: Absorbance Peaks

3.2 Energy gap

The bandgap energy (E_g) was evaluated using the Tauc plot equation given by:

$$\alpha h\nu = A(h\nu - E_g)^n \quad (3.1)$$

where h is Planck's constant, A is a constant, ν is the incident radiation frequency, n equals 2 for direct band gap materials, and α is the absorption coefficient, which was calculated from the relation:

$$\alpha = \frac{2.303A}{d} \quad (3.2)$$

where A is the measured absorbance, and d is the path length of light. The bandgap energy (E_g) can be estimated by plotting $(\alpha h\nu)^2$ versus the energy $h\nu$, and extrapolating the linear portion of the plot to the x-axis. From The Figures 3.2, 3.3, and 3.4 we found that band gap energy for pure PVC is 3.8 eV, 3.7 eV for PVC/1% Pbo, and 3.5 eV for PVC/2%, as shown in Table 3.1. Our result, which did not differ significantly from previous measurements, showed that the band gap of PVC was 4 eV[31].

sample	Optical band gap
PVC(pure)	3.8 ev
PVC/%1 Pbo	3.7 ev
PVC/%2Pbo	3.5 ev

Table 3.1: Valued for direct band gap

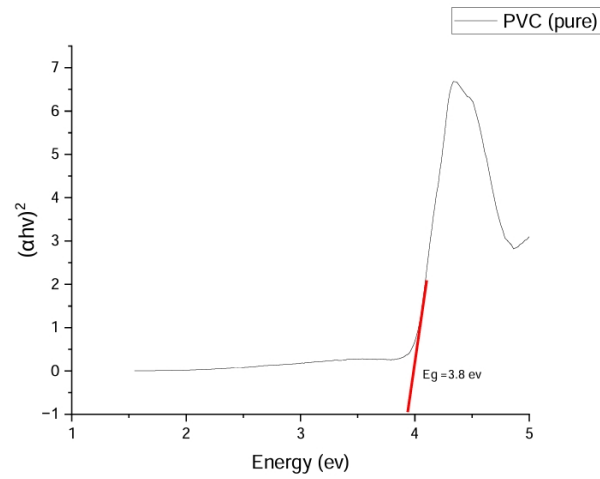


Figure 3.2: band gap of PVC(pure)

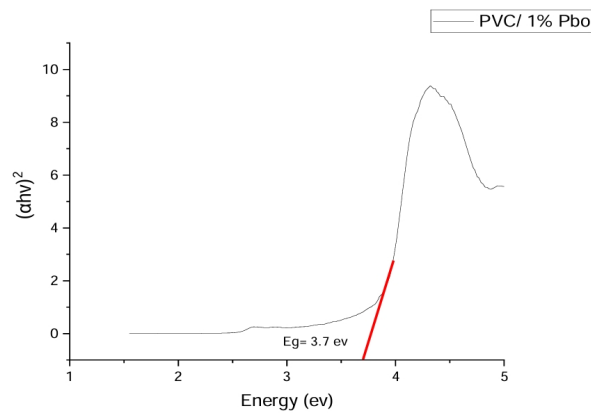


Figure 3.3: band gap of PVC/1% Pbo

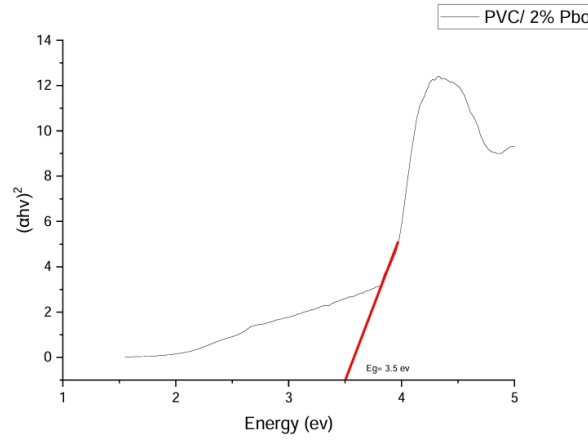


Figure 3.4: band gap of PVC/2% Pbo

3.3 Urbach Energy

The Urbach energy (EU) was calculated based on the band gap (Eg) value determined using UV-Vis measurements. According to the empirical Urbach relation, the Urbach energy was extracted by analyzing the exponential behavior of the absorption coefficient near the absorption edge, where the equation:

$$\alpha = \alpha_0 \exp\left(\frac{hv - E_g}{E_u}\right) \quad (3.3)$$

was applied. EU was determined from the experimental data using this equation, providing an accurate estimate of the Urbach energy associated with the density of states in the electronic bands of the studied materials. The results are presented in the table 3.2 below .

Sample	Urbach Energy (Eu)
PVC(pure)	0.172 ev
PVC/1% Pbo	0.872 ev
PVC/ 2%Pbo	0.95 ev

Table 3.2: Values for Urbach Energy of (Pbo)

As illustrated in Figures 3.5, 3.6, and 3.7, the Urbach energy (Eu) increases with the increasing concentration of the sample. This indicates a rise in structural defects and disorder within the electronic structure of the studied materials. The trend suggests that the increase in Urbach energy is linked to a higher density of localized states in the band structure, attributed to variations in composition, lattice distortions, and defects. This provides a better understanding of the optical and electronic behavior of the studied materials

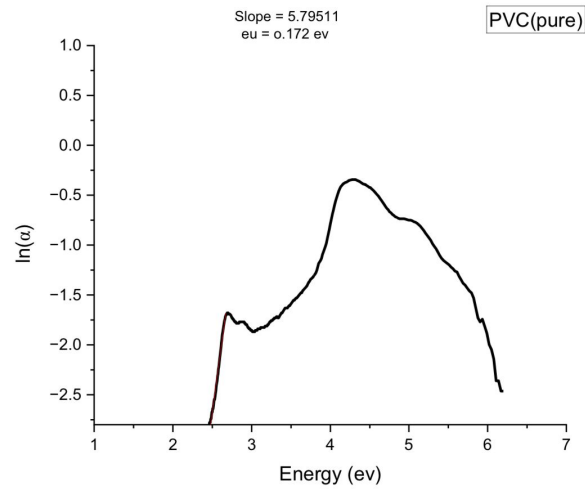


Figure 3.5: Urbach Energy of PVC(pure)

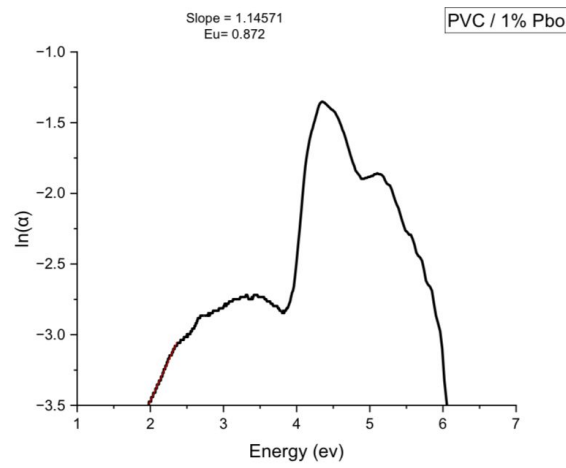


Figure 3.6: Urbach Energy of PVC/1% Pbo

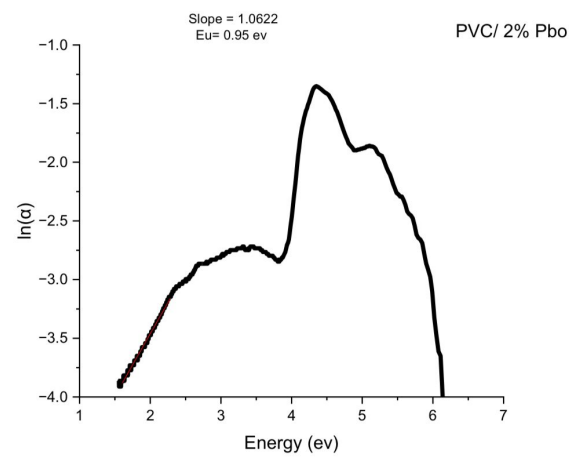


Figure 3.7: Urbach Energy of PVC/2% Pbo

Conclusion

In this study , lead oxide (PbO) was studied at different concentrations on nanocomposite films made from polyvinyl chloride (PVC) in diff concentrations PVC (pure) ,PVC/1% PbO and PVC/2% PbO The structural and optical properties of these films were investigated, noting the effect of increasing PbO concentration on the material's properties. It was observed that The direct optical band occurred and decreased with increasing PbO content. which was measured using a UV-Vis spectrophotometer, indicating an improvement in the optical properties due to the increased PbO concentration.

Reference

- [1] The Editors of Encyclopaedia Britannica. "Polymer." Encyclopaedia Britannica. Last. modified December 11, 2024. Revised by Erik Gregersen
- [2] Patrick, Stuart. Practical guide to polyvinyl chloride. iSmithers Rapra Publishing, 2005.
- [3] Patrick, Stuart. Practical guide to polyvinyl chloride. iSmithers Rapra Publishing, 2005. .
- [4] Yong, Ming, et al. "Properties of polyvinyl chloride (PVC) ultrafiltration membrane improved by lignin: Hydrophilicity and antifouling." Journal of membrane science 575 (2019): 50-59.
- [5] Khan, Ibrahim, Khalid Saeed, and Idrees Khan. "Nanoparticles: Properties, applications and toxicities." Arabian journal of chemistry 12.7 (2019): 908-931.
- [6] Biswas, Pratim, and Chang-Yu Wu. "Nanoparticles and the environment." Journal of the air & waste management association 55.6 (2005): 708-746
- [7] Kumari, Savita, and Leena Sarkar. "A review on nanoparticles: structure, classification, synthesis& applications." Journal of Scientific Research 65.8 (2021): 42-46.
- [8] Joudeh, Nadeem, and Dirk Linke. "Nanoparticle classification, physicochemical properties, characterization, and applications: A comprehensive review for biologists." Journal of Nanobiotechnology, vol. 20, 2022, article 262.
- [9] Alhalili, Zahrah. "Metal oxides nanoparticles: general structural description, chemical, physical, and biological synthesis methods, role in pesticides and heavy metal removal through wastewater treatment." Molecules 28.7 (2023): 30-86.
- [10] García-Ovando, Axel E., et al. "Biosynthesized nanoparticles and implications by their use in crops: Effects over physiology, action mechanisms, plant stress responses and toxicity." Plant Stress 6 (2022): 100-109.
- [11] Radu, A. I., et al. "Physical properties of metal oxide nanoparticles processed as thin films by MAPLE technique." Romanian Reports in Physics 72 (2020):

5032020.

[12] Adewuyi, Adewale, and Woei Jye Lau. "Nanomaterial development and its applications for emerging pollutant removal in water." Handbook of nanotechnology applications. Elsevier, 2021. 67-97.

[13] Grover, Jasmine. "Optics: Light, Optical Properties, Types, and Applications." Collegedunia, 3 Apr. 2019.

[14] Zwinkels, Joanne. "Light, electromagnetic spectrum." Encyclopedia of Color Science and Technology 8071 (2015): 1-8.

[15] Chouke, Prashant B., et al. "Bioinspired metal/metal oxide nanoparticles: A road map to potential applications." Materials Today Advances 16 (2022): 100-314.

[16] Sundarram, S., Y-H. Kim, and W. Li. "Preparation and characterization of poly (ether imide) nanocomposites and nanocomposite foams." Manufacturing of Nanocomposites with Engineering Plastics. Woodhead Publishing, 2015. 61-85 .

[17] Khan, Idrees, et al. "Polymer nanocomposites: an overview." Smart Polymer Nanocomposites (2023): 167-184.

[18] Beer, A. (1852). "Bestimmung der Absorption des rothen Lichts in farbigen Flüssigkeiten." Annalen der Physik und Chemie, 86(10), 78-88.

[19] Yu, P. Y., and Cardona, M. (2010). Fundamentals of Semiconductors: Physics and Materials Properties (4th ed.). Springer.

[20] Urbach, F. (1953). "The long-wavelength edge of photographic sensitivity and of the electronic absorption of solids." Physical Review, 92(5), 1324.

[21] Kuttithathil, Mohamed Shafi, et al. "Unlocking the dehalogenation potential of Lead Oxide (PbO) via its co-pyrolysis with polyvinyl chloride(PVC) and Novel Brominated Flame Retardants (NBFRs)." Case Studies in Chemical and Environmental Engineering (2024): 100-785.

[22] Yazdani-Darki, Sepideh, et al. "Preparation and structural characterization of PbO and WO₃-PVC hybrid nanocomposites for gamma ray radiation shielding." Radiation Physics and Chemistry 229 (2025): 112-489.

[23] Mohammed, Gh, Adel M. El Sayed, and W. M. Morsi. "Spectroscopic, thermal, and electrical properties of MgO/polyvinyl pyrrolidone/polyvinyl alcohol nanocomposites." Journal of Physics and Chemistry of Solids 115 (2018): 238-247.

[24] Raza, Junaid, et al. "Preparation and comparative evaluation of PVC/PbO and PVC/PbO/graphite based conductive nanocomposites." Zeitschrift für Physikalische Chemie 236.11-12 (2022): 1583-1601.

[25] Yazdani-Darki, Sepideh, et al. "Preparation and structural characterization of PbO and WO₃-PVC hybrid nanocomposites for gamma ray radiation shielding." Radiation Physics and Chemistry 229 (2025): 112-489.

-
- [26] El Sayed, A. M., et al. "Effect of PVA and copper oxide nanoparticles on the structural, optical, and electrical properties of carboxymethyl cellulose films." *Journal of Materials Science* 50 (2015): 4717-4728.
- [27] W.E. Mahmoud and A.A. Al-Ghamdi, *Polym. Compos.*, 32, 1143 (2011).
- [28] A. Olad and R. Nosrati, *Prog. Organ. Coat.*, 76, 113 (2013). 10. I.S. Elashmawi, N.A. Hakeem, L.K. Marei, and F.F. Hanna, *Phys. B*, 405, 4163 (2010).
- [29] El Sayed, A. M., and W. M. Morsi. "Dielectric relaxation and optical properties of polyvinyl chloride/lead monoxide nanocomposites." *Polymer Composites* 34.12 (2013): 2031-2039.
- [30] El Sayed, A. M., and W. M. Morsi. "Dielectric relaxation and optical properties of polyvinyl chloride/lead monoxide nanocomposites." *Polymer Composites* 34.12 (2013): 2031-2039.
- [31] El Sayed, A. M., and W. M. Morsi. "Dielectric relaxation and optical properties of polyvinyl chloride/lead monoxide nanocomposites." *Polymer Composites* 34.12 (2013): 2031-2039.