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

Optical Properties of Nano TiO_2|PVA Composite

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
Abeer Al-Kathiri

Supervisor
Prof. Wafaa Morsi

IMSIU-Riyadh-KSA
May , 2025

Contents

Table of Contents

List of Figures

List of Tables

Acknowledgements

I sincerely thank Allah, the Almighty, for giving me the strength and guidance to complete this research successfully. I’m very grateful to my supervisor, Professor Wafaa Morsi, for her valuable advice and continuous support throughout this project. Her expertise and encouragement were key to finishing this thesis. I also want to express my heartfelt thanks to the dedicated staff of the Central Laboratory at Imam Muhammad Ibn Saud Islamic University for their technical assistance and for providing the necessary equipment and support that were essential to the progress of this study. A big thanks goes to my beloved family for their constant support and motivation, which kept me going and helped me succeed. Lastly, I’m truly grateful to my dear friends for their moral support and encouragement, which helped me get through the tough times and made this journey easier.

Abstract

This study investigates the effect of incorporating titanium dioxide (TiO_2) nanoparticles into polyvinyl alcohol (PVA) on its optical properties. A concentration of 2.5% TiO_2 was used, and the results were compared with those of pure PVA. The optical properties were examined by measuring the absorption, optical band gap (Eg), and Urbach energy (EU) using a UV-Visible spectrophotometer. Additionally, the samples were analyzed using Fourier-transform infrared (FTIR) spectroscopy. The results showed that the addition of TiO_2 increased the absorption. Furthermore, the Urbach energy was found to be higher in pure PVA. These findings indicate that the incorporation of TiO_2 enhances the optical properties of PVA, suggesting its potential for improved performance in optical applications.

الملخص

تهدف هذه الدراسة إلى تحليل تأثير إضافة جسيمات نانوية من ثاني أكسيد التيتانيوم TiO_2 على الخصائص البصرية لمادة بولي فينيل الكحول (PVA). تم تحضير عينات من (PVA) تحتوي على نسبة 2.5% من TiO_2، ومقارنتها بعينة من PVA النقي. وقد تم تقييم الخصائص البصرية من خلال دراسة الامتصاص، وفجوة الطاقة البصرية (E_g)، وطاقة أورباخ (E_U)، باستخدام جهاز مطياف الأشعة فوق البنفسجية-المرئية (UV-Visible Spectrophotometer). بالإضافة إلى ذلك، تم تحليل العينات باستخدام جهاز FTIR. أظهرت النتائج أن زيادة تركيز TiO_2 يؤدي إلى ارتفاع في معامل الامتصاص، كما لوحظ انخفاض في طاقة أورباخ مع زيادة تركيز TiO_2، توضح هذه النتائج أن إضافة TiO_2 يُسهم في تحسين الخصائص البصرية لمادة PVA، مما يجعلها أكثر كفاءة للاستخدام في التطبيقات البصرية.

Chapter 1

The optical properties of materials refer to how a material interacts with light, These properties play a crucial role in many modern technological applications, such as optical devices, sensors, and solar cells. In nanomaterials, these properties can change significantly due to the interaction between light and the nanostructure of the material, opening new possibilities for enhanced performance in various applications.

1.1 Nanoparticles

Nanometers is used as a prefix for any unit such as a second or a meter, and it means a billionth of that unit. Hence, a nanometer (nm) is a billionth of a meter, or 10^{-9} meters.[1]

1.1.1 Nano types and shapes

Nanomaterials are classified based on the types of materials they are derived into four main categories:

1-Carbon-based materials:
These include substances such as graphene and nanodiamonds, which exhibit unique mechanical, electrical, and thermal properties due to their carbon-based molecular structures.

2-Organic nanomaterials:
These consist of compounds that contain carbon atoms typically bonded with hydrogen, and may also include other elements such as oxygen, nitrogen, and sulfur. They are often used in drug delivery systems and biodegradable materials.

3-Inorganic nanomaterials:
These do not contain carbon and include metals, metal oxides, and semiconductors. They are widely applied in fields such as catalysis, sensing, and electronics.

4-Composite nanomaterials:

These are combinations of two or more different types of nanoparticles, such as metals, ceramics, or polymers, designed to achieve enhanced or multifunctional properties. Composite nanomaterials are commonly used in commercial products, including vacuum cleaners, mobile phone covers, and structural components.

Nanomaterials can exhibit a wide range of shapes and sizes, which allows them to be tailored for diverse applications across science, industry, and medicine. They are also categorized by dimensionality into four types (0D, 1D, 2D, and 3D), depending on the number of dimensions within the nanoscale range.There are four different kinds of dimensions shown in the figure1.1:

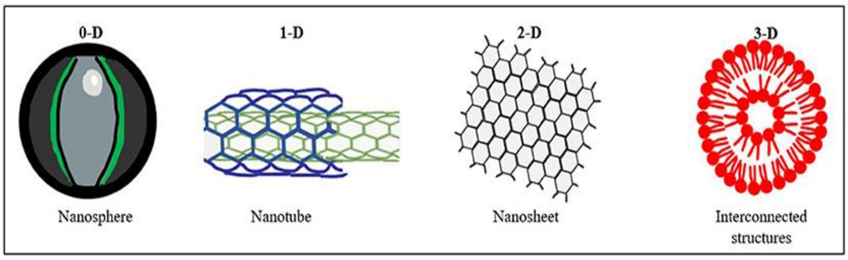

Figure 1.1: nanomaterials in different shapes and dimensions.

1. 0-D would be a tiny dot, like quantum dot nanomaterials.
2. 1-D would be a straight line, like nanorods.
3. 2-D would be a square/rectangle, like nanosheets.
4. 3-D would be two or more structures that are joined together.[2]

1.1.2 Metal oxide nanoparticles

Metal oxide nanoparticles is considered as one of the most emerging nanomaterials in many areas due to their unique physical and chemical properties, such as thermal conductivity and heat transfer In oil and gas industry.[3]

1.1.3 Optical Properties of TiO_2

Titanium dioxide and its modified forms are of interest for use in solar batteries and their ability to generate active radicals under ultraviolet radiation, which have oxidizing and bactericidal effects. These photochemical methods for cleaning air and water are being actively developed in many countries. Under UV irradiation, titanium dioxide can decompose water into molecular hydrogen and oxygen, while modified TiO_2 can achieve similar effects under sunlight. Materials based on titanium dioxide are considered promising for chemical sensors. Additionally, TiO_2 can facilitate the production of methane from water and carbon dioxide under UV irradiation. [4]

1.1.4 Applications of nanoparticles

The applications of nanoparticles include drug-delivery systems, cancer targeting, dentistry [5]

Figure 1.2: Nanomaterials applications

1.2 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. Polymers make up many of the materials in living organisms, including, for example, proteins, cellulose, and nucleic acids. Moreover, they constitute the basis of such minerals as diamond, quartz, and feldspar and such man-made materials as concrete, glass, paper.[6]

1.2.1 Polyvinyl Alcohol (PVA)

Polyvinyl alcohol (PVA) is a unique water-soluble polymer, widely used in papermaking, textiles, and a variety of coatings. This is a biocompatibility polymer which is used as scaffolding for cell cultures, embolic materials, contact lenses and wound dressings. This polymer is being used in an increasing number of applications for both environmental engineering and electrical materials.[7]

$[CH_2CH(OH)]_n$.

"It is prepared by the hydrolysis of polyvinyl acetate".[8]

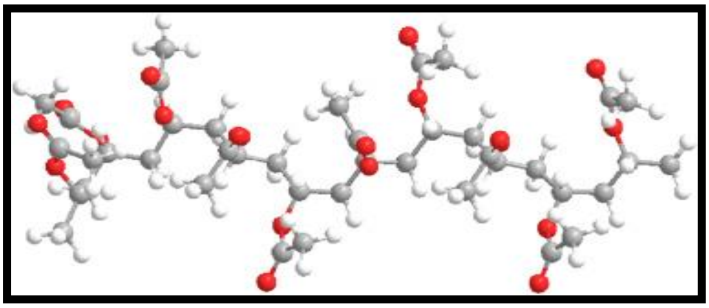

Figure 1.3: polyvinyl alcohol (PVA)

1.2.2 properties of polyvinyl alcohol (PVA)

a) Physical Properties of PVA:

1. PVA shows high tensile strength and flexibility.
2. It is soluble in water and has no odor.
3. PVA molecular weight or polyvinyl molecular weight ranges between 26,000-30,000.
4. Its melting point is 185°C.
5. It is insoluble in organic solvents but slightly soluble in ethanol.

b) Chemical Properties of PVA:

1. Polyvinyl alcohol can react with butyraldehyde and formaldehyde.
2. It is atactic type material and resistant to oil and grease.[9]

1.2.3 PVA NANOCOMPOSITES

A polymer composite is made of a polymer matrix and reinforcing fillers, which can be micro- or nanosized. These composites show new properties not found in the filler or matrix alone. Adding fillers changes the physical and chemical properties of the polymer. The final properties depend on the type, size, shape, amount, and interaction of the fillers. Common fillers include metal powders, chalk, polymer fibers, glass fibers, and carbon fibers. [10]

1.2.4 TiO2 PVA

A recent study investigated the effect of polymer chain size and polyvinyl alcohol (PVA) concentration on the thermal and electrical conductivity of TiO2-based nanofluids. The results showed that increasing the polymer concentration led to a decrease in thermal conductivity, while in nanofluids without polymer, thermal conductivity increased as particle concentration rose. This reduction is attributed to the presence of polymers at the interface or in the dispersion medium, which increases interfacial thermal resistance and reduces heat transfer. Additionally, the viscosity of the nanofluids increased with higher polymer concentration, affecting flow properties. The researchers concluded that to achieve a significant improvement in thermal conductivity, an optimal concentration of PVA must be used.[11]

1.3 Polymer nanocomposites

Polymer nanocomposites are the composites of nanosized inorganic particles dispersed in polymer matrix, Polymers are the combination of monomers with properties of flexible, lightweight and low-cost production,Inorganic nanomaterials have electrical, mechanical catalytic and magnetic properties. By combining both we get new material with different applications can be got.[12].

1.3.1 Applications of polymer nanocomposites

-Water Treatment

PNCs could be used in the field of water treatment to achieve various purposes, including the removal of dyes, metal ions, and microorganisms from water.

-Sensor Devices

Sensors have various applications, including chemical and toxic gas detection for safety, medical diagnosis, and defense. To be effective, sensors should be small, multifunctional, low-cost, reliable, and exhibit rapid response, high sensitivity, and selectivity. Rapid response and high sensitivity are linked to a large specific surface area, making polymer nanocomposites promising candidates for sensor fabrication.

-Food Packaging

Food packaging must effectively prevent microbial contamination and control moisture loss or gain, while also serving as a barrier against the permeation of oxygen, carbon dioxide, water vapor, and other volatile compounds that can affect taste and odor. Additionally, packaging materials should possess essential properties such as thermal stability, optical clarity, and mechanical strength, Polymer nanocomposites (PNCs) represent an innovative class of materials considered promising candidates for food packaging applications due to their outstanding thermal and mechanical properties, and excellent barrier performance. [13]

1.3.2 Advantages of polymer nanocomposites

Polymer nanocomposites have many advantages over traditional materials in different industries:

1) Mechanical, thermal, and electrical improvements: Adding nanoparticles makes the material stronger, more heat-resistant, and better at conducting electricity. This increases the durability and makes nanocomposites useful in advanced electronics.
2) Automotive industry: In cars, nanocomposites are lightweight but still very strong. This helps reduce the car's weight, save fuel, and improve overall performance without affecting safety.
3) Aerospace industry: In aircraft, these materials are important for making parts that are both light and tough. This helps airplanes perform better and use less fuel.
4) Electronics: Because of their excellent heat and electrical properties, nanocomposites are used to make smaller and more efficient electronic devices, such as smartphones, chips, and other smart technologies.
5) Biomedical field: Nanocomposites are used in medical tools like implants, tissue supports, and systems that release medicine slowly. They are safe to use inside the body and help create new ways to treat patients more effectively.[14]

1.4 Optical Properties

Optical properties are also a very important characteristic of glass. These properties determine how glass interacts with light and are generally divided into three main categories: refraction, absorption, and transmission of light.[15] In addition, spectrum in physics refers to the intensity of light as it varies with wavelength or frequency. Spectra are typically classified based on their origin into emission or absorption spectra.[16]

1.4.1 Absorption

Absorption spectra refer to the measurement of how much light is absorbed by a substance at different wavelengths. An absorption spectrum shows portions of a continuous spectrum that are missing because they have been absorbed by the medium through which the light has passed. These missing wavelengths appear as dark lines or gaps.[17]

1.4.2 Transmission

A transmission spectrum refers to the pattern of how light or other electromagnetic radiation passes through a material, shown as a function of wavelength. It helps in understanding how much light is transmitted at each wavelength.[18]

1.4.3 Refraction

Refraction, in physics, is the change in direction of a wave as it passes from one medium to another due to a change in its speed. This property affects how light bends when entering or exiting glass or any transparent material.[19]

1.5 Optical band gap

The band gap energy is defined as the width of the energy gap between the conduction band and the valence band. In the case of metals, it is necessary to specify which band gap is being referred to.Since absorbance is proportional to the absorption coefficient (α) according to Beer's law, the measured absorbance can be used as a substitute for the absorption coefficient to construct the absorption curve. The energy axis is obtained by converting the analyzed wavelength spectrum into energy using the relation:

$$\mathrm{E} = \frac{\mathrm{hc}}{\lambda} \qquad (1)$$

where E is the converted energy, c is the speed of light (3.0 x 108 m/s), h, as before, is Plank's constant and λ is the wavelength of light. By convention, the calculated energy is converted from J to eV.

While investigating the optical and electronic properties of amorphous germanium, Tauc et al. proposed and validated a method for determining the band gap. This approach was further developed in the more general work of Davis and Mott on amorphous semiconductors. They demonstrated that the optical absorption strength depends on the difference between the photon energy and the band gap, as expressed in (Eq. 2):

$$(\alpha h\nu)^{\frac{1}{n}} = A(h\nu - Eg) \quad (2)$$

where h is Planck's constant, ν is the photon's frequency, α is the absorption coefficient, Eg is the band gap and A is a proportionality constant. The value of the exponent denotes the nature of the electronic transition, whether allowed or forbidden and whether direct or indirect:

For direct allowed transitions $n = \frac{1}{2}$

For direct forbidden transitions $n = \frac{3}{2}$

For indirect allowed transitions $n = 2$

For indirect forbidden transitions $n = 3$

Typically, the allowed transitions dominate the basic absorption processes, giving either $n = \frac{1}{2}$ or $n = 2$, for direct and indirect transitions, respectively.

Thus, the basic procedure for a Tauc analysis is to acquire optical absorbance data for the sample in question that spans a range of energies from below the band gap transition to above it.[20]

1.5.1 Types of band gap

1. Direct Band Gap

A direct band gap is defined as one where the momentum (vector) of the highest states in the valence band is approximately the same as that of the lowest states in the conduction band. As shown in Figure 1.3, for a direct band gap, the minimum of the conduction band aligns with the maximum of the valence band. In this case, emission typically occurs with photon energies close to the band gap energy, while absorption can also take place at shorter wavelengths.

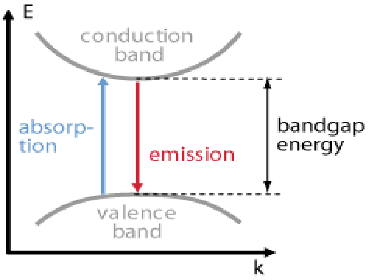

Figure 1.4 Direct Band Gap

2. Indirect Band Gap

In the case of an indirect band gap, the momentum (vector) of the lowest energy states in the conduction band differs significantly from that of the highest energy states in the valence band. As a result, absorption processes involving photon energies just above the band gap are limited because there are no available states in the conduction band that simultaneously match the required energy and momentum.

As illustrated in Figure 1.4, for materials with an indirect band gap, additional phonons must participate in the absorption and emission processes to provide the necessary change in electron momentum.[21]

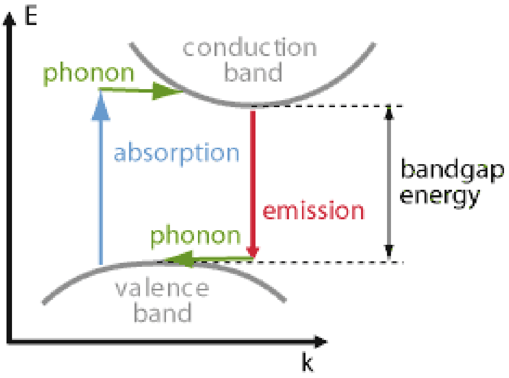

Figure 1.5 Indirect Band Gap

1.6 Urbach Energy

Urbach Energy is a physical parameter that characterizes the exponential tail in the optical absorption edge of materials, especially in amorphous and nanostructured semiconductors. It reflects the degree of structural or thermal disorder in a material.
Mathematically, it is described by the Urbach rule:

$$\alpha(E) = \alpha_0 e^{\left(\frac{E-E_0}{E_U}\right)}$$

Where:

- $\alpha(E)$ is the absorption coefficient at energy E,
- α_0 is a fitting constant,
- E_0 is the characteristic energy,
- E_U is the Urbach Energy.

The value of Urbach Energy provides insight into the material’s structural order; higher values indicate a greater degree of disorder. It is widely used to evaluate the optical quality and defect density of semiconducting materials, This equation is only valid when $\alpha \propto e^{E}$. [22]

1.7 Literature review

Polyvinyl alcohol (PVA) is a widely used polymer due to its excellent film-forming ability, biodegradability, and good mechanical properties. However, its optical and electronic characteristics are sometimes limited for advanced applications. To overcome this, researchers have incorporated metal oxide nanoparticles, especially Titanium Dioxide (TiO_2), into PVA to enhance its performance. TiO_2 is widely used due to its strong optical absorption, chemical stability, and high refractive index.

In a study conducted by Praveena et al. at Mangalore University in India, PVA/TiO_2 nanocomposite films were prepared with varying TiO_2 concentrations. The results showed that adding TiO_2 reduced the optical band gap and increased electrical conductivity, indicating improved optical and electrical properties of the material.[23]

Ibrahim Mourad from Suez University in Egypt also studied the effect of different TiO_2 concentrations on PVA films. His results revealed a decrease in the optical band gap from 3.87 eV to 2.79 eV, as well as an increase in the refractive index and electrical conductivity, confirming enhanced optical and electronic behavior.[24]

another study, Mohammed et al. from Al-Mustansiriyah University in Iraq prepared PVA/TiO_2 films using pulsed laser deposition. They observed a decrease in the optical band gap and an increase in optical conductivity after adding TiO_2, indicating improved optical performance.[25]

Chapter 2

Experimental and Theoretical background

2.1 Sample

In this study, pre-prepared samples of PVA films (pure) and PVA (2.5% TiO_2) as reported in Sol-Gel method were used [26]. Figure 2.1 shows the image of the TiO_2 rod nanoparticles in range 3 – 10 nm by TEM. The samples were measured and tested using a UV-Vis spectrophotometer.

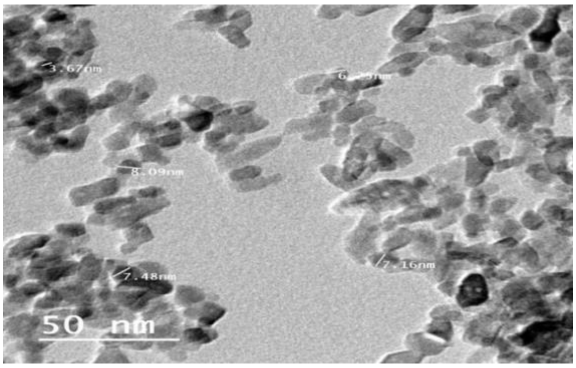

Figure 2.1: HR-TEM of TiO_2 nanoparticles

2.2 UV-VIS spectroscophotometer

UV-Vis spectroscopy is an analytical technique that measures the amount of discrete wavelengths of UV or visible light that are absorbed by or transmitted through a sample in comparison to a reference or blank sample. This property is influenced by the sample composition, potentially providing information on what is in the sample and at what concentration. Since this spectroscopy technique relies on the use of light.[27]

Figure 2.2: spectrophotometer UV-VIS Device

2.2.1 Principle of Spectrophotometer

The principle of a spectrophotometer is based on the Beer-Lambert Law, which describes the relationship between the absorbance of light by a sample and the concentration of the absorbing substance. When light passes through a sample, some wavelengths are absorbed by the material, while others pass through.[28]

2.2.2 Beer-Lambert law

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 2.3.[29]

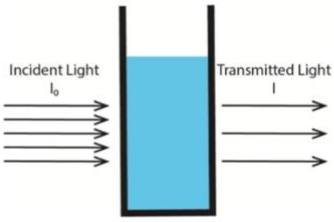

Figure 2.3: Beer Lambert diagram

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:

$$\frac{\mathrm{Io}}{\mathrm{I}} = \mathrm{e}^{-\,\alpha \mathrm{l}}$$

travels through the sample. Therefore, Where Io is the intensity of the incident light, I is the intensity of light transmitted through the sample, I is the thickness of the sample, and α is the absorption coefficient:

$$\log_{10}\frac{\mathrm{Io}}{\mathrm{I}} = \alpha \mathrm{l}\ \mathrm{loge}$$

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

$$A = \log_{10}\frac{\mathrm{Io}}{\mathrm{I}} = 0.4343\ \alpha l$$

2.5 FTIR spectroscopy

Attenuated total reflection-Fourier transform infrared (FTIR) spectroscopic imaging is a powerful imaging technique which is used to study a variety of materials and processes. The transmittance of samples were measured in range 4000 – 400nm. A large amount of useful information can be collected rapidly and easily in a single measurement, as every FTIR image, besides providing spatial information, contains the spectral data of each individual component in the sample. FTIR spectroscopic imaging therefore has a great advantage over other analytical tools when it comes to studying multi-component and dynamic systems. FTIR spectroscopy allows for the analysis of a range of sample forms, including solid samples, solutions and hydrated films, requiring minimal sample preparation.

In transmission mode, incident radiation passes directly through the sample, where infrared light is absorbed at specific wavelengths. The light that is not absorbed is transmitted onto a detector, resulting in an absorption spectrum.[30]

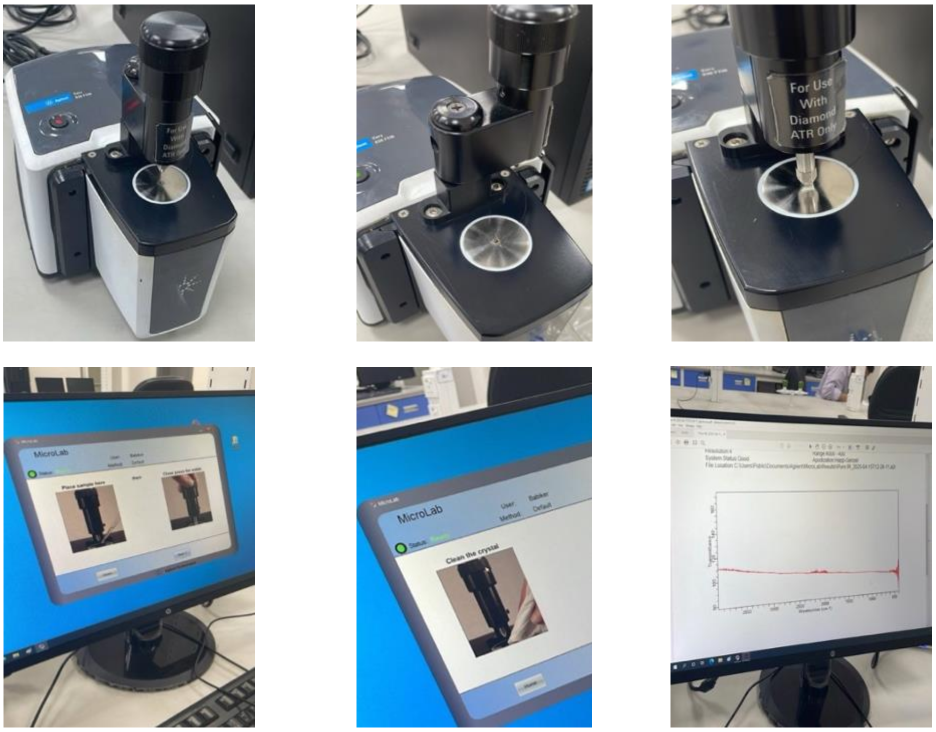

Figure 2.4: FTIR Device

2.6.1 FTIR Sample Measurements

For powders, thin films, or other solid samples, the sample is placed onto the FTIR crystal and pressed down using the swivel press to ensure optimal contact between sample and crystal. After the measurement, the sample can then be recollected, ideal for low-volume or expensive samples. The crystal can then be wiped clean using a light solvent, if necessary.[31]

2.6.2 FTIR Application Examples

FTIR analysis is used extensively throughout industry and academia in a wide range of applications, including in hand sanitizer analysis.

1. Pharmaceutical Packaging Materials Quality Control
2. Determination of Sucrose Levels in Infant Cereals
3. Fuel Blend Analysis
4. Analysis of Alcohol Levels in Hand Sanitizer
5. Cocaine Identification in Seized Drug Samples
6. Detection of Counterfeit Pharmaceuticals. [32]

Chapter 3

Result and Discussion

3.1 Spectrophotometer UV-VIS Device Result

The UV-Vis spectrum for TiO_2 is studied between 200 to 800 nm, encompassing the ultraviolet and visible regions, and The absorption Peaks of TiO_2 appear in two regions:

1. UV Region (200-400 mm): Strong absorption is typically obserred in this region due to electronic transitions in TiO_2. 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, The image shows the absorbance spectrum of a pure sample and another sample with 2.5% added TiO_2, within the wavelength range of 200 to 500 nm. The x-axis represents the wavelength in nanometers, and the y-axis represents absorbance in AU (Absorbance Units), which measures how much light is absorbed by the sample at each wavelength. The orange curve represents the pure sample, which shows relatively low absorbance that gradually decreases as the wavelength increases. This means the pure sample absorbs more in the UV region. In contrast, the purple curve represents the sample with 2.5% TiO_2 and shows higher overall absorbance, with clear peaks around 225 and 280 nm. These peaks and the increased absorbance indicate that the added material affects the electronic structure of the sample. The difference between the two curves highlights the role of TiO_2 in enhancing UV light absorption.

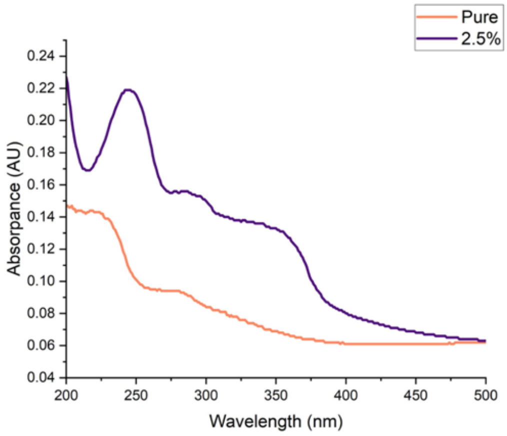

Figure 3.1: Absorpance peaks

3.2 Energy gap

Sample	Optical direct band gap	Optical indirect band gap
PVA (Pure)	4.55 eV	4.08 eV
PVA (2,5%)	4.15 eV	4.05 eV

Table 3.1: Valued for band gap

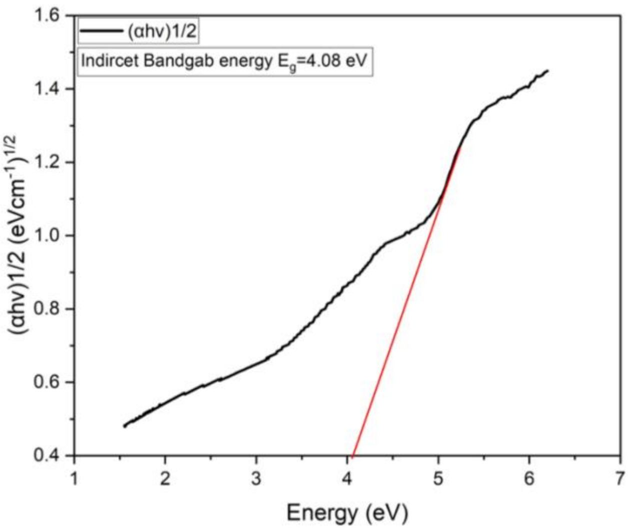

Figure 3.2: Indirect band gap of PVA (Pure)

Figure 3.2 shows the relationship between energy (eV) and $(\alpha h\nu)^{\frac{1}{2}}$, where the x-axis represents energy in electron volts (eV), and the y-axis represents $(\alpha h\nu)^{\frac{1}{2}}$, with α being the absorption coefficient and hν being the product of Planck's constant and frequency. The graph indicates a point at an energy of 4.08 eV, which is the indirect bandgap energy of pure PVA, representing the minimum energy required to free an electron.

The transition region appears as a flat section at the bottom, where the material does not effectively absorb energy in this range. As energy increases, the curve begins to rise, indicating a noticeable start in light absorption. The straight part of the curve that follows the transition region suggests a linear relationship, indicating that electronic transitions occur at a specific energy. This segment shows that the material follows an indirect transition model, where freeing electrons requires a certain amount of energy.

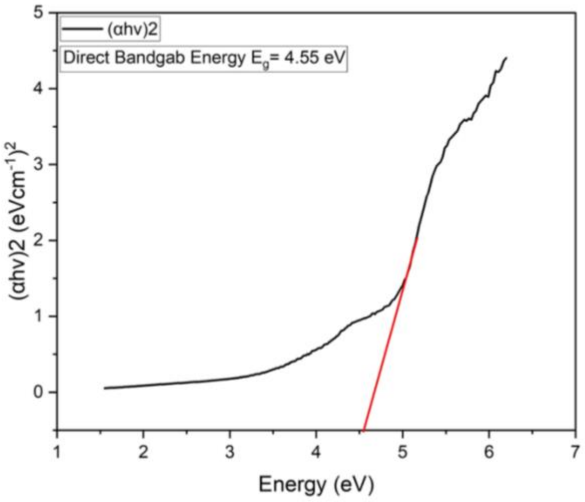

Figure 3.3: direct band gap of PVA (Pure)

Figure 3.3 shows the relationship between energy (eV) and $(\alpha h\nu)^2$. The x-axis represents energy in electron volts (eV), and the y-axis represents $(\alpha h\nu)^2$, where α is the absorption coefficient and hν is Planck's constant times frequency. The graph has a point at 4.55 eV, which is the direct bandgap energy of the material, meaning this is the minimum energy needed to free an electron.

The transition region is a flat section at the bottom, where the material does not absorb energy well, indicating weak absorption. As energy increases, the curve rises quickly, showing that light absorption begins significantly. The straight section that follows indicates a linear relationship, meaning electronic transitions happen at a specific energy, consistent with a direct transition model, where electrons can be easily freed at that energy.

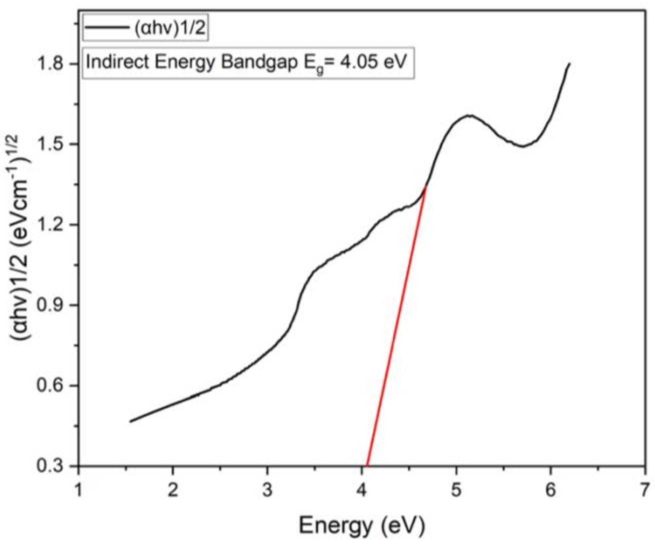

Figure 3.4: Indirect band gap of PVA (2.5% TiO_2)

Figure 3.4 shows the relationship between energy (eV) and $(\alpha h\nu)^{\frac{1}{2}}$ after adding 2.5% TiO_2. The x-axis represents energy in electron volts (eV), while the y-axis represents $(\alpha h\nu)^{\frac{1}{2}}$, where α is the absorption coefficient and hν is Planck's constant times frequency. The graph indicates an indirect bandgap energy (E_g) at 4.05 eV, which is the energy needed to free an electron in this material.

The curve starts at a low value and rises gradually, showing that the material does not absorb energy well at low energies. As energy increases, there is a noticeable rise, indicating that the material begins to absorb light more effectively. The straight section, highlighted in red, shows a direct relationship, confirming that electronic transitions occur at a specific energy level.

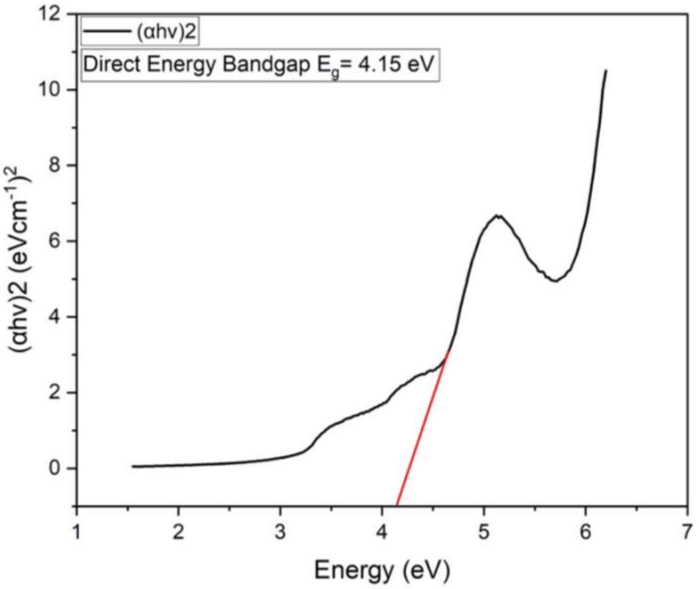

Figure 3.5: direct band gap of PVA (2.5% TiO_2)

Figure 3.5 shows the relationship between energy (eV) and $(\alpha h\nu)^2$ after adding 2.5% TiO_2. The x-axis represents energy in electron volts (eV), while the y-axis represents $(\alpha h\nu)^2$, where α is the absorption coefficient and hv is Planck's constant times frequency. The graph indicates a direct bandgap energy (E_g) at 4.15 eV, which is the energy needed to free an electron in this material.

The curve starts at a low value and rises sharply, indicating that the material begins to absorb light more effectively at higher energies. The straight section, highlighted in red, shows a linear relationship, confirming that electronic transitions occur at a specific energy level. This behavior is typical for materials with a direct bandgap, where electrons can be easily freed at the specified energy.

3.3 Urbach Energy

Sample	Urbach Energy $[\mathbf{E_U}]$
PVA (Pure)	3.42 eV
PVA 2.5% $\mathbf{TiO_2}$	1.25 eV

Table 3.2: Valued for Urbach Energy of $(\mathrm{TiO_2})$

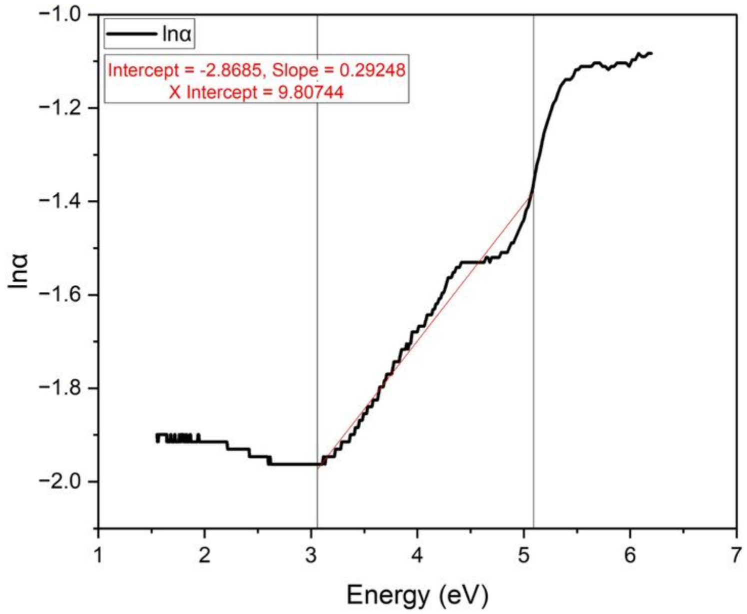

Figure 3.6: Urbach Energy of PVA (Pure)

Figure 3.6 shows the relationship between energy (eV) and $\ln(\alpha)$ for pure PVA material. The Urbach energy (E_U) can be calculated from the slope of the straight portion of the curve. The Urbach energy is given by the equation $(E_U) = \frac{1}{\text{slope}}$.

In this figure, the slope is measured at 0.29248, resulting in $E_U \approx 3.42\ \text{eV}$ This value indicates the level of disorder in the PVA structure. A higher Urbach energy suggests the presence of defects or weak bonds in the crystal structure.

This value of E_U implies that the material may exhibit some irregularities, which can affect its optical and electronic properties. These defects can enhance the material's ability to absorb light and influence its efficiency.

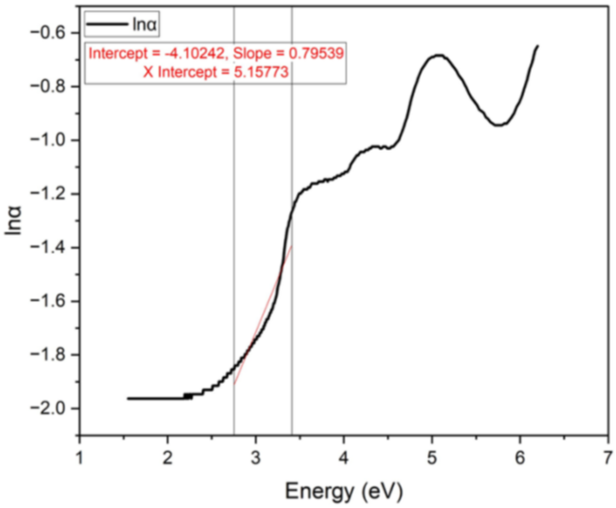

Figure 3.7: Urbach Energy of PVA (2.5% TiO_2)

Figure 3.7 shows the relationship between energy (eV) and ln(α) for PVA material with the addition of 2.5% TiO_2. The Urbach energy (E_U) can be calculated from the slope of the straight portion of the curve using the equation $(E_U) = \frac{1}{\text{slope}}$

In this figure, the slope is measured at 0.79539, resulting in $E_U \approx 1.25$ eV. This lower Urbach energy value compared to pure PVA indicates a reduction in disorder within the structure due to the addition of TiO_2.

The decreased E_U suggests that the incorporation of TiO_2 improves the structural integrity of the material, potentially reducing defects or weak bonds in the crystal lattice. This enhancement can positively influence the optical and electronic properties of the PVA-TiO_2 composite.

3.4 FTIR Device Result

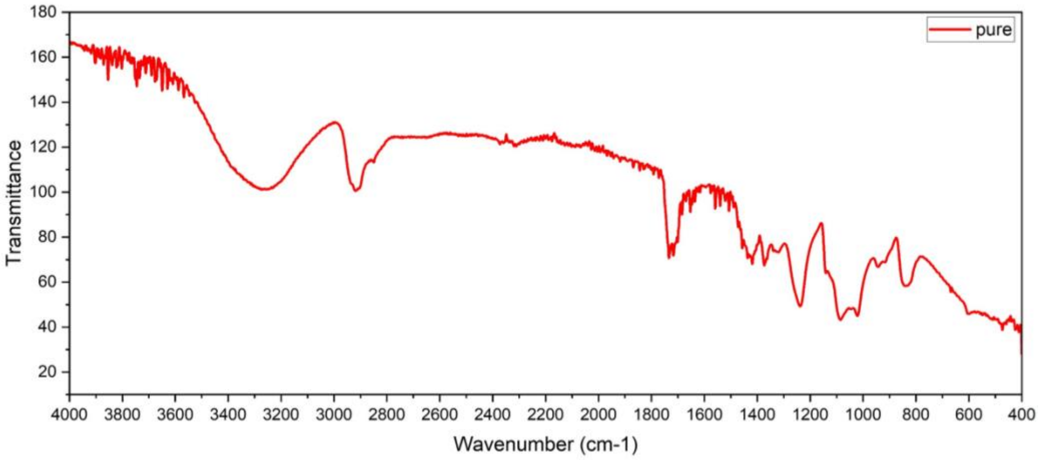

Figure 3.8: FTIR Spectrum of Pure PVA Film

The FTIR spectrum of the pure PVA film exhibited a broad absorption band around 3300 cm^{-1}, corresponding to the O–H stretching vibrations, which indicate the presence of hydroxyl (–OH) groups in the polymer structure.

A distinct peak also appeared at 2900 cm^{-1}, attributed to C–H stretching vibrations, which are characteristic of the carbon backbone in the polymer chains.

In the region between 1720 and 1000 cm^{-1}, a peak was observed at 1080 cm^{-1}, corresponding to C–O stretching vibrations, commonly found in alcohols and ether-based polymers.

Additionally, a peak around 1650 cm^{-1} was recorded, associated with H–O–H bending, likely due to moisture or bound water within the sample.

Finally, in the fingerprint region between 1200 and 600 cm^{-1}, several distinctive peaks were identified, reflecting the complex structure of PVA, although no signals related to inorganic additives were observed.

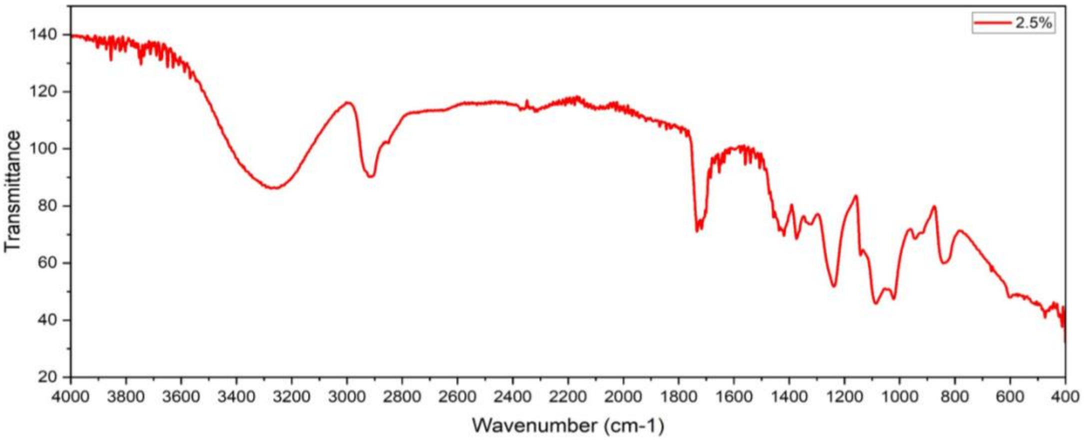

Figure 3.9: FTIR Spectrum of (2.5% TiO_2) PVA Film

When analyzing the PVA film after adding 2.5% TiO_2 nanoparticles, clear changes were observed compared to the pure sample.

The first noticeable change was the shift of the O–H peak from 3300 cm^{-1} to 3280 cm^{-1}, with increased sharpness, indicating the formation of hydrogen bonds between the hydroxyl groups in PVA and the surface of TiO_2.

Although the C–H peak remained at 2900 cm^{-1}, its intensity slightly decreased, suggesting a mild indirect effect from the nanoparticles.

Also, the C–O peak shifted from 1080 cm^{-1} to 1070 cm^{-1}, which indicates an interaction between TiO_2 and this functional group.

The H–O–H peak became more distinct at 1635 cm^{-1}, possibly due to water absorption from the surroundings as a result of the high surface activity of TiO_2.

Conclusion

In this study, the effect of adding titanium dioxide (TiO_2) to polyvinyl alcohol (PVA) nanofilms at different concentrations was explored, including pure PVA and PVA with 2.5% TiO_2. The goal was to understand how this addition affects the structural and optical properties. The band gap became smaller when TiO_2 was added, compared to the higher band gap of pure PVA. Also, the Urbach energy was higher in pure PVA and decreased with more TiO_2 which means the structure of the material became more regular.

The results showed that TiO_2 helped reduce defects in the crystal structure, leading to better bonding between molecules and increased structural stability. Additionally, the values of direct and indirect energy gaps decreased, making the material better at absorbing light at certain frequencies. The decrease in Urbach energy also indicated a more uniform distribution of energy levels within the material, which improves optical properties like transparency and light absorption.

Moreover, FTIR analysis confirmed interactions between TiO_2 nanoparticles and active groups in PVA. Shifts were observed in the O–H and C–O peaks, along with the appearance of peaks related to Ti–O bonds, indicating hydrogen bonding and molecular-level structural changes.

Overall, the results suggest that TiO_2 positively affects the structural and optical behavior of PVA films.

Reference

[1] Michael F Ashby, Paulo J Ferreira, Daniel L Schodek. Nanomaterials and Nanotechnologies, 22 April 2009.

[2] Nichole Donough, Vector Wepener, Taryn Lee Botha. Sizes, Shapes, and Types of Nanomaterials. Frontiers, 29 August 2024.

[3] Munawar Khalil,Mohammed Ali Berawi. Advanced nanomaterials in oil and gas industry: Design, application and challenges, 2022.

[4] Yu. M. Evtushenkoa, S.V.Romashkin, N.S. Trofimov, T.K. Chekhlova. Optical Properties of TiO2 Thin Films, 30 Jan 2015.

[5] Seyed Shahabeddin Mirsasaani,Danesh Arshadi Poshtiri. Nanotechnology and nanobiomaterials in dentistry, 2019.

[6] The Editors of Encyclopaedia Britannica. “Polymer”. Encyclopaedia Britannica Last Updated: Mar 17, 2025.

[7] Kantappa Halake, Jonghwi Lee. Recent application developments of water-soluble synthetic polymers, 2014.

[8] Gagandeep Kaur,Shivani Mishra. Toxicological effect of biopolymers and their applications, 2022.

[9] Ritika Singla. Polyvinyl Alcohol,2025. https://www.vedantu.com/chemistry/polyvinyl-alcohol

[10] Muhammad Aslam,Muhammad Mazhar Ali Kalyar. Polyvinyl alcohol: A review of research status and use of polyvinyl alcohol based nanocomposites. Article in Polymer Engineering and Science · April 2018.

[11] Letícia Oliveira, Anielle Silva, Noelio Dantas, Enio Filho. Thermophysical properties of TiO2-PVA/water nanofluids, Dec 2017.

[12] Muhammed Shameem, Sasikanth, Raja Annamalai, Ganapathi Raman. A brief review on polymer nanocomposites and its applications, 2021.

[13] Mohamed Darwish, Mohamed Mostafa, Laila Al-Harbi. Polymeric nanocomposites for environmental and industrial applications. International Journal of Molecular Sciences, 2022.

[14] Atif Suhail. Revolutionizing Industries: Innovative Applications of Polymer Nanocomposites, 11 Apr 2024.

[15] updated by Amy Tikkanen. https://www.britannica.com/science/refraction, 14 Mar 2025.

[16] Erik Gregersen. Spectrum physics. https://www.britannica.com/science/spectrum ,21 Feb 2025.

[17]Ojha,Swarupa. Metal Oxide Glass Nanocomposites, 2020 (17.4.3 Optical properties).

[18] Recent Advances in Multidisciplinary Applied Physics. Absorption Spectra, 2005.

[19] generated definition based on: Progress in Quantum Electronics, Transmission Spectrum,2001.

[20] Brian Viezbicke, Shane Patel, Benjamin Davis, Dunbar Birnie. Evaluation of the Tauc Method for Optical Absorption Edge Determination: ZnO Thin Films as a Model System, 2015.

[21] Paschotta R. Band Gap RP Photonics Encyclopedia, RP Photonics Consulting GmbH, https://www.rp-photonics.com/band_gap.html .

[22] https://en.wikipedia.org/wiki/Urbach_energy?utm_source=chatgpt.com.

[23] Praveena M, Prasanna K, Prasad G, Shashikala D. Structural, thermal and dielectric properties of TiO_2 filled polyvinyl alcohol nano composite films, Polymer Composites, 2013.

[24] Mourad A. Optical and Electrical Properties of TiO_2/Polymers Nano composites, 2020.

[25] Mohammed J, Ibrahim A, Mahdi S. Optical Properties of (PVA–TiO_2) Nano composite Thin Films Prepared by Pulsed Laser Deposition. Mustansiriyah Journal of Science, 2015.

[26] Gh.Mohammed, Adel ElSayed, WM .Morsi. Spectroscopic, thermal, and electrical properties of MgO/polyvinyl pyrrolidone/polyvinyl alcohol nanocomposites. Journal of Physics and Chemistry of Solids, 2018.

[27] Justin Tom. UV-Vis Spectroscopy: Principle, Strengths and Limitations and Applications, 18 Dec 2023.

[28] Sagar Aryal. Spectrophotometer: Principle, Instrumentation, Applications, 1 May 2024.

[29] Bee A. Bestimmung der Absorption des rothen Lichts in farbigen Flüssigkeiten, 1852.

[30] Céline van Haaren, Marieke De Boc , Sergei G Kazarian. Advances in ATR-FTIR Spectroscopic Imaging for the Analysis of Tablet Dissolution and Drug Release, 12 Jun 2023.

[31] Agilent Technologies. https://www.agilent.com/en/product/molecular-spectroscopy/ftir-spectroscopy/atr-ftir-spectroscopy?utm_source=chatgpt.com, 2025.

[32] ATR Sampling Accessories for the Agilent Cary 630 FTIR Spectrometer. www.agilent.com/chem/cary630,
19 Jan 2022.