Ministry of Higher Education and Scientific Research

University of Babylon, College of Education for Pure Sciences

Department of Physics

Optical Characterization of Polymer Nanocomposites

A research submitted to the College of Education for Pure Sciences Council as part of the requirements for a bachelor's degree in the College of Education, Department of Physics.

By

Dargam Mohammed Hassan

Supervisor

Dr.Mohammed Jawad Kadhim

2026 A.D 1446A.H

Abstract

In this research, the optical properties for (Polymer- nanomaterials) nanocomposites have been studied.

As the study of the absorbance, the study of the absorption areas, the direct electronic transitions, and the indirect electronic transitions of these nanocomposites, as well as the study of the optical constants, which are the absorption coefficient, refraction coefficient, extinction coefficient, real and imaginary dielectric constant.

Chpter three : Optical Properties

Chapter One

“ Nano Composites “

1.1 Introduction

In the past few decades, the field of materials science has undergone a dramatic transformation catalyzed by advances in Nanotechnology the science and engineering of controlling matter at dimensions ranging from approximately 1 to 100 nanometers. At such a nanoscale, materials often exhibit markedly different chemical, physical, mechanical, thermal, and optical properties compared to their bulk counterparts .

Among the most significant innovations emerging from nanotechnology is the development of **nanocomposites** composite materials in which a “matrix” (e.g., polymer, metal, or ceramic) is reinforced with “nanofillers” such as nanoparticles, nanofibers, or nanosheets. This hybridization harnesses the exceptional surface-to-volume ratios and quantum or size-effect-induced properties of the nanofillers to achieve a synergy: the resulting material often demonstrates superior performance in multiple domains simultaneously from mechanical strength and stiffness,

to thermal and electrical conductivity, to enhanced durability and resistance to degradation [1] .

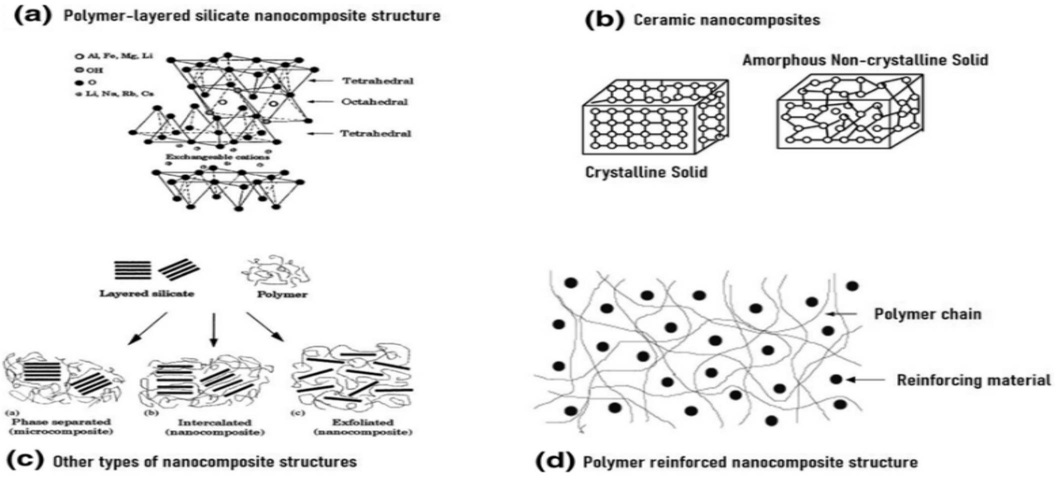


Figure 1. Schematic representation of a nanocomposite structure showing the matrix andnanoscale fillers.

Nanocomposites is Matter

The motivation behind engineering nanocomposites stems from the increasingly demanding requirements of modern technologies and industries. Conventional materials frequently face trade-offs: for example, metals may offer strength but are heavy; polymers may be lightweight but too soft or thermally limited. Nanocomposites, however, can combine the best of multiple worlds:

- **Enhanced mechanical properties**: Even a small addition of nanofillers (often well below 5 % by volume) can significantly improve stiffness, tensile strength, toughness, and wear resistance compared to the pure matrix [2 , 3].
- **Improved thermal and electrical properties**: Depending on the type of filler (e.g., graphene, metal nanoparticles, carbon nanotubes), nanocomposites can show dramatically increased thermal conductivity, improved heat dissipation, or enhanced electrical conductivity properties critical for electronic, aerospace, or thermal-management applications [4].
- **Multifunctionality & design flexibility**: By choosing different matrix-filler combinations, varying filler shapes (particles, fibers, sheets), controlling dispersion, and optimizing filler content and orientation — researchers can “tune” properties to meet diverse demands: lightweight structural materials, conductive polymers, thermally stable composites, biocompatible materials, etc [5].

This versatility is what makes nanocomposites a central pillar in the evolution of “advanced materials” for the 21st century enabling breakthroughs in aerospace, automotive, electronics, energy, biomedicine, and beyond .

State of Research & Recent Advances

Recent literature highlights remarkable progress in the synthesis, characterization, and application of nanocomposites. A comprehensive review from 2024 details how different preparation methods (e.g., melt blending, sol-gel, in-situ polymerization, layer-by-layer assembly) influence the structure and, hence, the final properties of nanocomposites .

Moreover, hybrid nanocomposites those combining multiple types of fillers (e.g., graphene + metal nanoparticles, or natural fibers + synthetic nanofillers) have shown synergistic effects: achieving enhancements in thermal conductivity, mechanical strength, or multifunctional behavior that surpass what single-filler composites can achieve [6].

Such advances not only deepen our scientific understanding of nanoscale interactions, dispersion and interfacial bonding, but also expand the application horizon paving the way for high-performance, lightweight, and multifunctional materials that were previously unattainable with traditional composites .

1.2 Literature Review

Nanocomposites are composite materials in which at least one component possesses dimensions in the nanoscale range (1–100 nm). The incorporation of nanoscale fillers into a matrix (polymer, metal, or ceramic) enables the creation of materials with significantly enhanced properties compared to their bulk counterparts. These enhancements include increased mechanical strength, thermal stability, electrical conductivity, and durability. The high surface area to volume ratio of nanoparticles results in stronger interfacial interactions with the matrix, which is a key factor in property improvement Nanofillers can take various forms including particles, fibers, and sheets, each contributing differently to the composite's performance. The selection of filler type, size, and loading fraction critically influences the structural, thermal, mechanical, and electrical properties of the resulting nanocomposite.

Synthesis and Fabrication Methods [7] .

Several methods have been developed to fabricate nanocomposites, each influencing the dispersion of nanoparticles and the resulting properties of the material. Common techniques include:

- **In-situ polymerization**: Nanofillers are incorporated during the polymerization process, resulting in improved interfacial bonding (ResearchGate, 2021).
- **Melt blending**: Nanoparticles are physically mixed with a molten matrix, commonly used for thermoplastics (MDPI, 2024).
- **Sol-Gel method**: A chemical route where precursors in solution form a gel that solidifies into a nanocomposite with uniform nanoparticle distribution.
- **Layer-by-layer assembly**: Sequential deposition of layers of matrix and nanoparticles to control composition and structure precisely.

The choice of fabrication method directly affects nanoparticle dispersion, interfacial adhesion, and, consequently, the performance of the nanocomposite.

Physical, Mechanical, and Thermal Properties

Nanocomposites demonstrate superior physical and mechanical properties relative to traditional composites. For instance, even low nanoparticle loading (<5 wt%) can enhance tensile strength, Young's modulus, and toughness. The improvements arise due to effective stress transfer between the matrix and the nanoparticles and the prevention of crack propagation [8].

Thermal and electrical properties are also significantly influenced by the type of nanofiller. Graphene or carbon nanotubes, for example, can substantially increase thermal conductivity, whereas metallic nanoparticles enhance electrical conductivity. The morphology, size, and dispersion state of the nanofillers are critical parameters that determine the final properties [9].

Applications of Nanocomposites

Nanocomposites have a wide range of industrial and technological applications due to their multifunctional properties:

- **Aerospace and Automotive**: Lightweight, high-strength components.
- **Electronics**: Conductive polymers and thermal interface materials.
- **Energy**: High-efficiency solar cells and batteries.
- **Biomedicine**: Drug delivery systems and medical implants.

These applications demonstrate the potential of nanocomposites to surpass traditional materials in performance and functionality (Journal of Babylon, 2021; ResearchGate Infographic, 2022).

Research Gaps

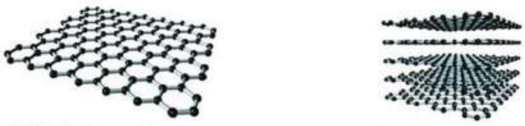
Despite extensive studies, several gaps remain in the current literature:

- The correlation between nanoparticle structural characteristics (size, shape, and morphology) and composite properties is not fully understood.
- The effect of different dispersion techniques on final performance requires further investigation.
- Comparative studies evaluating the same nanocomposite for multiple industrial applications are limited.

Addressing these gaps is crucial for optimizing nanocomposite design and for enabling targeted applications in emerging technologies.

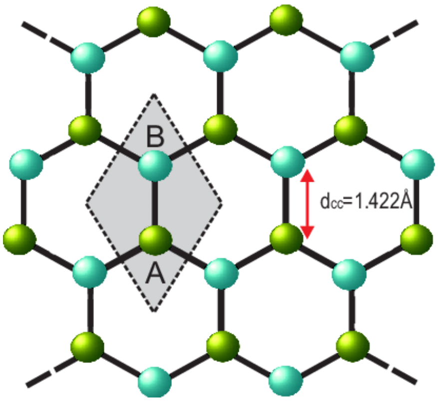
Graphene

Graphene (C) is a unique form of carbon, represented chemically by the symbol **C**, consisting of a single, atomically thin layer of carbon atoms arranged in a two-dimensional hexagonal lattice. This remarkable structure gives graphene its extraordinary physical properties. Mechanically, it is exceptionally strong—much stronger than steel—yet extremely lightweight and flexible, capable of bending without breaking. Its stiffness and tensile strength make it ideal for reinforcing materials in advanced composites. Graphene also exhibits outstanding thermal conductivity, efficiently transferring heat, which is highly beneficial in applications requiring thermal management. In addition, its electrical conductivity is excellent, with electrons able to move through the lattice at exceptionally high speeds, making it suitable for high-performance electronic devices. Physically, graphene is nearly transparent, allowing about 97% of light to pass through, and its large surface area relative to its volume enhances its interaction with other materials[10 , 11].



(a) Single-layer graphene (b) Multi-layer graphene

(c) GO (d) rGO



(Figure 2 , 3) . Its structure, the arrangement of its atoms, and its distinctive (hexagonal lattice) shape, in addition to diagrams highlighting some of its physical properties in terms of strength, conductivity, transparency, and others.

Graphene plays a central role in the development of nanocomposites due to its extraordinary physical and chemical properties. When incorporated into polymeric, metallic, or ceramic matrices, graphene acts as an efficient **nanofiller**, enhancing the performance of the composite materials even at very low concentrations. Its extremely high mechanical strength and flexibility significantly improve the **tensile strength, stiffness, and durability** of nanocomposites, making them suitable for applications where lightweight yet strong materials are required [12].

Beyond mechanical reinforcement, graphene contributes to **enhanced electrical and thermal conductivity** within nanocomposites. This property is particularly valuable in electronic devices, conductive polymers, and thermal interface materials, where efficient charge transport or heat dissipation is critical. Additionally, the large surface area of graphene enables excellent interfacial interaction with the surrounding matrix, improving load transfer and stability, and minimizing the risk of structural failure under stress.

Graphene-based nanocomposites have also been applied in **functional and protective materials**. For instance, the incorporation of graphene can provide anticorrosive properties, chemical resistance, or even antimicrobial activity, depending on the matrix and functionalization. Its high surface reactivity allows for chemical modification, which further extends the range of applications of graphene nanocomposites in areas such as energy storage, sensors, biomedical devices, and advanced coatings [13].

Despite these advantages, challenges remain in the fabrication of graphene nanocomposites. Achieving **uniform dispersion** of graphene sheets within the matrix is critical to fully exploit their reinforcing capabilities. Agglomeration of graphene layers can reduce performance, and production costs of high-quality graphene remain significant. Nonetheless, due to its **unique combination of mechanical, electrical, thermal, and chemical properties**, graphene continues to be one of the most promising nanofillers for creating high-performance nanocomposite materials [14].

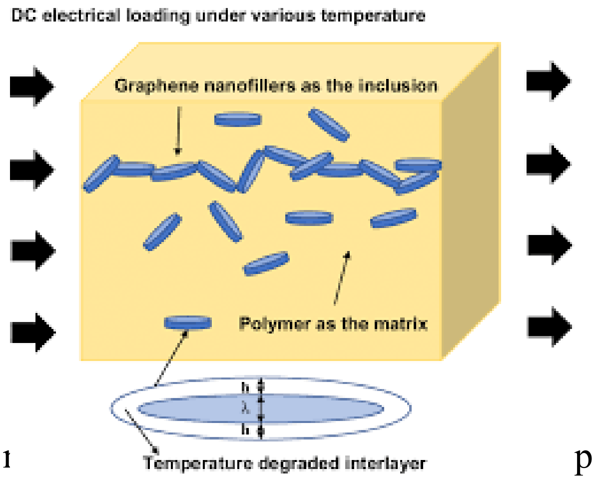


Figure 4 . graphene ı polymer which helps to understand the structure of the nanocomposite (e.g., “exfoliated” shape or uniform distribution).

1.3 Aim of This Study

Given the rapid evolution of nanocomposite science and its vast potential, this research aims to investigate a specific class of nanocomposites (to be defined based on chosen matrix and nanofiller) with the goal of elucidating how key parameters such as filler type, filler concentration, filler morphology (particles, fibers, sheets), and dispersion method affect the physical, mechanical, thermal, and possibly electrical properties of the composite material.

By systematically studying and characterizing these relationships, this work seeks to contribute to the fundamental understanding of structure–property correlations in nanocomposites, and to provide insights relevant for real-world applications from structural materials to electronics or thermal management systems.

Furthermore, this research intends to situate its findings within the broader scientific and industrial context, offering recommendations for optimizing nanocomposite design and processing for future applications.

Chapter TWO

“ Polymer & Nano “

2.1 Introduction

Polymers represent one of the most important classes of materials in modern science and engineering due to their wide range of physical, chemical, and mechanical properties. The term *polymer* is derived from the Greek words *poly* (many) and *meros* (parts), referring to substances composed of long chains of repeating molecular units known as monomers. These materials play a crucial role in various industrial, biomedical, and technological applications, ranging from packaging and construction to electronics and biomedical devices (Odian, 2004) .

The increasing demand for lightweight, cost-effective, and versatile materials has significantly expanded the use of polymers in both traditional and advanced engineering fields. Unlike metals and ceramics, polymers offer advantages such as low density, ease of processing, corrosion resistance, and high design flexibility. These properties make polymers suitable for integration with advanced materials, including nanomaterials, to form high-performance composites (Young & Lovell, 2011) .

2.1.1 General Concept of Polymers

Polymers are macromolecules composed of repeating structural units connected by covalent bonds. These repeating units originate from small molecules called monomers, which undergo chemical reactions such as addition or condensation polymerization. The resulting polymer chains may vary in length, structure, and molecular weight, all of which significantly influence the material's physical and mechanical behavior (Sperling, 2006).

Polymers can be classified based on several criteria, including their origin (natural or synthetic), molecular structure (linear, branched, or crosslinked), and thermal behavior. Thermoplastic polymers soften upon heating and can be reshaped multiple times, while thermosetting polymers undergo irreversible chemical changes when heated, forming rigid three dimensional networks. Elastomers, another important class, exhibit rubber like elasticity due to their flexible molecular chains (Callister & Rethwisch, 2018).

2.1.2 Physical and Mechanical Properties of Polymers

The physical properties of polymers are strongly influenced by their molecular architecture and intermolecular forces. Properties such as density, glass transition temperature (Tg), melting temperature (Tm), and crystallinity determine how polymers behave under different environmental conditions. Mechanically, polymers exhibit a wide range of behaviors, from rigid and brittle to soft and highly elastic, depending on their chemical composition and processing conditions.

One of the most significant advantages of polymers is their high strength to weight ratio, which makes them attractive for lightweight structural applications. Additionally, polymers often exhibit excellent resistance to corrosion, chemicals, and moisture, making them suitable for harsh environments. Their electrical insulation properties also make them widely used in electronic and electrical applications (Young & Lovell, 2011).

2.1.3 Polymers in Advanced Materials and Nanotechnology

In recent years, polymers have become essential components in advanced material systems, particularly in the development of nanocomposites. When combined with nanoscale fillers such as carbon nanotubes, graphene, or metallic nanoparticles, polymers can exhibit significantly enhanced mechanical, thermal, and electrical properties. This synergy allows polymers to overcome their traditional limitations and expand their application into high-performance fields such as aerospace, biomedical engineering, energy storage, and nanoelectronics (Sperling, 2006).

The versatility of polymers, combined with their ability to interact effectively with nanomaterials, makes them an ideal matrix for nanocomposite systems. This characteristic forms the foundation for the integration of advanced nanomaterials such as silver nanoparticles and graphene into polymer matrices, which will be discussed in subsequent sections of this chapter.

2.2.1 Poly(methyl methacrylate) (PMMA)

Poly(methyl methacrylate), commonly known as **PMMA**, is one of the most widely used synthetic polymers due to its excellent optical, mechanical, and chemical properties. It is a transparent thermoplastic polymer derived from the polymerization of methyl methacrylate (MMA) monomers. PMMA is often referred to by commercial names such as *Plexiglas*, *Acrylic*, or *Lucite*, and it is widely used as a lightweight and durable alternative to glass in many industrial and scientific applications (Young & Lovell, 2011).

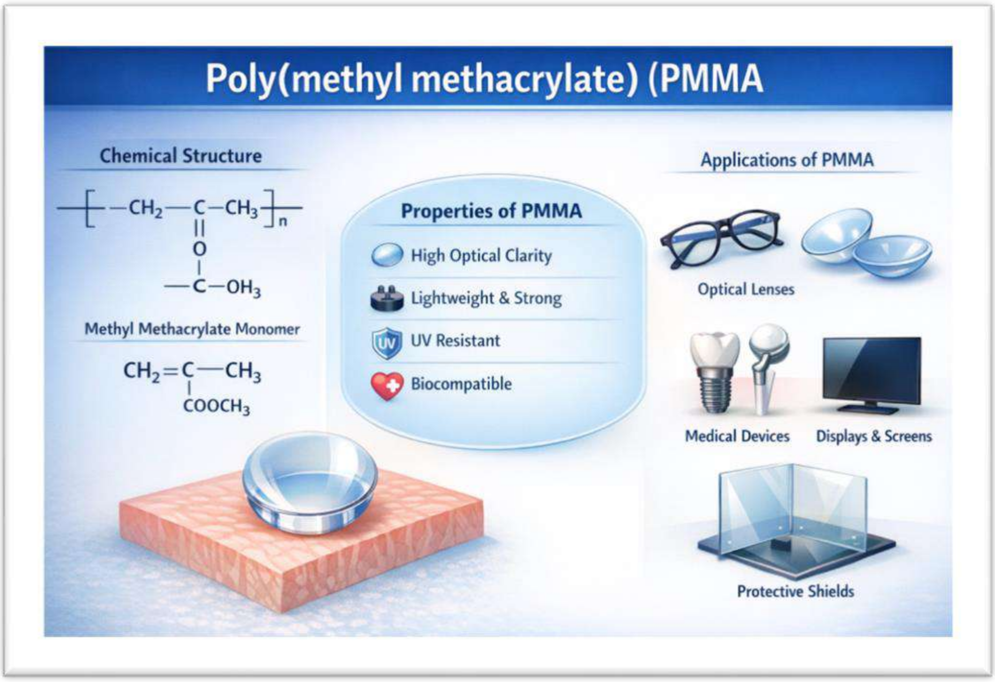


Figure 1. Illustration of Poly(methyl methacrylate) (PMMA): structure, properties, and applications.

PMMA is classified as a **thermoplastic polymer**, meaning it softens upon heating and can be reshaped without undergoing chemical degradation. This characteristic makes it highly suitable for molding, extrusion, and fabrication processes. Its amorphous molecular structure contributes to its high optical clarity and dimensional stability, which are essential properties in optical and electronic applications (Callister & Rethwisch, 2018).

2.2.2 Physical and Mechanical Properties of PMMA

PMMA exhibits excellent physical and mechanical properties that make it attractive for both structural and functional applications. It is known for its high transparency, allowing up to 92% of visible light to pass through, which is higher than that of conventional glass. In addition, PMMA demonstrates good surface hardness, scratch resistance, and weather stability, making it suitable for outdoor use (Odian, 2004).

From a mechanical perspective, PMMA possesses moderate tensile strength and stiffness, along with good impact resistance compared to many other transparent polymers. However, it is relatively brittle when subjected to sudden or excessive mechanical stress, which limits its use in high-impact environments. This limitation has driven extensive research toward reinforcing PMMA using fillers and nanomaterials to enhance its toughness and durability (Sperling, 2006).

2.2.3 Thermal and Chemical Properties of PMMA

Thermally, PMMA exhibits a relatively high glass transition temperature (Tg), typically around 105 °C, which allows it to maintain structural stability under moderate heat conditions. However, its thermal resistance is lower than that of some engineering polymers, which restricts its use in high-temperature environments. PMMA also shows good resistance to ultraviolet (UV) radiation, which contributes to its long-term optical clarity and outdoor durability (Callister & Rethwisch, 2018).

Chemically, PMMA exhibits good resistance to many dilute acids, alkalis, and inorganic salts, but it can be affected by strong solvents such as ketones, esters, and aromatic hydrocarbons. This chemical behavior is an important factor when selecting PMMA for applications involving chemical exposure or surface modification processes.

2.2.4 PMMA in Advanced Applications and Nanocomposites

Due to its transparency, biocompatibility, and ease of processing, PMMA is widely used in biomedical devices, optical components, protective coatings, and electronic applications. In recent years, PMMA has gained significant attention as a **polymeric matrix in nanocomposites**, particularly when combined with nanomaterials such as graphene, carbon nanotubes, and metallic nanoparticles.

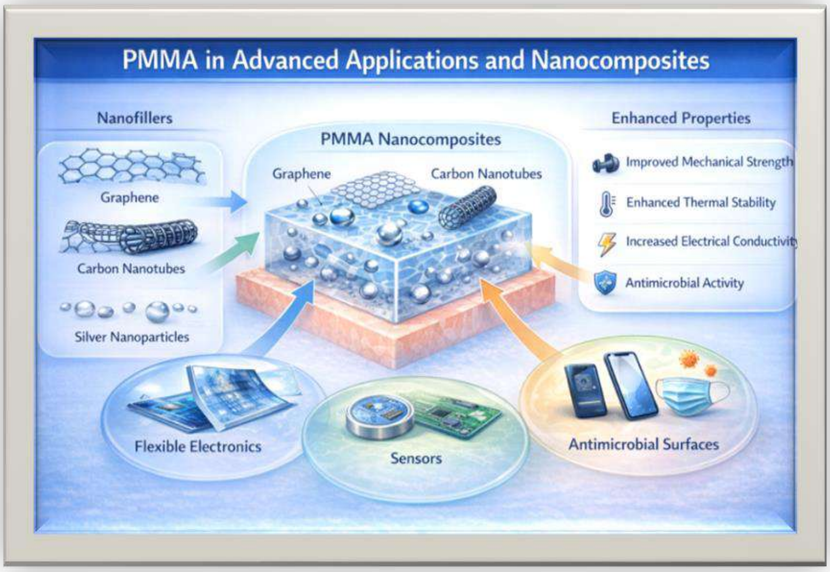


Figure 2 . PMMA nanocomposites with embedded nanofillers: enhanced properties and advanced applications.

The incorporation of nanofillers into PMMA can significantly improve its mechanical strength, thermal stability, electrical conductivity, and functional performance. These enhancements make PMMA-based nanocomposites suitable for advanced applications such as sensors, flexible electronics, antimicrobial surfaces, and optical devices. The compatibility of PMMA with various nanomaterials, along with its ease of processing, makes it one of the most widely studied polymer matrices in nanotechnology research (Sperling, 2006; Young & Lovell, 2011).

Nanotechnology and Nanomaterials

2.3.1 Introduction to Nanotechnology

Nanotechnology is one of the most advanced and rapidly growing scientific fields, focusing on the design, characterization, production, and application of materials at the nanoscale. The term "nano" refers to dimensions ranging from 1 to 100 nanometers, where materials exhibit unique physical, chemical, and biological properties that differ significantly from their bulk counterparts. At this scale, quantum effects and surface phenomena become dominant, leading to enhanced mechanical strength, electrical conductivity, optical behavior, and chemical reactivity (Bhushan, 2017).

The emergence of nanotechnology has revolutionized various scientific disciplines, including materials science, medicine, electronics, energy, and environmental engineering. Its ability to manipulate matter at the atomic and molecular levels has opened new pathways for designing materials with tailored properties that cannot be achieved using conventional methods (Roco, 2011).

2.3.2 Concept and Classification of Nanomaterials

Nanomaterials are materials that possess at least one dimension in the nanoscale range. They can be classified based on their dimensionality into zero-dimensional (0D), one-dimensional (1D), two-dimensional (2D), and three-dimensional (3D) nanostructures. Examples include nanoparticles (0D), nanowires and nanotubes (1D), nanosheets such as graphene (2D), and nanostructured bulk materials (3D). Each category exhibits distinct physical and chemical behaviors due to differences in surface area, atomic arrangement, and quantum confinement effects (Poole & Owens, 2003).

One of the most significant characteristics of nanomaterials is their extremely high surface area-to-volume ratio. This property enhances surface interactions, chemical reactivity, and catalytic activity, making nanomaterials particularly valuable in applications such as sensing, catalysis, energy storage, and biomedical engineering.

2.3.3 Physical and Chemical Properties of Nanomaterials

Nanomaterials exhibit exceptional physical and chemical properties compared to their bulk counterparts. Mechanically, they often show enhanced strength, hardness, and flexibility. Electrically, many nanomaterials demonstrate improved conductivity or tunable electronic behavior, which is essential for nanoelectronics and sensor technologies. Thermally, nanomaterials can exhibit either enhanced or reduced thermal conductivity depending on their structure and composition (Bhushan, 2017).

Chemically, nanomaterials possess high surface reactivity due to the presence of a large number of surface atoms. This feature allows easy functionalization and strong interaction with surrounding materials, making them ideal candidates for composite systems and surface-modified applications. These characteristics are particularly beneficial when nanomaterials are incorporated into polymer matrices to form nanocomposites with superior performance.

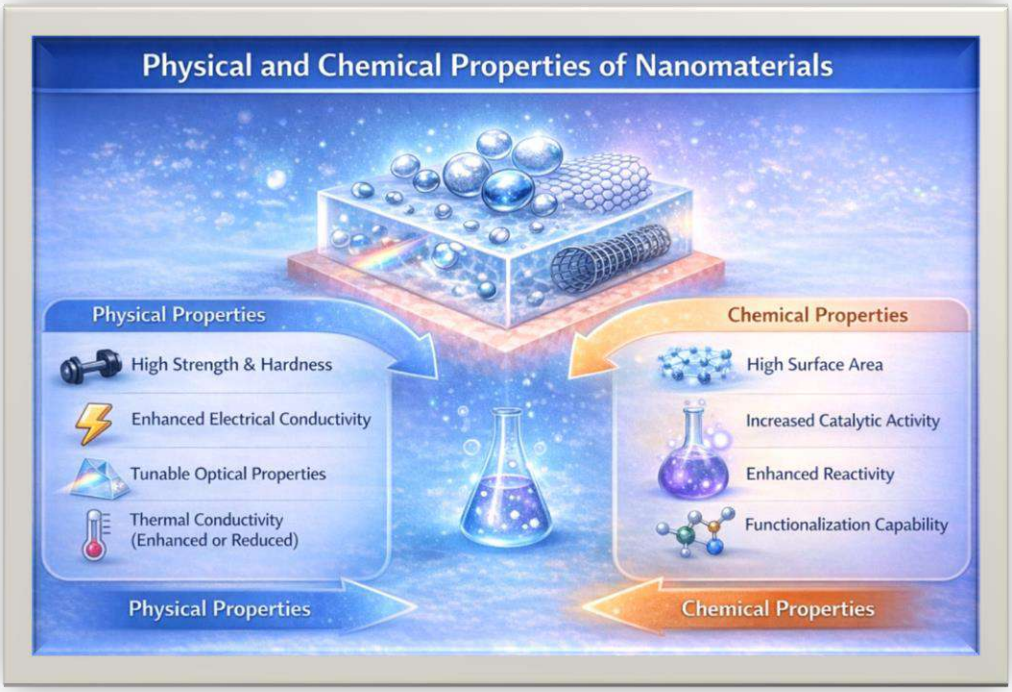


Figure 3. Physical and chemical properties of nanomaterials: key features and examples.

2.3.4 Nanomaterials in Polymer-Based Systems

In polymer based systems, nanomaterials play a crucial role in enhancing mechanical strength, thermal stability, electrical conductivity, and barrier properties. Even a small concentration of nanomaterials can significantly improve the overall performance of polymer matrices due to effective stress transfer and strong interfacial interactions. This behavior makes nanomaterials highly attractive for developing advanced polymer nanocomposites used in aerospace, biomedical devices, flexible electronics, and packaging industries (Ajayan, Schadler, & Braun, 2003).

The incorporation of nanomaterials into polymers also enables multifunctional behavior, such as self-cleaning surfaces, antimicrobial activity, and improved electrical responsiveness. These advantages have positioned nanotechnology as a foundational component in the development of next generation composite materials.

2.3.5 Importance of Nanotechnology in Modern Applications

Nanotechnology has become a cornerstone of modern scientific innovation due to its ability to enhance material performance while reducing weight and material consumption. Its integration with polymers enables the production of high performance nanocomposites that meet the growing demands of advanced engineering applications. As a result, nanotechnology continues to play a pivotal role in fields such as renewable energy, medical diagnostics, electronics, and environmental protection (Roco, 2011).

Silver Nanoparticles (Nano Ag)

2.4.1 Introduction to Silver Nanoparticles

Silver nanoparticles (AgNPs), commonly referred to as **Nano Ag**, are among the most widely studied and utilized nanomaterials due to their unique physical, chemical, and biological properties. These nanoparticles typically range in size from 1 to 100 nanometers and exhibit characteristics that differ significantly from bulk silver. At the nanoscale, silver demonstrates enhanced surface reactivity, optical behavior, and antimicrobial efficiency, making it highly valuable in scientific and industrial applications (Rai, Yadav, & Gade, 2009).

The growing interest in silver nanoparticles is largely attributed to their strong antimicrobial activity, high surface area, and excellent compatibility with polymer matrices. These properties have led to their extensive use in medical devices, coatings, electronics, environmental applications, and polymer-based nanocomposites.

2.4.2 Physical and Chemical Properties of Nano Ag

Silver nanoparticles possess distinctive physical and chemical properties that arise from their nanoscale dimensions. One of the most important features of

Nano Ag is its **high surface-to-volume ratio**, which significantly enhances its chemical reactivity and interaction with surrounding materials. This property allows silver nanoparticles to exhibit strong antimicrobial and catalytic behavior even at low concentrations (Sharma et al., 2009).

From a physical perspective, Nano Ag exhibits unique optical properties due to a phenomenon known as **surface plasmon resonance (SPR)**. This effect occurs when conduction electrons on the surface of the nanoparticles interact with incident light, resulting in strong absorption and scattering in the visible region. This property is widely exploited in sensing, imaging, and optical devices (Kelly et al., 2003).

Chemically, silver nanoparticles demonstrate high stability when properly synthesized and stabilized, yet they can also interact effectively with polymers and biological systems. Their surface can be functionalized with various chemical groups to improve dispersion, compatibility, and performance within composite materials (Rai et al., 2009).

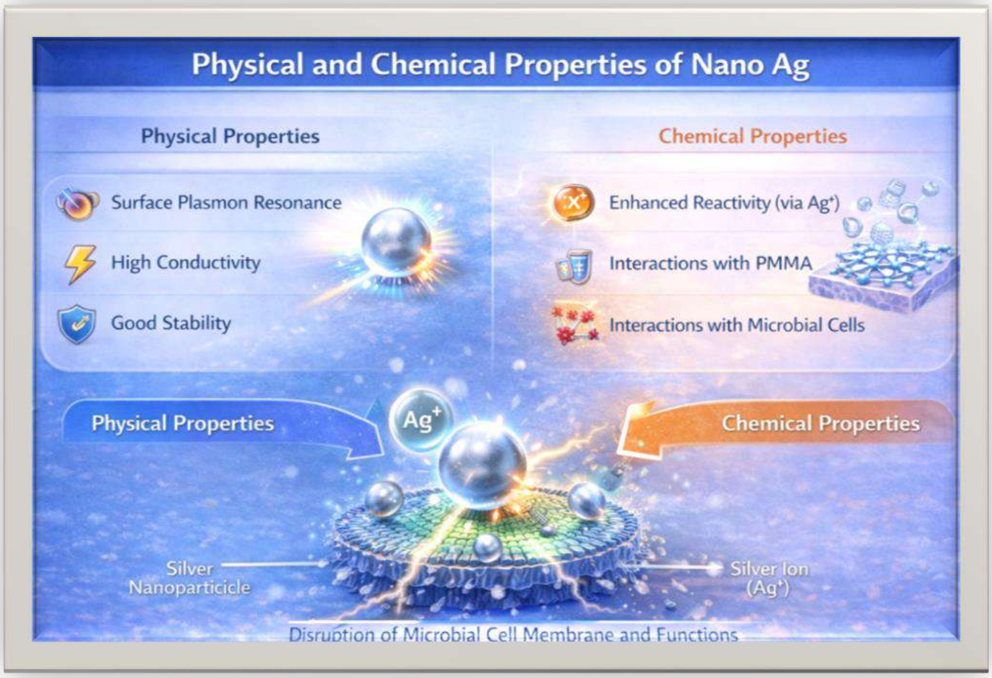


Figure 4. Physical and chemical properties of silver nanoparticles (Nano Ag) and their interactions.

2.4.3 Synthesis Methods of Silver Nanoparticles

Silver nanoparticles can be synthesized using several methods, broadly classified into physical, chemical, and biological approaches. Physical methods include evaporation–condensation and laser ablation, which produce high-purity nanoparticles but often require high energy input. Chemical reduction methods are among the most widely used techniques, where silver ions (Ag^+) are reduced to metallic silver using reducing agents such as sodium borohydride or citrate. These methods allow better control over particle size and morphology (Iravani, 2011).

Biological or "green" synthesis methods have gained increasing attention due to their environmental friendliness. These methods utilize plant extracts, bacteria, or fungi as reducing and stabilizing agents, offering an eco-friendly alternative for nanoparticle production while maintaining good stability and biocompatibility.

2.4.4 Role of Silver Nanoparticles in Polymer Nanocomposites

Silver nanoparticles play a significant role in enhancing the performance of polymer nanocomposites. When incorporated into polymer matrices such as PMMA, they improve mechanical strength, thermal stability, electrical conductivity, and antimicrobial efficiency. The uniform dispersion of Nano Ag within the polymer matrix is crucial for achieving optimal performance, as agglomeration can reduce effectiveness (Ajayan et al., 2003).

One of the most important applications of Ag-based nanocomposites is in antimicrobial materials. The release of silver ions (Ag^+) disrupts microbial cell membranes and interferes with cellular metabolism, making these materials highly effective against bacteria, fungi, and viruses. This property makes PMMA/Ag nanocomposites suitable for medical devices, dental materials, coatings, and water purification systems.

2.4.5 Importance of Nano Ag in Advanced Applications

Silver nanoparticles are widely used in medical, environmental, and industrial fields due to their multifunctional nature. In biomedical applications, they are used in wound dressings, implants, and drug delivery systems. In electronics, Nano Ag enhances conductivity and improves device performance. Additionally, in polymer-based nanocomposites, Nano Ag contributes to multifunctionality by combining mechanical reinforcement with antimicrobial and electrical properties (Rai et al., 2009).

Figure 5. Importance of silver nanoparticles (Nano Ag) in advanced applications across medicine, environment, and industry.

The integration of Nano Ag into polymer matrices such as PMMA represents a significant advancement in materials science, enabling the development of smart, durable, and multifunctional nanocomposites suitable for modern technological applications.

Chapter three

“ Optical Properties “

3.1 The Optical Properties

The investigation of optical properties is a fundamental pillar in the characterization of nanocomposite materials. These properties describe how a medium responds to the electromagnetic field of incident light. In the realm of physics, when light (photons) interacts with a solid-state material, several phenomena occur simultaneously: transmission, reflection, scattering, and absorption. For nanocomposites which typically consist of a host matrix (like a polymer or glass) and an inorganic filler (nanoparticles) the optical behavior is not merely an average of the two components but a complex result of the "Interface" effects and quantum confinement.

The optical response of these materials is governed by the electronic transitions between energy levels. In a semiconductor or insulator nanocomposite, the most vital feature is the **Optical Band Gap (E_g)**. This represents the minimum energy required to excite an electron from the filled valence band (VB) to the empty conduction band (CB). The study of these properties allows researchers to tailor materials for specific applications, such as solar cells, optical filters, and sensors (Smith, 2021, p. 48).

3.1.1 Absorptance (*A*)

Absorptance is a dimensionless quantity that represents the ratio of the energy absorbed by the material to the total energy of the incident light. In nanocomposites, the absorption mechanism is highly sensitive to the concentration of the dopant (nanoparticles). At low wavelengths (high energy), the absorptance usually increases significantly as the photon energy becomes sufficient to overcome the bandgap.

Mathematically, the relationship between Absorptance (A), Transmittance (T), and Reflectance (R) is derived from the principle of conservation of energy:

$$A + T + R = 1$$

If the material is deposited as a thin film on a transparent substrate, the absorptance is often derived from the absorbance (*Abs*), which is the logarithmic ratio of incident to transmitted intensity. The relationship is given by: (Johnson & Lee, 2019, p. 115).

$$A = 1 - 10^{-Abs}$$

3.1.2 Fundamental Absorption Edge

The fundamental absorption edge is the most striking feature in the optical spectrum. It is the threshold where the material changes from being transparent to being opaque. In crystalline materials, this edge is very sharp, but in nanocomposites, it often appears "smeared" or shifted.

- **Blue Shift:** If the nanoparticles are extremely small (less than the Bohr exciton radius), the absorption edge shifts toward shorter wavelengths (higher energy) due to **Quantum Confinement**.
- **Red Shift:** This occurs if the addition of nanoparticles introduces new localized states within the bandgap, effectively narrowing the energy required for transition (Miller, 2020, p. 92).

3.1.3 Absorption Regions

The absorption spectrum of a nanocomposite can be analyzed by dividing it into three distinct physical regions based on the photon energy (*hv*):

1. **The High Absorption Region (** $a \geq 10^{-4}$ cm^{-1} **)**In this region, the energy of the incident photons is greater than the bandgap (*hv* > E). Absorption here is dominated by "Interband Transitions," where electrons jump directly from the valence band to the conduction band.
2. **The Urbach Tail Region (The Exponential Edge):** Here, the absorption coefficient follows an exponential law:

$$\alpha(h\nu) = \alpha_0 \exp\left(\frac{h\nu}{E_U}\right)$$

Where E_U is the **Urbach Energy**. This region represents the transitions involving "Tail States" created by structural disorder, defects, or the internal strain caused by the interface between the nanoparticles and the matrix (Urbach, 1953, p. 1324).

The Weak Absorption Region: This occurs at low energies ($h\nu < E_g$) where absorption is minimal and usually caused by impurities or transitions between localized states (Davis & Mott, 2018, p. 215).

3.1.4 The Electronic Transitions

Electronic transitions are the heart of optical physics in solids. When a photon is absorbed, an electron moves to a higher energy state. These transitions are governed by "Selection Rules" and are classified into two main types:

- **Direct Transitions:** These occur in materials where the maximum of the valence band and the minimum of the conduction band lie at the same point in the Brillouin zone (same wave vector k). The momentum of the electron remains constant during the jump. The relation for the absorption coefficient in this case is:

$$\alpha h\nu = C(h\nu - E_g)^{1/2}$$

Indirect Transitions: In many nanocomposites, the band extrema are at different k values. For an electron to jump, it must interact with both a photon (for energy) and a **Phonon** (a lattice vibration, for momentum). Because this is a three-particle process, it is less probable than a direct transition. The relation is:

$$a\, h\nu = \mathrm{C}\,(\,h\nu - \mathrm{E_g} \pm \mathrm{E_{ph}}\,)^{2}$$

Where E_{ph} is the phonon energy (Garcia, 2021, p. 38).

3.2 Optical Constants

Optical constants are the parameters that characterize the propagation of electromagnetic waves through a medium. For nanocomposites, these constants are not only dependent on the wavelength of the incident light (λ)but also on the volume fraction and the nature of the interface between the nanofiller and the host matrix. Understanding these constants is vital for calculating the energy loss and the dispersion of light within the material (Wilson, 2017, p. 105).

3.2.1 Absorption Coefficient(α)

The absorption coefficient ($\boldsymbol{\alpha}$) is a measure of the rate of decrease in the intensity of an electromagnetic wave as it passes through a medium. It represents the distance over which the light intensity falls to $1/\boldsymbol{e}$ of its original value. In physics, $\boldsymbol{\alpha}$ is determined by the electronic structure and the density of states.

For a thin film of a nanocomposite with thickness (t), the absorption coefficient is calculated from the absorbance (A) using the Beer-Lambert law:

$$\boldsymbol{\alpha} = 2.303\left(\frac{A}{t}\right)$$

In the high-absorption region, α follows Tauc's relation, which is used to determine the optical energy gap (E_g) :

$$(\alpha h\nu) = B(h\nu - Eg)^{r}$$

Where B is a constant called the Tauc parameter, $h\nu$ is the photon energy, and r is an index that characterizes the type of electronic transition (r =1/2 for direct and r=2 for indirect transitions)

(Brown, 2022, p. 59).

3.2.2 Refractive Index (*n*)

The refractive index is one of the most significant optical constants. It describes the phase velocity of light in the medium relative to its velocity in a vacuum. In nanocomposites, the refractive index often follows the Maxwell-Garnett effective medium theory, which relates the effective index of the composite to the indices of the matrix and the nanoparticles.

Experimentally, n can be calculated using the reflectance (R) and the extinction coefficient (k) through the following relation:

$$n = \left(\frac{1+R}{1-R}\right) + \sqrt{\frac{4R}{(1-R)^2} - K^2}$$

If the absorption is very low ($k \approx 0$), the formula simplifies to:

$$n = \frac{1+\sqrt{R}}{1-\sqrt{R}}$$

The refractive index is highly dependent on the "Dispersion" of light, which can be analyzed using models like the Wemple-DiDomenico (W-D) single oscillator model (Taylor, 2020, p. 155).

3.2.3 Extinction Coefficient (*k*)

The extinction coefficient (k) represents the imaginary part of the complex refractive index. It accounts for the energy lost due to absorption and scattering as the wave propagates. A high value of k indicates that the light is rapidly attenuated. It is directly proportional to the absorption coefficient (α) and the wavelength (λ):

$$K = \frac{\alpha\lambda}{4\pi}$$

In the visible range, k usually decreases as the wavelength increases for most dielectric nanocomposites, reflecting the transparent nature of the material in that region (Garcia, 2021, p. 40).

3.2.4 Dielectric Constant (ε)

The dielectric constant (or relative permittivity) describes the polarization of the material under an external electric field. In optical physics, we deal with the Complex Dielectric Constant ($\varepsilon^* = \ \varepsilon\iota + i\varepsilon i$) , which is related to the complex refractive index ($N = n + ik$) by the relation $\varepsilon^* = N^2$

1. **1-** The Real Part ($\varepsilon\iota$) : Represents the ability of the material to store electrical energy and is related to the dispersion of light:

$$\varepsilon\iota = \ n^2 - k^2$$

2. **2-** The Imaginary Part ($\varepsilon\iota$): Represents the energy dissipation (loss) within the material:

$$\varepsilon\iota = 2nk$$

The study of ε provides information about the density of states and the polarizability of the dipoles at the nanoparticle-matrix interface (Taylor, 2020, p. 162).

References

1. Ajayan, P. M., Schadler, L. S., & Braun, P. V. (2003). Nanocomposite science and technology. Wiley-VCH Verlag.

2. Al-Mutairi, N. H., Mehdi, A. H., & Kadhim, B. J. (2021). Nanocomposites via layer-by-layer assembly (LbL).

3. Bhushan, B. (2017). Springer handbook of nanotechnology (4th ed.). Springer.

4. Brown, D. (2022). Optical characterization techniques. CRC Press.

5. Callister, W. D., & Rethwisch, D. G. (2018). Materials science and engineering: An introduction (10th ed.). Wiley.

6. Coetzee, D., Venkataraman, M., Militky, J., & Petru, M. (2020). Influence of nanoparticles on thermal and electrical conductivity of composites. Polymers, 12(4), 742.

7. Davis, E. A., & Mott, N. F. (2018). Conduction in non-crystalline materials. Oxford University Press.

8. El Hawary, A., et al. (2019). A review on processing and applications of nanocomposites. Journal of Composites and Biodegradable Polymers.

9. Garcia, M. (2021). Semiconductor optics and applications. Elsevier.

10. George, J., & Bhattacharyya, D. (2023). Graphene: An introduction. In Recent advances in graphene and graphene-based technologies (pp. 1–24). IOP Publishing.

11. Iravani, S. (2011). Green synthesis of metal nanoparticles using plants. Green Chemistry, 13(10), 2638–2650.

12. Jiang, Y., Song, S., Mi, M., Yu, L., Xu, L., Jiang, P., & Wang, Y. (2023). Improved electrical and thermal conductivities of graphene–carbon nanotube composite film. Energies, 16(3), 1378.

13. Johnson, R., & Lee, T. (2019). Fundamentals of optical materials. Springer.

14. Jovanović, S., Huskić, M., Kepić, D., et al. (2023). A review on graphene composites for electromagnetic shielding. Graphene and 2D Materials, 8, 59–80.

15. Kelly, K. L., Coronado, E., Zhao, L. L., & Schatz, G. C. (2003). The optical properties of metal nanoparticles. The Journal of Physical Chemistry B, 107(3), 668–677.

16. Miller, A. (2020). Nanostructures and optical behavior. Wiley.

17. Müller, K., Bugnicourt, E., Latorre, M., et al. (2017). Polymer nanocomposites and nanocoatings review. Nanomaterials, 7(4), 74.

18. Odian, G. (2004). Principles of polymerization (4th ed.). Wiley.

19. Patnaik, S., Behera, A., & Parida, K. (2021). g-C3N4/graphene nanocomposites review. Catalysis Science & Technology, 11, 6018–6040.

20. Poole, C. P., & Owens, F. J. (2003). Introduction to nanotechnology. Wiley.

21. Puggal, S., Dhall, N., Singh, N., & Singh, M. (2016). Polymer nanocomposites review. Indian Journal of Science and Technology, 9(4), 1–6.

22. Rai, M., Yadav, A., & Gade, A. (2009). Silver nanoparticles as antimicrobials. Biotechnology Advances, 27(1), 76–83.

23. Rana, S., & Gupta, A. (2022). Hybrid nanocomposites. Nanomaterials, 12(6), 1012.

24. Roco, M. C. (2011). Nanotechnology development overview. Journal of Nanoparticle Research, 13, 427–445.

25. Shahil, M. F., & Balandin, A. A. (2012). Graphene-based nanocomposites. Applied Physics Letters.

26. Sharma, V. K., Yngard, R. A., & Lin, Y. (2009). Silver nanoparticles synthesis. Advances in Colloid and Interface Science, 145(1–2), 83–96.

27. Shiju, J., Al Sagheer, F., & Ahmad, Z. (2020). Thermal mechanical properties of graphene nanocomposites. Polymers, 12(11), 2740.

28. Smith, J. (2021). Optical properties of nanocomposite materials. Academic Press.

29. Sperling, L. H. (2006). Introduction to physical polymer science (4th ed.). Wiley.

30. Taylor, S. (2020). Optical constants and dispersion models. Cambridge University Press.

31. Urbach, F. (1953). Optical absorption edge. Physical Review, 92(5), 1324.

32. Wilson, P. (2017). Electromagnetic wave propagation in materials. McGraw-Hill.

33. Young, R. J., & Lovell, P. A. (2011). Introduction to polymers (3rd ed.). CRC Press.

جمهورية العراق

وزارة التعليم العالي والبحث العلمي

جامعة بابل

كلية التربية للعلوم الصرفة

قسم الفيزياء

الخصائص البصرية للمتراكبات النانوية البوليمرية

بحث مقدم الى مجلس كلية التربية للعلوم الصرفة
كجزء من متطلبات نيل شهادة البكلوريوس في كلية التربية / قسم الفيزياء

من قبل الطالب

ضرغام محمد حسن

بأشراف

أ.م.د محمد جواد كاظم البيرماني

1446هـ 2026م

بِسۡمِ ٱللَّهِ ٱلرَّحۡمَٰنِ ٱلرَّحِيمِ

{ قالوا سبْحَانَكَ لا عِلْمَ لَنَا إِلَاّ مَا عَلَّمْتَنَا
إِنَّكَ أَنْتَ الْعَلِيمُ الْحَكِيمُ }

صدق الله العلي العظيم

[سورة البقرة: الاية 32]

إهداء

إلى...

الفاتح لما أغلق * والخاتم لما سبق * والناصر للحق بالحق * والهادي الى الصراط المستقيم * سيد الخلق وحبيب الحق * نبينا محمد عليه وعلى اله وصحبه أفضل الصلاة والتسليم *

إلى...

من أوصى الله بطاعتهما ..... والدي العزيزين * حسباً وتقديراً وعرفاناً بالجميل *

إلى...

كل من ساندني وأزرني خطوة بخطوة على هذا الطريق * رمز النقاء والوفاء والمحبة ونبض القلب * أصدقائي وأخوتي *

إلى...

إلى اساتذتي الافاضل وكل من ساهم في تعليمي *

أهدي ثمرة جهودي وأرجو قبولها

شكر وتقدير

الحمد لله رب العالمين والصلاة والسلام على أشرف الخلق والمرسلين الرسول الكريم محمد وعلى أله الطيبين الطاهرين .

أتوجه بالشكر الجزيل الى جميع اساتذتي الافاضل في قسم الفيزياء كلية التربية للعلوم الصرفة جامعة بابل الذين بذلوا جهداً في توجيهي وامدادي بما احتجت اليه من النصيحة .

وأرى أن اقف شاكراً لأستاذي الفاضل الدكتور محمد جواد البيرماني الذي بذل جهده معي وأعاني ووجهني في كتابتي لهذا البحث.

وأشكر كل من ساعدني وأعانني من الأصدقاء على انجاز هذا البحث فلهم في النفس منزلة وان لم يسعف المقام لذكرهم فهم اهل للفضل والخير والشكر .

الخلاصة

تم خلال هذا البحث دراسة الخصائص البصرية للمتراكبات النانوية (البوليمر- المواد النانوية) وكما تم دراسة الامتصاصية ودراسة مناطق الامتصاص والانتقالات الكترونية المباشرة والانتقالات الكترونية غير المباشرة لهذة المتراكبات النانوية وكذلك دراسة الثوابت البصرية وهي عبارة عن معامل الامتصاص ومعامل الانكسار ومعامل الخمود وثابت العزل الحقيقي والخيالي.