Kingdom of Saudi Arabia
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Faculty of Sciences – Department of Physics

Optical modelling of core-shell plasmonic nanoparticles

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

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بسم الله الرحمن الرحيم

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الملخص

العنوان : "النمذجة البصرية للجسيمات النانوية البلاتينية ذات النواة والغلاف"

يستعرض هذا المشروع خصائص امتصاص الضوء لجزيئات نانوية كروية من الفضة (Ag) والذهب (Au) في شكل نواة وقشرة باستخدام نظرية ميا. لقد تحققنا من كيفية تأثير قطر جزيئات الفضة (Ag) على كفاءة الامتصاص. وقد لوحظ أنه مع زيادة نصف قطر جزيئات الفضة، تتحول رنات البلازمون السطحية نحو أطوال موجية أطول (انزياح نحو الأحمر). في تكوين نواة وقشرة من Ag/Au، مع قطر ثابت لجزيئات الفضة يبلغ 50 نانومتر وسماكة قشرة الذهب (Au) المتغيرة من 4 إلى 14 نانومتر، يصبح طيف الامتصاص أكثر تعقيدًا، مما يكشف عن أوضاع بلازمون أعلى. يبرز هذا البحث العلاقة بين حجم الجسيمات النانوية، وهيكل النواة والقشرة، وسلوك رنين البلازمون السطحي، مما يبرز الخصائص الضوئية القابلة للتعديل التي تفيد في التطبيقات المتعلقة بتوصيل الأدوية المستهدفة، والتصوير البيولوجي، والعلاج الضوئي الحراري.

Abstract

This project examines the light absorption properties of spherical Ag/Au core-shell nanoparticles using Mie theory. We investigated how the diameter of the silver (Ag) nanoparticles influences absorption efficiency. It was observed that as the radius of the Ag nanoparticles increases, their surface plasmon resonances shift towards longer wavelengths (red shift). In the Ag/Au core-shell configuration, with a fixed Ag diameter of 50 nm and varying gold (Au) shell thickness from 4 to 14 nm, the absorption spectrum becomes more complex, revealing higher-order plasmon modes. This research highlights the relationship between nanoparticle size, core-shell structure, and surface plasmon resonance behavior, emphasizing the tunable optical properties that are beneficial for applications in targeted drug delivery, bioimaging, and photothermal therapy.

Chapter 1: Introduction to Light and Its Properties

1.1. Light:

Light is a form of electromagnetic radiation that allows us to perceive the world around us. It travels as waves and does not require a medium, enabling it to move through the vacuum of space. Light waves are transverse waves. It is produced by alternating electric and magnetic fields perpendicular to the propagation of the wave (Figure 1). Light is essential in our daily lives; it provides energy, supports plant growth through photosynthesis, and is integral to technologies such as lasers, fiber optics, and cameras. The speed of light in a vacuum is approximately 299,792 kilometers per second. Additionally, light exhibits wave-particle duality, behaving both as a wave and as a particle.

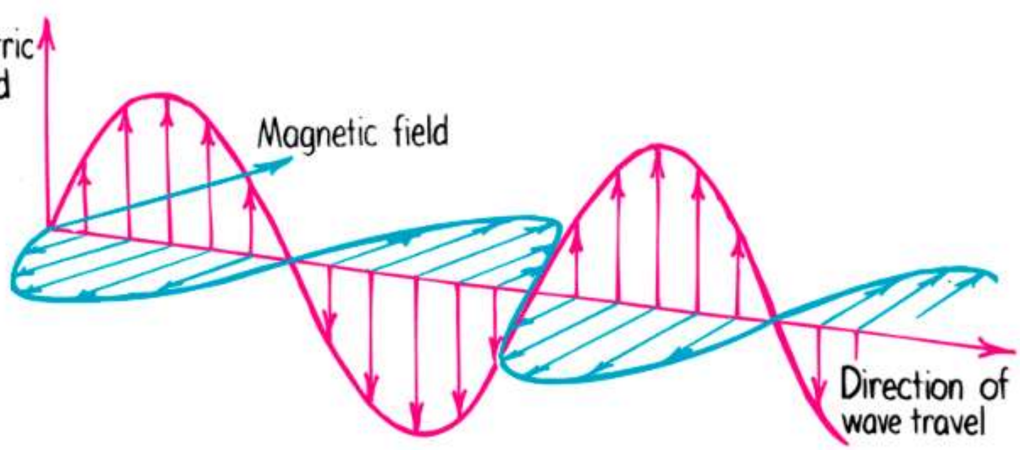

Figure 1.1. Light as a transverse electromagnetic wave.

1.2. Photon:

A photon is the fundamental particle of light, representing a quantum of electromagnetic energy. It is considered massless, which allows it to travel at the speed of light. Photons are emitted when atoms absorb energy and become excited; as they return to a lower energy state, they release energy in the form of photons. The energy carried by a photon depends on its frequency or wavelength: high-energy photons, such as X-rays, have shorter wavelengths, while low-energy photons, like radio waves, have longer wavelengths.

1.3. Light Properties:

Light exhibits several key properties that define its behavior and interactions with materials, including wavelength, frequency, speed, energy, amplitude, and polarization [1][2]. The wavelength determines the color of visible light, while the frequency relates to the energy of the photons. Light can be reflected, refracted, absorbed, transmitted, and scattered, and it can also interfere with other light waves and become polarized. Understanding these properties is essential in fields such as optics, astronomy, and telecommunications.

1.4. Absorption:

Absorption occurs when a material takes in the energy of light and converts it, typically into heat. Different materials absorb various wavelengths of light depending on their composition. For example, black objects absorb more light and thus become warmer, while white objects reflect most of the light and remain cooler. Absorption is crucial in solar energy applications, where solar panels absorb sunlight and convert it into electricity. It also plays a significant role in vision, as pigments in the eye absorb specific wavelengths of light.

Chapter 2: Plasmonic Nanoparticles: Concepts and Theories

1.2 Maxwell's Equations:

Maxwell's Equations are a set of four fundamental equations that form the foundation of classical electromagnetism. They describe how electric and magnetic fields interact and how these interactions give rise to electromagnetic waves, including light. Formulated by James Clerk Maxwell in the 19th century, these equations are essential for understanding a wide range of physical phenomena and modern technologies.

Gauss's Law for Electricity: Gauss's Law states that the electric flux through a closed surface is proportional to the total electric charge enclosed within that surface. This law implies that electric charges are the source of electric fields. It is expressed by the equation:

$$\nabla \cdot E = \rho / \varepsilon_0 \tag{2.1}$$

Gauss's Law for Magnetism: Gauss's Law for Magnetism indicates that there are no magnetic monopoles; magnetic field lines always form closed loops. It is expressed by the equation:

$$\nabla \cdot B = 0 \tag{2.2}$$

Faraday's Law of Induction: Faraday's Law explains that a changing magnetic field induces an electric field. This principle is fundamental in the operation of electric generators and transformers. It is expressed by the equation:

$$\nabla \times E = - \partial B / \partial t \tag{2.3}$$

Ampère-Maxwell Law: The Ampère-Maxwell Law describes how magnetic fields are generated both by electric currents and by changing electric fields. The addition of the displacement current term by Maxwell was key in predicting electromagnetic waves. It is expressed by the equation:

$$\nabla \times B = \mu_0 J + \mu_0 \varepsilon_0 \, \partial E / \partial t \tag{2.4}$$

Table 2-1: Symbols of Maxwell's Equations

Symbol	Meaning
$\boldsymbol{E}$	Electric field
D	Electrical displacement
H	Magnetic field stength
$\boldsymbol{B}$	Magnetic field
σ	Charge density
ε_0	Permittivity of free space
μ_0	Permeability of free space
$\boldsymbol{J}$	Current density
$\nabla \cdot$	Divergence operator
$\nabla \times$	Curl operator

2.2. Plasmonic Resonance:

Plasmonic resonance is a phenomenon that occurs when electromagnetic waves, such as light, interact with the free electrons on the surface of a metal, typically gold or silver. Under specific conditions, the incident light induces a collective oscillation of these electrons around positive ion cores within the nanoparticles, resulting in what is known as surface plasmon resonance (SPR) (see Figure 9). The Coulomb force between the negatively charged electrons and the positively charged nucleus acts to restore the electrons to their equilibrium positions [3]. This phenomenon is characterized by longitudinal oscillations and typically occurs at the interface between the metal and a dielectric material, leading to the creation of a strong localized electromagnetic field. At plasmonic resonance, maximum absorption of incident light causes significant kinetic energy transfer to the electrons, enhancing the collective oscillation of conduction electrons within the material. Plasmonic resonance is significant because it enables the control of light at scales smaller than its wavelength. This capability opens up new opportunities for developing miniaturized optical components and for exploring light-matter interactions in unprecedented ways. It serves as a bridge between photonics and electronics in nanoscale devices, facilitating advancements in various applications, including sensing, imaging, and telecommunications.

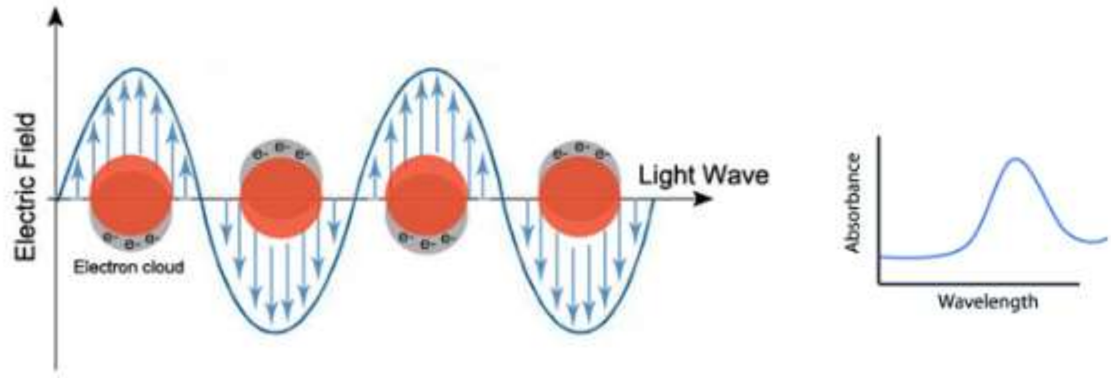

Figure 2.1. Plasmonic resonance in metal nanoparticles.

2.3. Applications for SPR:

Plasmonic resonance has several important applications, particularly in the fields of nanotechnology and optics as present in Table 3

Biosensing: SPR sensors are widely used for detecting biomolecular interactions, such as antigen-antibody binding.

Photovoltaics: Enhances the efficiency of solar cells by improving light absorption.

Imaging: Super-resolution microscopy techniques utilize plasmonics to surpass the diffraction limit.

Nano-optics: Enables the guiding and manipulation of light at the nanoscale using plasmonic waveguides.

Table 2-2: The different applications of surface plasmon resonance (SPR) with a brief description of each application

Plasmonic Resonance Application	Description
Biosensing	SPR sensors used for detecting biomolecular interactions such as antigen-antibody binding.
Photovoltaics	Improves the efficiency of solar cells by enhancing light absorption.
Imaging	Used in super-resolution microscopy techniques to surpass the diffraction limit.
Nano-optics	Guiding and manipulating light at the nanoscale using plasmonic waveguides.

2.4 Mie Theory

Mie theory, formulated by the German physicist Gustav Mie in 1908, provides a comprehensive analytical solution to Maxwell's equations that describe the scattering of electromagnetic radiation, particularly light, by spherical particles. It is a cornerstone in the study of light-particle interactions across various scientific domains.

At its core, Mie theory offers detailed insights into how light is absorbed, scattered, and extinguished by spherical particles. The theory predicts not only the total intensity of scattered light but also its angular distribution, polarization characteristics, and spectral behavior. These optical responses are quantified using key dimensionless parameters, including scattering efficiency, absorption efficiency, extinction efficiency, and the asymmetry parameter, all derived from solutions involving spherical Bessel and Hankel functions. Additionally, Mie theory accounts for the complex refractive index of both the particle material and the surrounding medium, further influencing scattering and absorption profiles.

Although Mie theory is most accurate for homogeneous, isotropic, and perfectly spherical particles, its principles have been extended to more complex geometries, including ellipsoids, cylinders, and multilayered particles. Computational implementations of Mie theory, including numerical solvers and software tools, have made it accessible to researchers across various disciplines, allowing for precise simulation of light-particle interactions. In the context of shells or coatings, Mie theory is indispensable for both theoretical modeling and experimental interpretation.

2.5 Applications of Mie Theory

One of the primary reasons for the enduring relevance of Mie theory is its wide range of applications:

Atmospheric Physics: Mie theory is employed to analyze the scattering of sunlight by water droplets, aerosols, and particulate matter. This enables accurate modeling of phenomena such as cloud brightness, sky coloration, and atmospheric visibility. The theory also explains why clouds appear white and why certain particles lead to optical effects like halos or glories.

Biomedical Optics: Mie theory simulates the interaction of light with biological tissues, blood cells, and nanoparticles used as contrast agents or drug carriers. It aids in the design of optical imaging techniques, such as optical coherence tomography (OCT) and diffuse optical spectroscopy, by providing insights into how light penetrates and scatters within tissues.

Nanoscience and Nanotechnology: Mie theory plays a crucial role in the study and design of metal and dielectric nanoparticles. When nanoparticles are coated with metallic shells—creating core-shell nanostructures—their scattering and absorption behaviors exhibit sharp resonances known as localized surface plasmon resonances (LSPRs). Mie theory provides the mathematical framework to predict these resonances, which are highly sensitive to the particle's size, shell thickness, refractive index, and dielectric environment. This sensitivity is leveraged in the development of plasmonic sensors, photothermal therapy agents, and tunable optical devices.

Characterization of Nanoparticle Suspensions: Mie theory is foundational in enabling researchers to extract size distributions, refractive indices, and concentration information from experimental data using techniques like dynamic light scattering (DLS) and UV-Vis spectroscopy. These capabilities are critical in materials science, pharmaceuticals, and colloid chemistry.

2.7 Core-Shell Nanoparticles

Core-shell nanoparticles are a class of engineered nanostructures composed of a central "core" material surrounded by a distinct outer "shell" layer, as illustrated in Figure 11. This design enables the combination of different physical, chemical, and optical properties within a single particle, offering a high degree of tunability and functionality. The core and shell can be made from various materials, such as metals, semiconductors, oxides, or polymers, with combinations chosen based on the desired application.

The core often determines the primary functional properties of the nanoparticle, such as magnetism, fluorescence, or catalytic activity. In contrast, the shell can serve multiple roles: enhancing stability, providing biocompatibility, improving dispersibility in solvents, or modulating the particle's interaction with electromagnetic radiation. For instance, a dielectric or semiconductor core coated with a thin metallic shell—typically gold or silver—can exhibit surface plasmon resonance (SPR), where conduction electrons on the metal surface resonate with incident light at specific wavelengths. This plasmonic effect leads to strong absorption and scattering peaks that can be precisely tuned by altering the core size, shell thickness, or surrounding refractive index.

Core-shell structures are particularly advantageous in optical and biomedical applications. In biosensing, the enhanced optical response of metal-coated nanoparticles is utilized to detect changes in the local environment, such as binding events with target biomolecules. In photothermal therapy, the shell's ability to absorb light and convert it into heat allows for the targeted destruction of cancer cells upon irradiation.

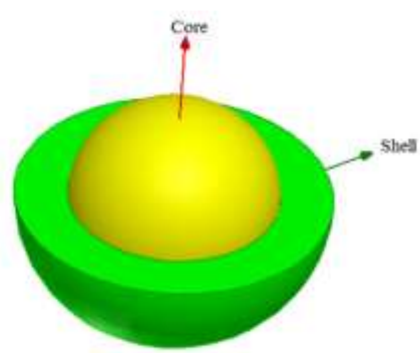

Figure 2.2. core-shell nanoparticles structure.

Chapter 3: Results and discussion

3.1 Effect of Ag nanoparticle diameter on the light absorption cross-sectional area

The absorption cross-sectional area of pure Ag nanoparticles was calculated using Mie theory, with nanoparticle radii ranging from 20 to 50 nm in air, as illustrated in Figure 3.1. Each nanoparticle diameter exhibits a peak in the Mie resonance wavelength, where the resonance peak shows the highest amplitude across all curves. Following this peak, scattering decreases rapidly. As the nanoparticle diameter increases, these peaks not only grow in amplitude but also shift towards longer wavelengths. This shift is attributed to the plasmon resonance of the Ag nanoparticles, which significantly influences the electromagnetic wave and enhances scattering at longer wavelengths. The coherent oscillations of free electrons within the plasmonic nanoparticles respond to the alternating electric field of the incident light, producing surface polarization around the nanoparticles. As the size of the nanoparticles increases, the charge separation between the negative charges (free electrons) and positive charges (ionic metal core) also increases. Consequently, the Coulomb attraction force between the oscillating electrons and the ionic core diminishes. This results in a decrease in plasmon resonance energy, leading to a red shift in the resonance peak [4]. Figure 3.2 illustrates the relationship between the Ag nanoparticle diameter and the Mie resonance wavelength peak. The peak position increases sharply with the diameter of the Ag nanoparticles, shifting from 354 nm to 567 nm as the radius increases from 20 nm to 50 nm.

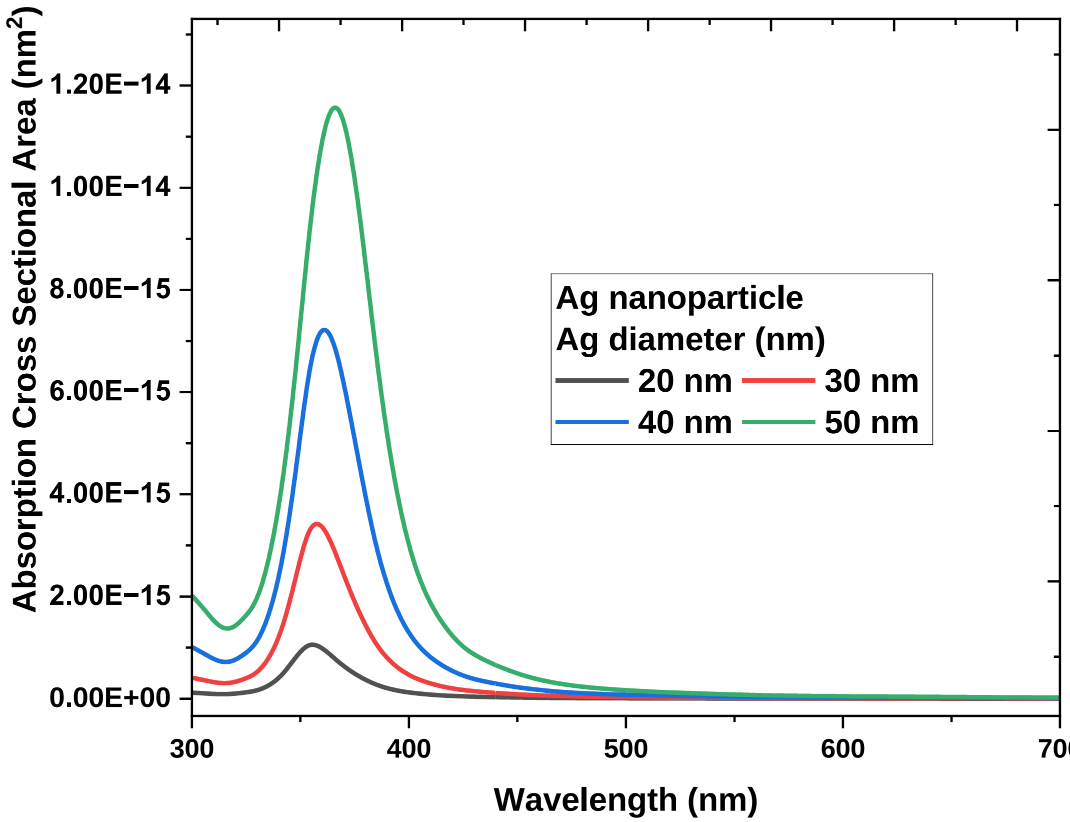

Figure 3.1. Absorption cross-sectional area of Ag nanoparticles with diameters between 20 and 50 nm in air.

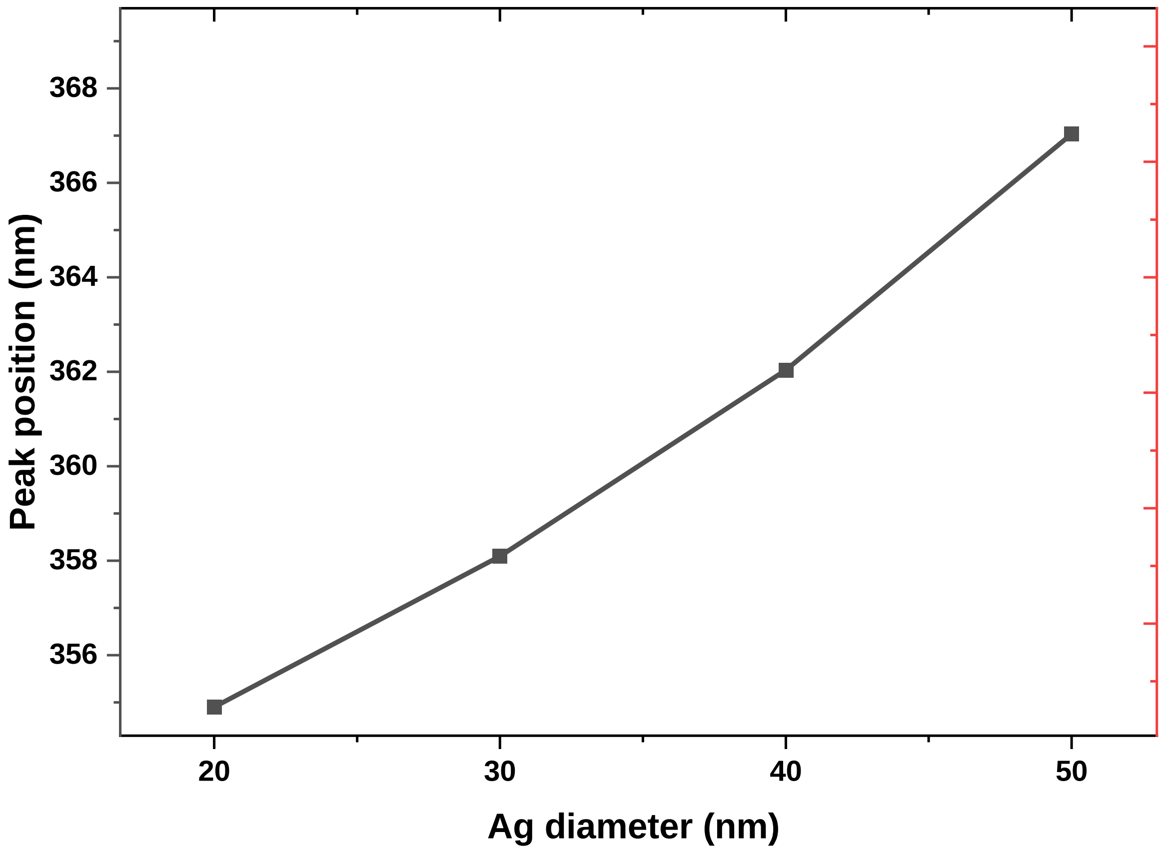

Figure 3.2. Resonance wavelength peak positions as a function of the radius of Ag nanoparticles.

3.2 Effect of Au shell thickness on light absorption cross-sectional area for Ag/Au core/shell nanoparticle

The absorption cross-sectional area for the Ag/Au core-shell model was calculated in air, focusing on nanoparticles with a fixed silver (Ag) diameter of 50 nm while varying the thickness of the gold (Au) shell from 4 to 14 nm. Silver is well-known for its strong surface plasmon resonance (SPR), which enhances its ability to absorb and scatter light effectively. However, silver is also prone to oxidation, which can diminish its performance over time. In contrast, gold is highly stable and resistant to oxidation, providing a protective layer that improves the overall durability of the core-shell nanoparticle. This design harnesses the advantageous properties of both metals, making the nanoparticles suitable for various biomedical applications.

The absorption spectra of the Ag/Au core-shell nanoparticles differ significantly from those of pure silver nanoparticles, as illustrated in Figure 3.3. This difference is attributed to the influence of the gold shell on the plasmonic behavior of the silver core. When the gold shell is thin (4 and 8 nm), the core-shell nanoparticles exhibit a single oscillation mode, indicating a fundamental surface plasmon mode. As the shell thickness increases to 10 and 14 nm, the number of peaks in the scattering spectra also rises, suggesting that thicker shells facilitate more complex plasmonic interactions and allow for the excitation of higher-order plasmon modes.

The behavior of SPR modes is closely tied to the size and shape of the nanoparticles. In smaller core-shell configurations, the electric field of the incident light remains uniform across the nanoparticle, leading to coherent oscillation of all electrons in phase, which produces only the fundamental surface plasmon mode. However, as the size of the core-shell nanoparticle increases, the polarization of the electric field becomes more inhomogeneous. This variation in polarization induces dynamic polarization effects, enabling the excitation of higher-order modes. These higher-order modes contribute to the richer scattering spectra observed with increased Au shell thickness. This tunability in the optical properties of core-shell nanoparticles is particularly advantageous for applications such as targeted drug delivery, bioimaging, and photothermal therapy, where specific absorption and scattering characteristics are crucial for effectiveness.

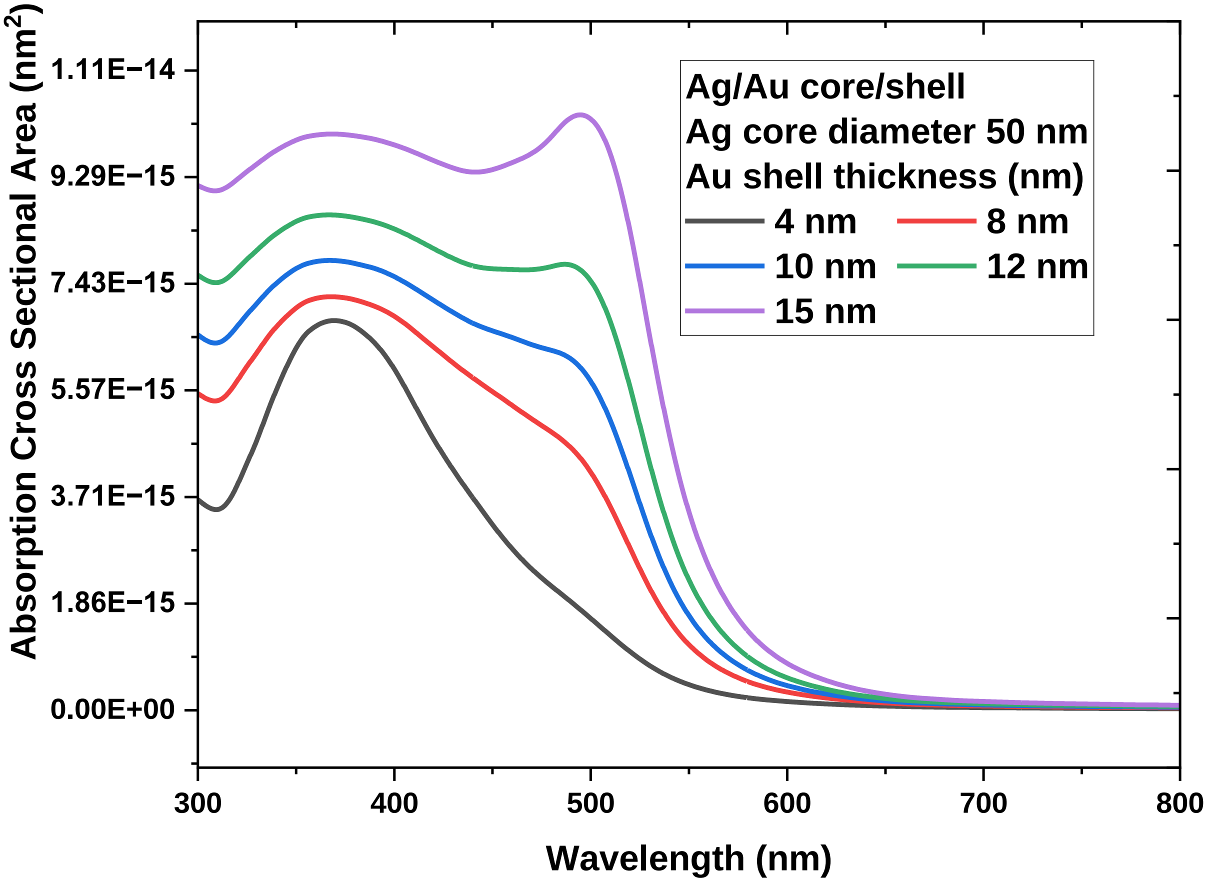

Figure 3.3. Absorption cross-sectional area of Ag/Au cor-shell nanoparticles with the Ag core having a diameter of 50 nm and varying Au shell thicknesses from 4 to 15 nm in air.

Conclusion

This study examined the optical properties of spherical Ag/Au core-shell nanoparticles, specifically their light absorption characteristics influenced by the size of the silver core and the thickness of the gold shell. We found that increasing the diameter of the Ag nanoparticles results in a red shift of their surface plasmon resonances, indicating altered interactions with light. Additionally, for Ag/Au core-shell nanoparticles, varying the Au shell thickness from 4 to 14 nm leads to more complex absorption spectra, characterized by the emergence of higher-order plasmon modes. The ability to tune these optical properties presents significant potential for improving the efficacy of applications such as targeted drug delivery, bioimaging, and photothermal therapy.

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