



THE EFFECT SURFACE PLASMON RESONANCE ON SPHERICAL MAGNETO PLASMONIC $Fe_3O_4@Au$ CORE-SHELL NANOPARTICLES.

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Abstract

this thesis, study the characteristics of the scattering cross section, the permeability, permittivity, the electric polarizability, extinction cross section and absorption cross section of light on the surface of the plasmon resonance at the spherical magneto plasmonic (Fe_3O_4/Au)core/shell nanoparticle with different value of wave length, metal fraction (β), host matrix (ε_h) and a constant value of factorize(f) and a radius of the shell(a_s).

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Chapter 1

Background of the study

1.1 Introduction

Nanomaterials attract much attention due to their interesting properties and have wide scientific and technical applications [1,2]. The rapid advances of nanotechnologies during the last decades made it possible to design compounds and materials with strictly tailored dimensions, compositions, structures, and other parameters [3,4]. This structures tunability can potentially give rise to new technologies for even more complex field of chemistry, and material science [5]. Nanomaterials forms heterogeneous structures composed of a noble metal and a semiconductor. Noble metals such as Au and Ag, strongly absorbed light in the visible region due to coherent collisions of the metal conduction band electrons in strong resonance with visible frequencies of light. This phenomenon known as surface plasmon resonance (SPR) and is highly dependent on NPs size, shape, surface, and dielectric properties of the surrounding medium. Light absorbed by nanoparticles is readily dissipated as heat. Due to their large absorption cross sections, plasmonic NPs can generate a significant amount of heat and increase temperature in their vicinities [6, 7, 8, 9, 10,]. These peculiar types of systems offer to design materials with novel and unique physical

chemistry and properties. Iron oxides nanoparticles play a major role in many areas of chemistry, physics and material science.

surface plasmons resonance have been used to enhanced the surface sensitivity of several spectroscopic measurements including fluorescence, Raman scattering and second harmonic generation. However, in their simplest form, SPR reflectivity measurements can be used to detect molecular adsorption, such as polymers DNA or proteins etc [11]

magneto plasmonic nanoparticles are one of the emerging multifunctional materials in the field of nanomedicine. Nanomedicine, which is based on successful administration of nanomaterials to prevent diagnose and treat diseases has attracted for the last few decades. magnetic nanoparticles on Au nanoparticles possess promising properties for theragnostic (combination of diagnosis and therapy).

composite nanomaterials are a built of core (the inner material) and shell (the outer material layer), both layers having nanometer sizes [12] in view of the ever-rising interest to potentially multifunctional nanomaterials core-shell nanostructures are increasingly attracting attention [8-10]. The composition of the core and shell in core-shell nanoparticles (NPs) can be constituted from organic and inorganic materials and compounds [13]. The appearance of synergism makes these nanomaterials useful in biotechnology, nanomedicine, nanooptics, magnetic devices, fuel cells, nano catalysis, and so on [14,15].

Core shell nanoparticles are essentially heterogeneous NPs composed of two or more materials (metal, element, or biomolecules); one nanomaterial acts as a core in the center while the other materials behave as a shell [16]. Core/shell composite nanostructures (NSs) exhibit many unique properties, including mono- dispersion,

core/shell operability, stability and self- assembly. Those materials have a good surface plasmon resonance at their interface and the noble metal/semiconductor core /shell composite NS has been one of the most promising composite NSs of the recent decades [17]. Magnetic/plasmonic nanostructures demonstrate multiple properties not present in individual nanomaterials. Magnetic-plasmonic core shell (NPs) possess dual magnetic plasmonic properties and have widespread applications in biomedical fields. The magnetic core such as iron-oxide(Fe_3O_4) are greatly desired for applications such as magnetic separation, magnetic resonance imaging or magnetic guided drug delivery. A magnetic resonance imaging (MRI) medical imaging techniques using a strong magnetic field and radio wave for body diagnosis is the major application of magnetite(Fe_3O_4) [21,22]. Moreover, typical metal nanoparticles (NPs) of gold and silver have a great attractive in many application [23,24] due to exhibits of surface plasmon resonance phenomena and optical activity.

Bifunctional nanomaterials Fe_3O_4 @Au core-shell is a kind of nanoparticles that includes magnetic iron oxide core with gold coated. It can be used in can achieve controllable and tunable electromagnetic field enhancement and may open exciting opportunities to engineer a new material used in biomedical and another application.

1.2 Statement of the problem

The characteristics of scattering, the absorption, and the extinction cross sections of Fe_3O_4 @Ag core/shell spherical nanoparticles has been studied by different researchers. However, it shows that we still have a lot of work to do in terms of the importance of the technology. Therefore, as I have understood there is necessity to do a research based of the noble metal nanoparticles. That's why the research

question have an objective to studies the characteristics of scattering, absorption, extinction cross section and the theoretical model of the spherical core/shell $Fe_3O_4@Au$ nanoparticles.

1.3 Basic research questions

- What is the electrical polarizability of the surface plasmon resonance on spherical magneto plasmonic $Fe_3O_4@Au$ core - shell nanoparticles?
- What is the absorption cross section of the surface plasmon resonance on spherical magneto plasmonic $Fe_3O_4@Au$ core - shell nanoparticles?
- What is the scattering cross section of the surface plasmon resonance on spherical magneto plasmonic $Fe_3O_4@Au$ core - shell nanoparticles?
- What is the extinction crosssection of the surface plasmon resonance on spherical magneto plasmonic $Fe_3O_4@Au$ core - shell nanoparticles?

1.4 Objective of the study

1.4.1 General objective

To investigate the characteristics of surface plasmon resonance on spherical magneto plasmonic $Fe_3O_4@Au$ core - shell nanoparticles

1.4.2 Specific objective

- To analysis the electrical polarizability of the surface plasmon resonance on spherical magneto plasmonic $Fe_3O_4@Au$ core - shell nanoparticles

- To determine the absorption cross section of the surface of surface plasmon resonance on spherical magneto plasmonic $Fe_3O_4@Au$ core-shell nanoparticles
- To identify the scattering cross section of the surface plasmon resonance on spherical magneto plasmonic $Fe_3O_4@Au$ core - shell nanoparticles
- To determine the extinction cross section of the surface plasmon resonance on spherical magneto plasmonic $Fe_3O_4@Au$ core - shell nanoparticles

1.5 Scope of the study

The scope of this study is limited to study the characteristics of the real and the imaginary part of the polarizability, the absorption cross section ,scattering cross section and the extinction cross section versus wave length of different value of β and host matrix ε_h and with fixed value of frequency and radius of the shell(a_s)

1.6 Significant of the study

The benefit of this research paper is many. As you know nanotechnology is very useful for the level we have reached now. Because it helps us use for different purpose. Therefore, this paper is introducing some advantage of surface plasmon resonance and spherical of $Fe_3O_4@Au$ core/shell for the nanotechnology, nanomedicine and so on. But it does not focus on this one, the paper focus, how to analysis theoretically the scattering cross section, absorption cross section, extinction cross section and electrical polarizability of the spherical $Fe_3O_4@Au$ core/shell nanoparticles.

Chapter 2

Review Related of Literature

2.1 Introduction

The concept of nanotechnology was introduced for the first time Richard Feynman during 1959. According to Richard Feynman, nanotechnology is a science and art that produced a material at nanoscale and it is used to create material on atomic scale. it depend on the ability to manipulated each individual atom and molecules for the case of assembling them into a bigger structure. Those materials that made of this process is called nanostructures. Such artificial nanostructures, usually fabricated by using self-assembly phenomena. And also, nanostructure is intermediate size between macroscopic and molecular structures.

Nanostructures with combining both magnetic and plasmonic properties becomes an active research topic in recent years, Armelles et al. (2013), Maksymov et al. (2015). Nanoparticles made of noble metals like Ag and Au exhibit surface plasmonic resonance (SPR) under special conditions. Plasmonic effect in enhance absorbance and scattering at plasmonic resonance. Moreover, the intensity and position of plasmon resonance in absorbance spectrum depend on the shape, size and the embedding

medium. SPR has been used for biosensing, photothermal therapy applications, Brullot et al. (2012), conde et al. (2011). The ability of magnetical manipulating and guiding of nanostructure are important in biomedicine. Magnetic material such as magnetite and maghemite have been used in biomedicine due to low toxicity and high magnetic susceptibility, Brullot et al. (2012). Core shell noble metal - magnetic nanoparticles provide both magnetic and plasmonic behaviors. Therefore these composites have great potential due to multifunctionalities. $Fe_3O_4@Au$ nanoparticles are promising structures for using in biomedical applications due to their magnetic and plasmonic characteristics. $Fe_3O_4@Au$ can be prepared by available chemical method in different diameters of shell and core. Therefore, desired optical properties can be achieved at manageable dimensions. These multifunctional structures have extensive applications such as using them for magnetic resonance imaging (MRI), drug release and photothermal therapy, Brullot et al. (2012), conde et al. (2011).

Many researchers have attempted to combine Fe_3O_4 and Au as nanocomposite devices. These attempts were challenged by the core/shell $Fe_3O_4@Au$ due to surface enhanced Raman scattering (SERS) effect and localized surface plasmon resonance (LSPR). LSPR cause some suitable characteristics such as enhancement of electric field, localization of energy at nanometer scale, and strongly enhanced absorption and scattering. In Ref. [7], it is reported that the synthesis characterization of core-shell NPs with a magnetic core and a gold shell can be done by varying the concentration ratio of the reduction agent so that gold is deposited on the magnetite. Gold coating was achieved by adding butylamine as a weak reducing agent of $AuNO_3$ in foregoing solution. And they have been dealing with ferromagnetic metal coating noble metal

developed a sequence synthesis method of gold shell in surface Fe_3O_4 with high mono dispersity and controllable. Mostly, core -shell nanoparticles are manufactured by a consecutive two- step process: a core is first fabricated, then a shell is grown over [22]. The most important points in manufacturing these structures are coverage uniformly and careful regulation of the shell thickness. Surfactants and polymers can serve for this purpose; they can change the surface the surface change and selectivity of the core to generate a homogeneous shell that can would be completely coat the core [23].

Recently, much attention has been paid to the fabrication of core -shell nanostructures comprising magnetic iron oxides coated with a shell of noble -metal (gold, platinum, silver, and palladium) nanoparticles The properties of the nanosized materials appreciably differ from the properties of their bulk analogues, so they can be used in some advanced functional technologies. Noble metal nanoparticles, have high catalytic properties surface modifying versatility and unique biocompatibility [24]

To investigate the optical properties and response (absorption and scattering) of NPs with light (electromagnetic radiation) interaction, one has to measure the effective permittivity, ϵ_{eff} , and permeability, μ_{eff} , [25]. In this paper, we intended the magneto optical response of the theoretically modelled spherical core-shell NPs. Gold nanoparticle was selected as a shell on magnetic nanospheres, due to its nontoxic, strong absorption in the UV and visible spectrum [19] and surface plasmon resonance (SPR) which play great role in determining the optical response of nanoparticles. In this research the theoretical investigation of the basic optical absorption properties of $Fe_3O_4@Au$ core shell with the plasmon resonance wave length, light scattering,

absorption extinction cross section of core/shell are affected shell thickness, core diameter, electronic properties of the shell and surrounding environment at the two different interfaces (outer surface between the surface and the incident light, and inner interface between metal and semiconductor). And this paper structure as follow: In section 2, the effective permittivity, permeability of the theoretical modelled magnetic semiconductor- semiconductor/metal/shell spherical NPs embedded in a dielectric host matrix and the equation for the effective polarizabilities, absorption cross-section and scattering cross section are derived. In section 3 the methodology of the research is described. The numerical results will present and discussed in section 4. Detailed analysis of the magneto optical responses of $Fe_3O_4@Au$ core/shell NPs namely the electric polarizability, absorption cross-section, scattering cross-section and extinction cross section will present. Finally, concluding remarks are presented in section 5.

2.2 Theoretical model

the core-shell model was employed to characterize the Fe_3O_4 nanoparticles coated with a gold shell. The fitting geometrical parameter for this model are: the core radius(a_c),the shell radius(a_s) and the total radius(a_t). In the present work, we considered a model of $Fe_3O_4@Au$ spherical core- shell NPs, which is composed of magnetic-half metallic iron(III) oxide (Fe_3O_4) core of radius (a_c) and an outer metallic(Au) shell of radius a_s embedded in a dielectric host matrix as shown in Fig. 1, where $a_c < a_s$. Because of the core material the magnetic is with permeability, $\mu \gg 1$, the magneto optical properties of the system require determination of its effectivity ε_{eff} and permeability μ_{eff} . Based on electrostatic approximation and the Maxwell-

Garent effective medium theory, theoretically analysis have be done to derive y ε_{eff} and μ_{eff} . Moreover, using these theoretically determined values, calculations has been done on the magneto-optical parameters such as, the electric polarizability, absorption and scattering cross-sections.

2.3 Effective permittivity and permeability

The dielectric constant of the gold- shell is a function of frequency of the incident electromagnetic wave. Indeed, the interaction between an electromagnetic wave or with a $\phi(\omega)$ and a metal will lead to polarization of the medium. This polarization will then generate a change in complex refractive index, $n(\omega)$, which was relative to the relative dielectric constant, $\varepsilon(\omega)$. we drive the effective dielectric function of the core- shell composite material which is obtained to be:

$$\varepsilon_1 = \varepsilon_s \frac{\varepsilon_c(\frac{3}{\beta} - 2) + 2\varepsilon_s}{\varepsilon_c + \varepsilon_s(\frac{3}{\beta} - 1)} \quad (2.3.1)$$

where

$$\beta = 1 - v_f \quad (2.3.2)$$

$$v_f = \left(\frac{a_c}{a_s}\right)^3 \quad (2.3.3)$$

Here we consider a system composed of a finite number of core -shell NPs uniformly dispersed in a host matrix.

As shown in the above fig suppose N is the desity of number of the inclusions(NPs) in the system, then the effective polarizability of the system can be described by using the clausius - mossotti relation together with the maxwell- Garent mixing formula.

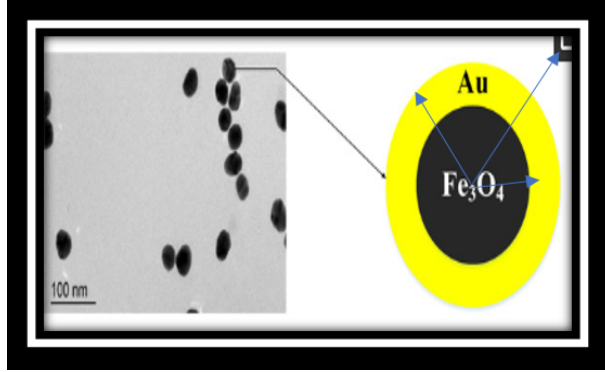


Figure 2.1: schematic of a core-shell spherical with the radius of core and shell NPs.

Accordingly the electric polarizability and the effective permittivity are related by [21].

$$\frac{N\alpha}{3} = \frac{\mu_{eff} - \mu_h}{\mu_{eff} + 2\mu_h} \quad (2.3.4)$$

Rearranging and carrying out some mathematical manipulation, the effective dielectric function "eff" of the system and polarizability are given by

$$\varepsilon_{eff} = \varepsilon_h \left(\frac{1 + 2\alpha_{eff}}{1 - f\alpha_{eff}} \right) \quad (2.3.5)$$

Where, f is the filling factor of the core-shell NPs defined by

$$f = \frac{4\pi r_s^3 N}{3} \quad (2.3.6)$$

and

$$\alpha_{eff} = \left(\frac{\varepsilon_1 - \varepsilon_h}{\varepsilon_1 + 2\varepsilon_h} \right) \quad (2.3.7)$$

similarly, we previously derived[20] that the effective magnetic permeability of the composite material and dimensionless magnetic polarizability are found to be given by

$$\mu_1 = \mu_s \left[\frac{\mu_c \left(\frac{3}{\beta} - 2 \right) + 2\mu_s}{\mu_c + \mu_s \left(\frac{3}{\beta} - 1 \right)} \right] \quad (2.3.8)$$

Using the Clausius - Mossotti relation and the maxwell - Garnet mixing theory, the magnetic polarizability are related

$$\frac{N_{km}}{3} = \frac{\mu_{eff} - \mu_h}{\mu_{eff} + 2\mu_h} \quad (2.3.9)$$

Where μ_{eff} is the effective magnetic permeability of the ensemble. After some manipulation, we obtained

$$\mu_{eff} = \mu_h \left(\frac{1 + 2fk_{eff}}{1 - fk_{eff}} \right) \quad (2.3.10)$$

Where $f = \frac{4\pi r_s^3 N}{3}$ is the filling factor of the core shell NPs and k_{eff} the dimensionless magnetic polarizability which is given by

$$k_{eff} = \frac{\mu_1 - \mu_h}{\mu_1 + 2\mu_h} \quad (2.3.11)$$

2.4 Optical properties of $Fe_3O_4@Au$ nanoparticles

In this section we present the equations for the optical parameters, i.e the absorption, scattering, and extinction cross sections with the help of polarizability equations for a system composed of $Fe_3O_4@Au$ core/shell NPs embedded in a liquid/water medium. Hence, in order to get an explicit expression for the absorption and scattering cross - section, we must fix the magnetic core, magnetic shell, and host matrix.

The response of 'bare' metallic (Au) shell to incident electromagnetic wave (EMW) is solely described by the dielectric function (permittivity) with permeability being equal to unity ($\mu_s = 1$). Therefore, we choose the frequency dependent complex dielectric function of the metal (Au) shell to have the drude form given by

$$\varepsilon_s(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega(\omega + i\gamma)} \quad (2.4.1)$$

Where the constant ε_∞ is the permittivity at high frequencies, ω_p is the plasma frequency, γ is the damping parameter, and ω is the frequency of the incident radiation. Further, separating the real and the imaginary part of Eq. (2.4.1), i.e., $\varepsilon_s = \varepsilon'_s + i\varepsilon''_s$, we obtain the following:

$$\varepsilon'_s(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + \gamma^2} \quad (2.4.2)$$

and

$$\varepsilon''_s(\omega) = \frac{\gamma\omega_p^2}{\omega(\omega^2 + \gamma^2)} \quad (2.4.3)$$

Where $\varepsilon'_s(\omega)$ and $\varepsilon''_s(\omega)$ are imaginary and real respectively, part of $\varepsilon_s(\omega)$. It was well understood that the dielectric function of materials specifically that of noble and alkali metals, very significantly as a function of the frequency of the incident light in the visible spectra region, but that of magnetite is constant or very little. Hence, we assume that both the permittivity (ε_c) and permeability (μ_c) of magnetite as well as the permittivity of the host (ε_h) to be real constants and independent of frequency.

2.5 Effective electric and magnetic polarizabilities

The effective (dimensionless) electric polarizability of the system is given by [24,25]

And the corresponding electric polarizability becomes

$$\alpha_e = 4\pi a_s^3 \alpha_{eff}. \quad (2.5.1)$$

Because ε_{eff} for the system is complex, the effective electric polarizability α_{eff} , defined by Eq. (2.5) is also complex, which may be written as

$$\alpha_{eff} = \alpha'_{eff} + i\alpha''_{eff}, \quad (2.5.2)$$

Where the α'_{eff} and $i\alpha''_{eff}$ are its real and imaginary parts, respectively. Substituting $\varepsilon_s = \varepsilon'_s + i\varepsilon''_s$ into Eq. (2.5.2), we get different equations. where

$$\phi' = \varepsilon_h(\frac{3}{\beta} - 1),$$

$$\eta = \phi' + \varepsilon_c(\frac{3}{2\beta} - 1),$$

$$\varphi' = (\varepsilon_s)^2 - (\varepsilon''_s)^2 + \varepsilon_s\eta + \varepsilon_c\varepsilon_h,$$

$$\psi = 2\varepsilon_s\varepsilon''_s + \varepsilon''_s.$$

2.6 Absorption, scattering, and Extinction cross - sections

The absorption cross- section, σ_{abs} , of the system consisting of spherical core-shell composite NPs embedded in a host matrix is given by [25]

$$\sigma_{abs} = kIm[\alpha_e + \alpha_m], \quad (2.6.1)$$

where $k = 2\pi\sqrt{\varepsilon_h/\lambda}$. Note that α_m is a real constant. In addition, we consider that the lose electromagnetic wave upon propagation through the spherical nanoinclusions results by means of the generation of heat and scattering. The scattering cross section, σ_{sc} , of the system can be shown to have the following form:

$$\sigma_{sc} = \frac{k^4}{6\pi}|\alpha_e + \alpha_m|^2 \quad (2.6.2)$$

Furthermore, the extinction cross- section, σ_{ext} , of the system is given by

$$\sigma_{ext} = \sigma_{sc} + \sigma_{abs}, \quad (2.6.3)$$

where σ_{sc} and σ_{abs} are given by eqs(2.6.2) and eq(2.6.1) respectively.

Chapter 3

Research Methodology

3.1 Materials and methods

3.1.1 Materials

The study is purely theoretical. The main source are, published articles, books, thesis, application of pc, mathematical software.

3.1.2 mathematical program methodology

This one type of which used to modifying or which used to describe the effect of surface plasmonic resonance on aspherical magneto plasmonic $Fe_3O_4@Au$ nanoparticles. Like the cross section, the permeability, permittivity, the electric polarizability, scattering, extinction cross section and absorption cross section versus wave length at different value of β and ε_h .

Chapter 4

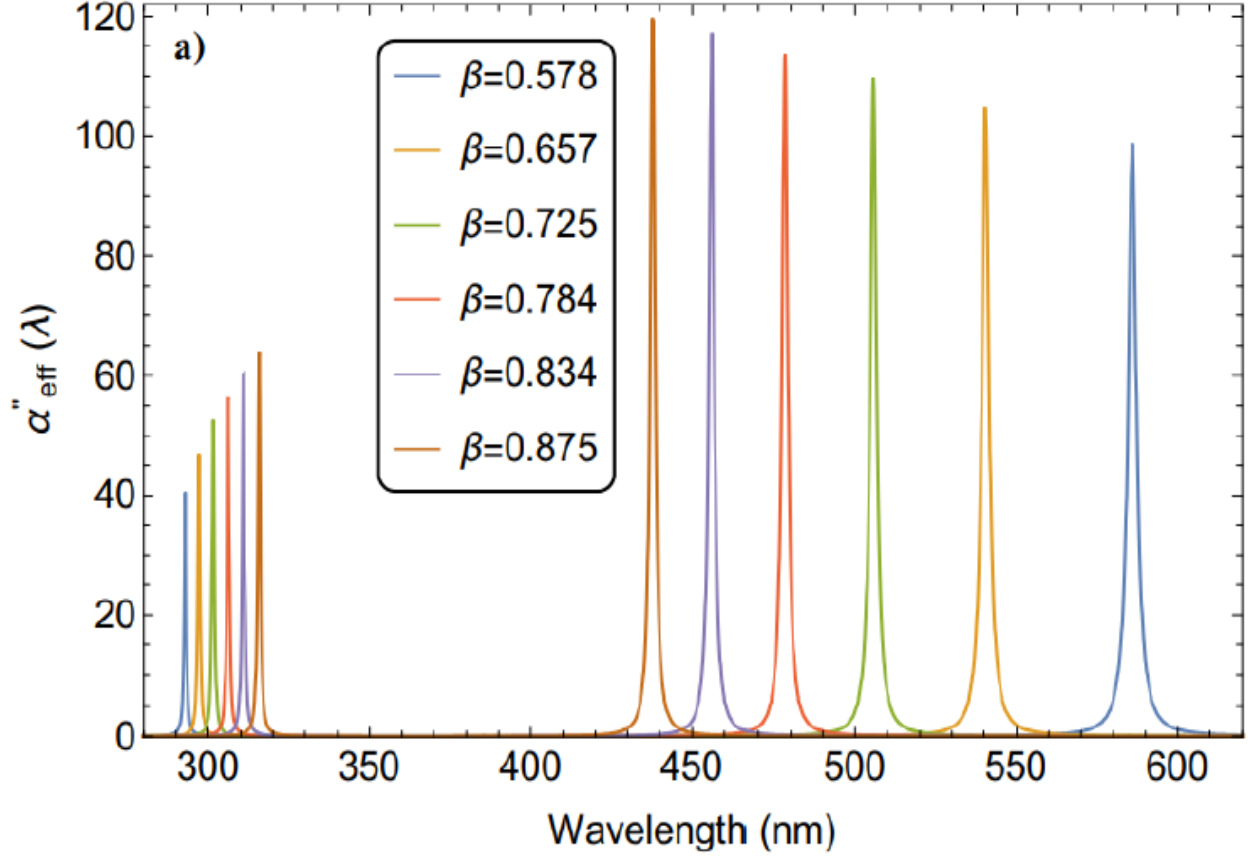
Results and discussion

Next we discuss the results of the polarizability as well as the absorption, scattering, and extinction cross-sections of the theoretically modelled spherical $Fe_3O_4@Au$ core/shell NPs embedded in a dielectric host matrix. These optical parameters are analyzed by varying the material parameters β and ε_h . For the numerical evaluations we used mathematical version 7.1.1 software. The following parameter values are used in the stimulation: $\varepsilon_\infty = 4.5$, $\omega_p = 1.46 \times 10^{16} rad/s$ and $\gamma = 1.67 \times 10^{13} rad/s$ for the golds hell; and $\varepsilon_c = 5.85$ and $\mu_c = 9.0$ for the magnetite.

4.0.3 Electric polarizability

Fig 4.1, depicts the real and imaginary parts of the frequency dependents complex electric polarizability (α_{eff} and α''_{eff}) of the spherical $Fe_3O_4/@Au$ nanoinclusions as a function of the wave length of the incident radiation for the different value of metal fraction, β , and fixed values of $\varepsilon_h = 1.77$ and NPs size $a_s = 10nm$. It shows that:

Both α_{eff} and α''_{eff} possess two sets of resonance peaks the first in the vicinity of the wavelength $\lambda = 300nm$ and the second peak in the visible spectra region above the



wave length of $\lambda = 430nm$. The first set of peaks for both real and imaginary parts are blue shifted as β decrease and second sets of peaks are red shifted as β decreases. The first and the second sets of peaks arise due to the coupling of the surface plasmon oscillations of the gold shell at the inner semiconductor /metal ($Fe_3O_4@Au$ interface and outer (Au/host matrix) interface respectively.

Furthermore ,it is found that the value of both α'_{eff} and α''_{eff} increases as the value of core radius a_c is decreased (or equivalently as the metal fraction β is increased). Besides ,the first set of resonance peaks are less intense than the second set

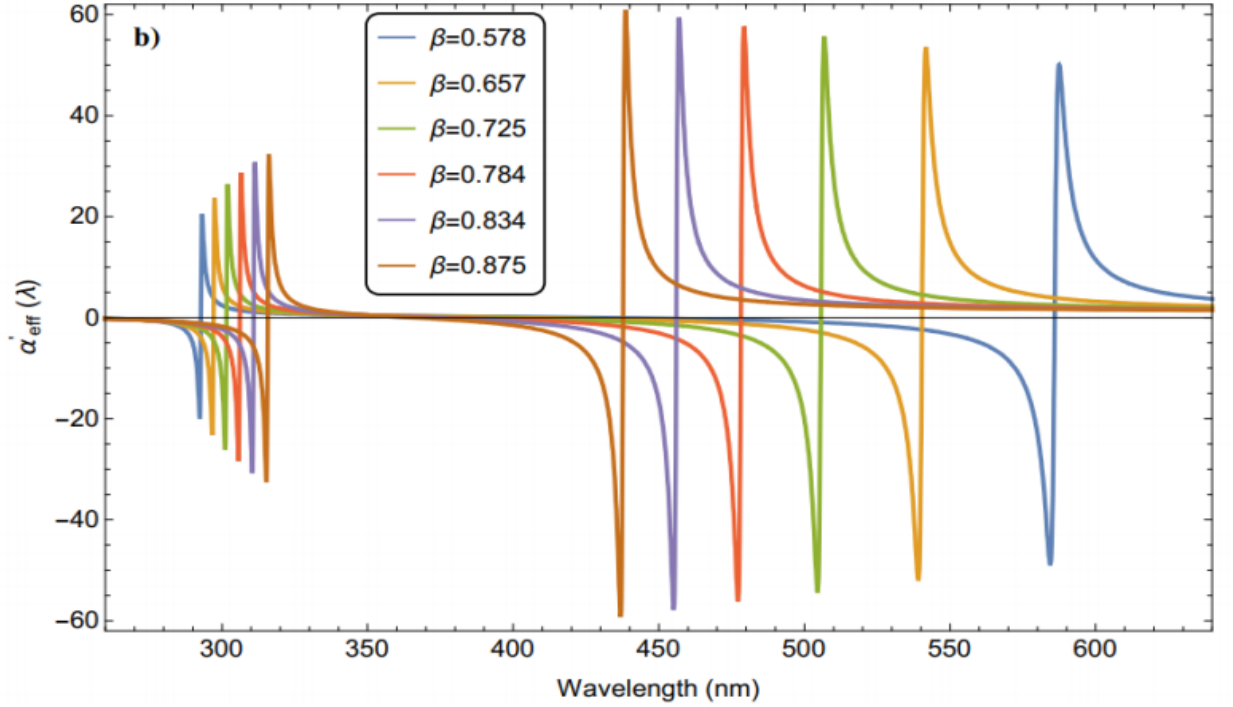
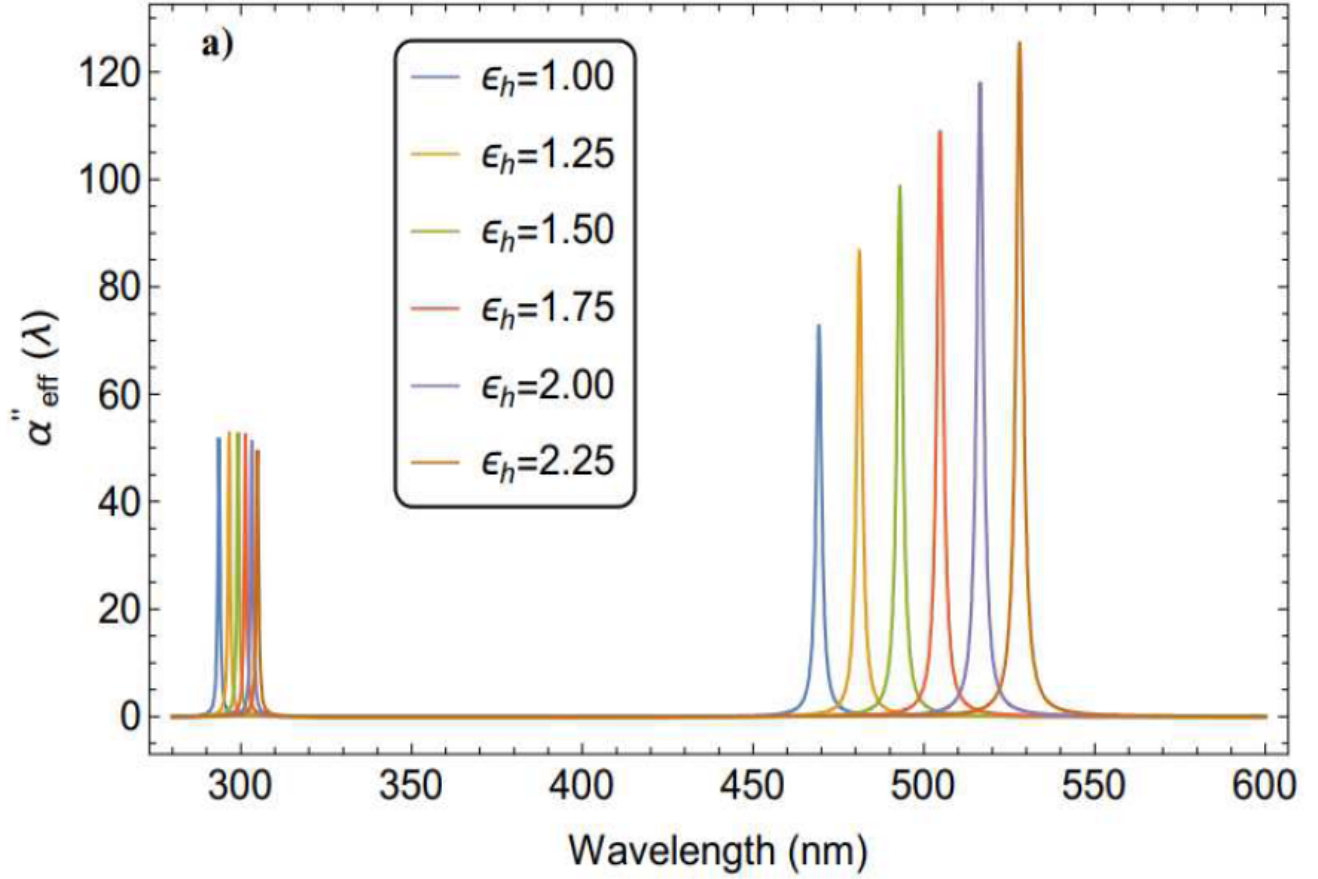


Figure 4.1: the real a) and the imaginary b) parts of the electric polarizability versus wave length for different values of β ; with $\varepsilon_h = 1.77$ and $a_s = 10\text{nm}$.

of peaks. This may be explained with the fact that the surface area of the outer surface (Au/host matrix interface) of the Au shell is larger than that of the inner surface area (magnetite/Au interface), and hence large number of the carriers available at the outer interface than the inner.

Moreover the results shows that when β is increased the first set of peaks in the uv region are red -shifted which is mainly attributed to the decrease of the size the NPs, i.e ,the semiconductoring Fe_3O_4 /core. Conversely, the second set of peaks are blue-shifted when β is incresead, due to an increase in the thickness of the metallic shell. Certainly, the two resonance peaks corresponding to each NPs become closer

and closer to each other as β is increased indicating that the metallic shell plays the dominant role in determine both the real and imaginary parts of the electric polarizability.



Similarly, the graphs of α'_{eff} and α''_{eff} as a function the wavelength of the incident EMW for the spherical nanoinclusions for different dielectric function of the host, ϵ_h and fixed values of $\beta = 0.725$ and $a_s = 10nm$ are shown in fig 4.2;. From the figures it is obvious that both α'_{eff} and α''_{eff} possess two set of resonance peaks the first in the UV region in the vicinity of the wave length $\lambda = 300nm$. and the second peak

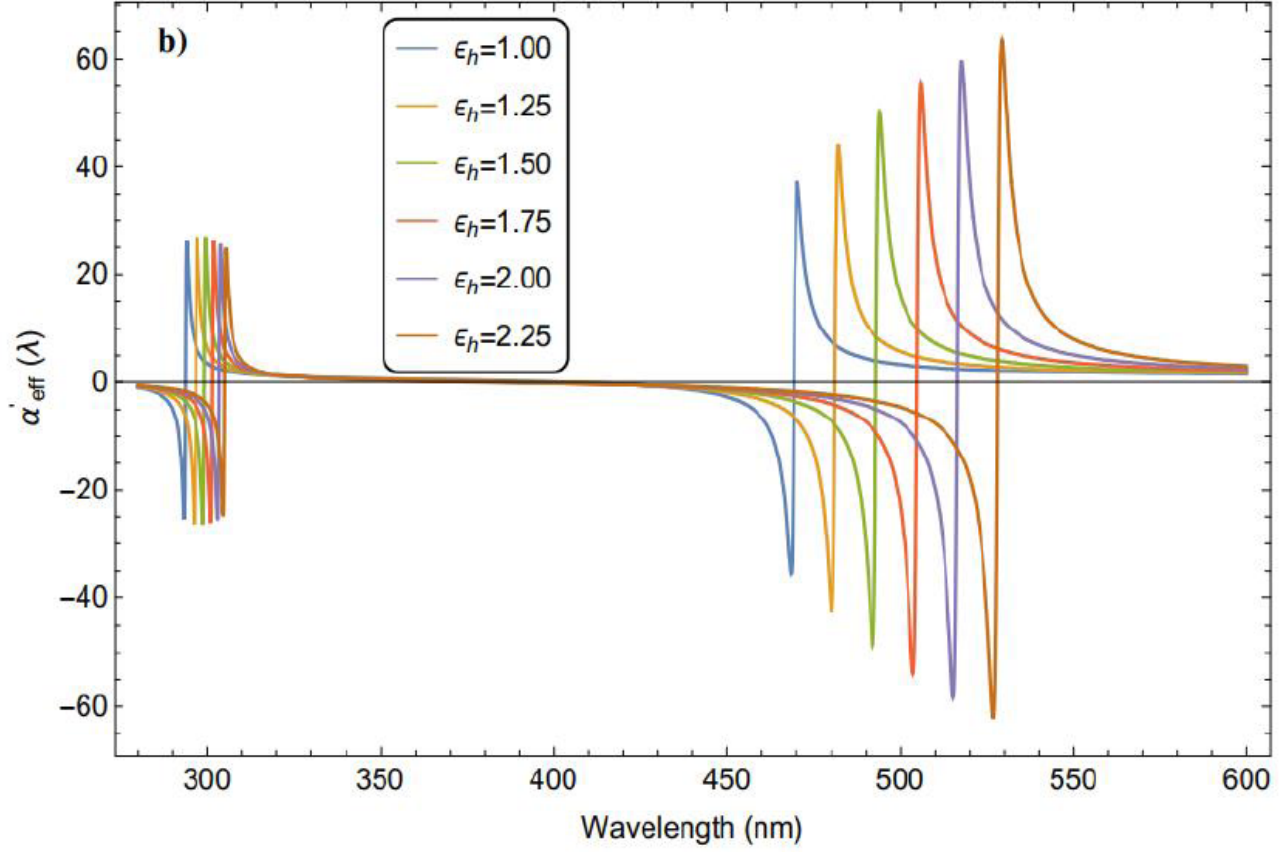


Figure 4.2: the real a) and the imaginary b) parts of the electric polarizability versus wave length for different value of ϵ_h ; with $\beta=0.75$ and $a_s = 10$ nm fixed constant

in the visible spectral region above the wave length of $\lambda=450$ nm. The first and the second set of peaks are red- shifted as ϵ_h increases.

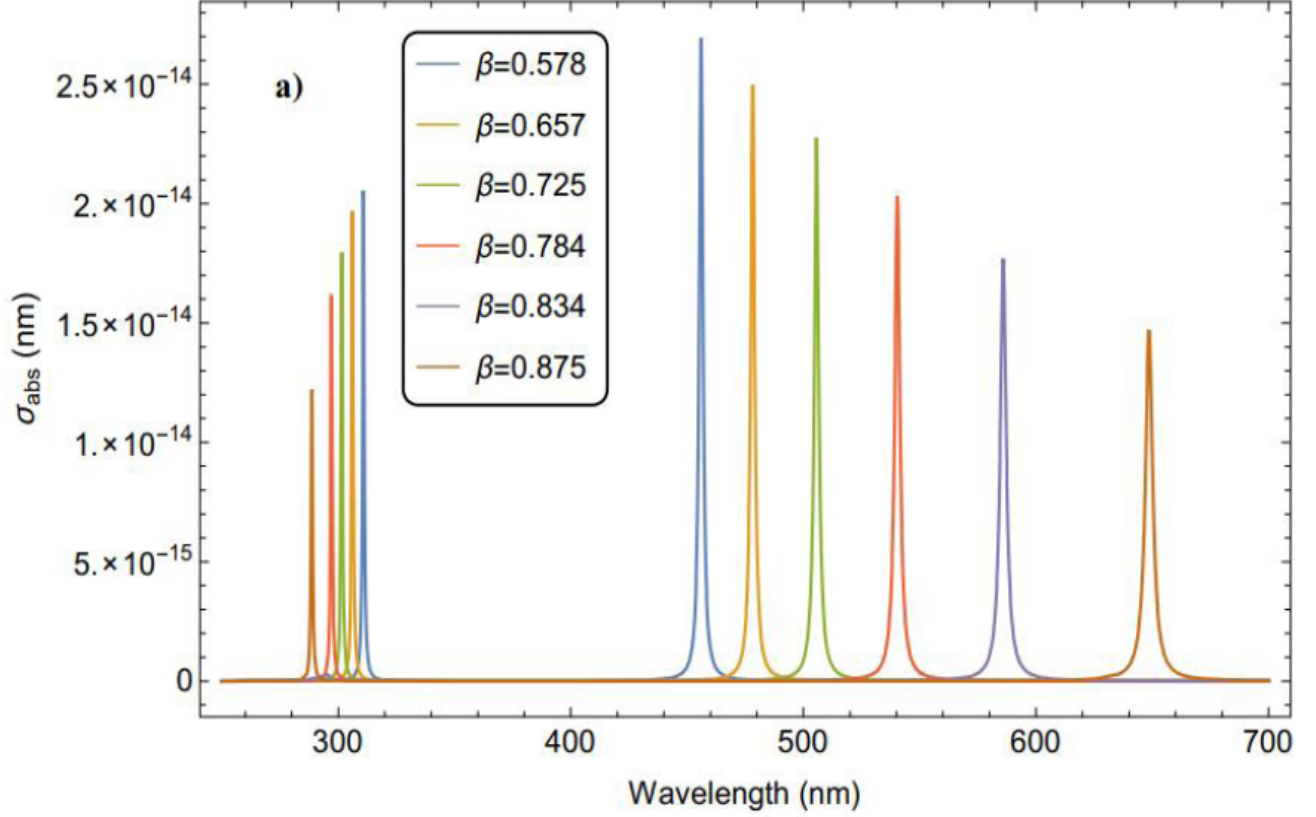
Likewise, it is found that the polarizabilities, α'_{eff} and α''_{eff} increase in the second set of peaks. While significant change takes place in the first set of resonance peaks as the value of the ϵ_h increase besides second set of resonance peaks are more pronounced than the first set of peaks. Note also that when ϵ_h is increase the two set of resonance

peaks far apart each other, for both the real and imaginary parts of the polarizability (see Fig. 4.2), gets more pronounced in the second peaks than the first.

4.0.4 Absorption cross section

the absorption cross section of $Fe_3O_4@Au$ core shell spherical nanoinclusions are numerically analyzed using Eq(2.6.1) together corresponding expression for α_e and α_m , i.e., Eq(2.5.1). The absorption cross section (σ_{abs}) of the spherical nanoinclusion as a function of the wavelength of the incident EMW for different values of β and ε_h as shown in the Figs.4.3a) and 4.3b). The graph possesses two sets of resonance peaks, the first set of peaks in both case are located in the vicinity of $\lambda = 300nm$ in the UV region which are attributed to the interaction at the inner (Fe_3O_4/Au) interface. The second set of peaks are found above wavelength of $\lambda = 450nm$ all in the visible spectral region, which are corresponds to the resonance at the outer (Au/host) interface. As β increases the two sets of peaks gets far apart from each other accompanied with a spectral shift toward lower wavelengths in the first sets of peaks and shifted to the higher wavelengths in the second set of peaks than the first set of peaks.

As it seen from the graphs, the effect of rapid on set of strong absorption, occurring in the UV region for all dielectric medium/host ε_h , is dependent on the particles size. That is when the value of β is increased, the absorption peaks sharply drops (less intense) for both the first and second peaks (see Fig.4.3a) for a constant $\varepsilon_h = 1.77$. On the other hand, for a particular value of $\beta = 0.725$, the absorption cross section for both the first and second sets of peaks sharply increases and red-shifted as shown in Fig.4.3b).



4.0.5 scattering cross section

Figures 4.4a and 4.4b depict the scattering cross-section as a function of the wavelength of the incident EMWs for different value of β and ε_h . In each case figures there are two sets resonance peaks. The first of resonance peaks positioned near to $\lambda = 300nm$ in the UV region and its associated with the inner (magnetite/Au) interface. The second set of peaks which are connected to Au/host interface are located above the wave length of $\lambda = 450nm$ all in the visible spectral region. Figures (4.4a illustrate that, scattering of light is sharply increased (more scattering takes place) in the first

set of peaks than the second set of peaks and gates sharply decreased as β increases. Furthermore, the two sets of peaks increase as ε_h increases as shown in the FIG. 4.4b. from both FIGS. 4.4a and 4.4b, it is observed that the first resonance peaks are more pronounced than the second set of peaks. As the size of the system of core/shell nanoparticles gets smaller and smaller, the metal fraction, β is also decreased. This leads to the decrease in the scattering cross sections.

In fig. 4.4a) the two set of resonance gets closer each other as β decrease accompanied by the shift toward the higher energy in the second peaks and emission spectral shift to lower energy in the first peaks. Both set of resonance peaks are reds-shifted(see Figs. 4b) as ε_h increased. For both figures 4.4a and 4.4b there are no noticeable peaks found in the first sets of peaks at particular values $\beta = 0.725$ and at $\varepsilon_h = 1.50$. This may be due to the fact that the absorption is more likely to dominate over scattering processes at the particular values of $\beta = 0.725$ and at $\varepsilon_h = 1.50$. On the other hand, the dielectric medium at the value of $\varepsilon_h = 1.50$ in the host matrix may affect the propagation of the incident electromagnetic wave.

4.0.6 Extinction cross section

Figures 4.5 depicts the graph of extinction cross section, σ_{ext} as a function of wave length for different values β and ε_h for the spherical nanoinclusions. As it is seen from the graphs, the extinction cross section possess two sets resonance peaks. The first set of peaks for Figs. 4.5a and 4.5b, the resonance peaks are located close to $\lambda = 300nm$ in the UV region and the first set of peaks are due to resonance at the inner (magnetite/Au) interface. The second set of peaks are those found above the wave length of about $\lambda = 450nm$ all in the visible spectral region. As Fig. 4.5a) depicts, the two sets of resonances gets closer to each other as β is decreased and the

spectra shift towards lower frequency in the first set of peaks, and shift toward higher frequency for the second set of peaks. Both sets resonance peaks are red -shifted (see Fig. 4.5b as ε_h is increasing).

The extinction cross section depends on the chemical composition of the particles, their size, shape, orientation, the surrounding medium, the number of the particles, and the polarization state and frequency of the incident EMWs[13]. The system of the spherical core /shell nanoparticles that is considered in this study composed of two chemically dissimilar nanoparticles one as the semiconducting core and the other as a plasmonic shell. We found that the extinction cross section is dependent on the size and on the chemical composition of the semiconducting core or the metallic shell.

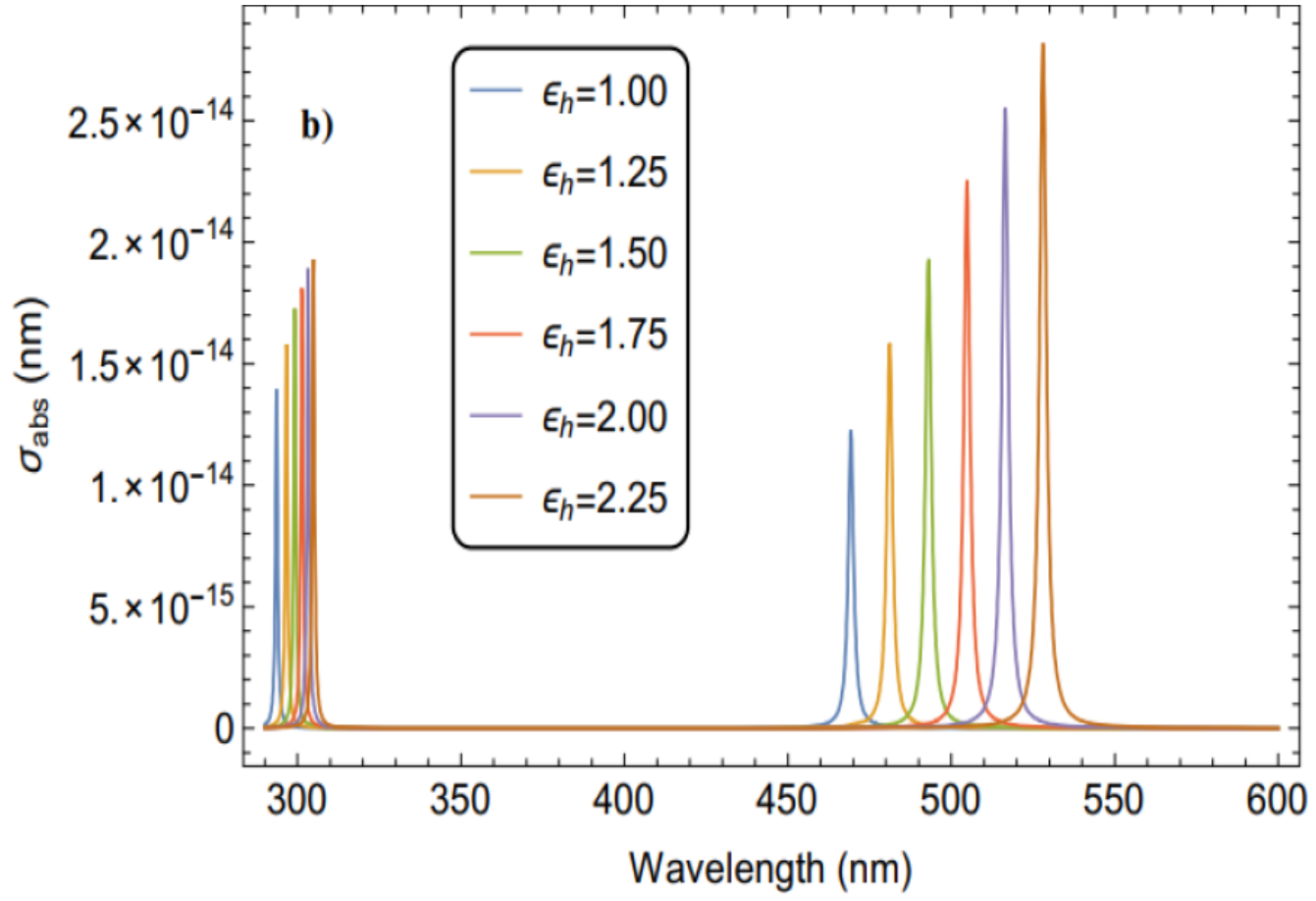
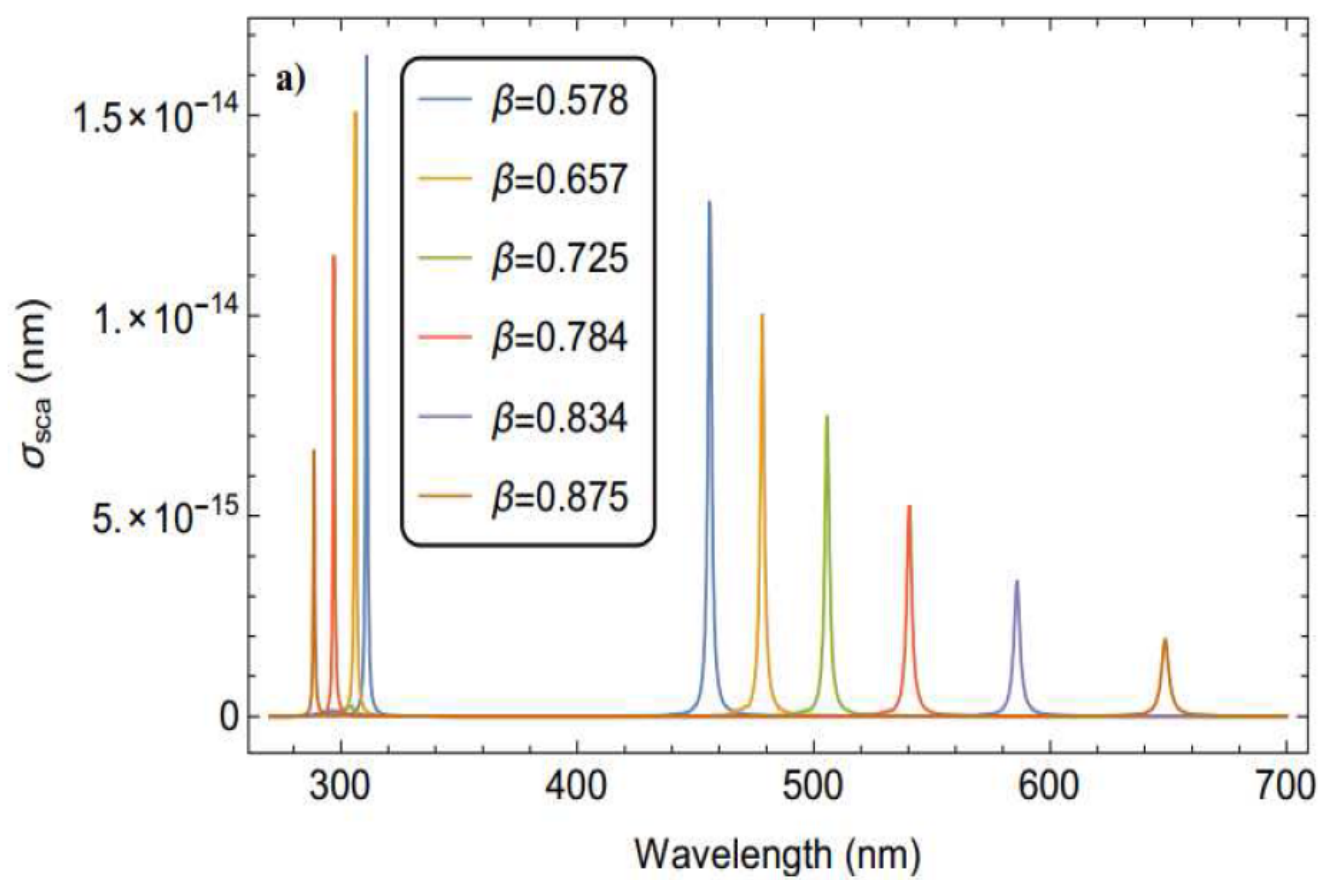


Figure 4.3: the absorption and cross section versus wavelength a) for different value of β and b) for different value of ϵ_h ; with $f=0.003$ and $a_s = 10\text{nm}$



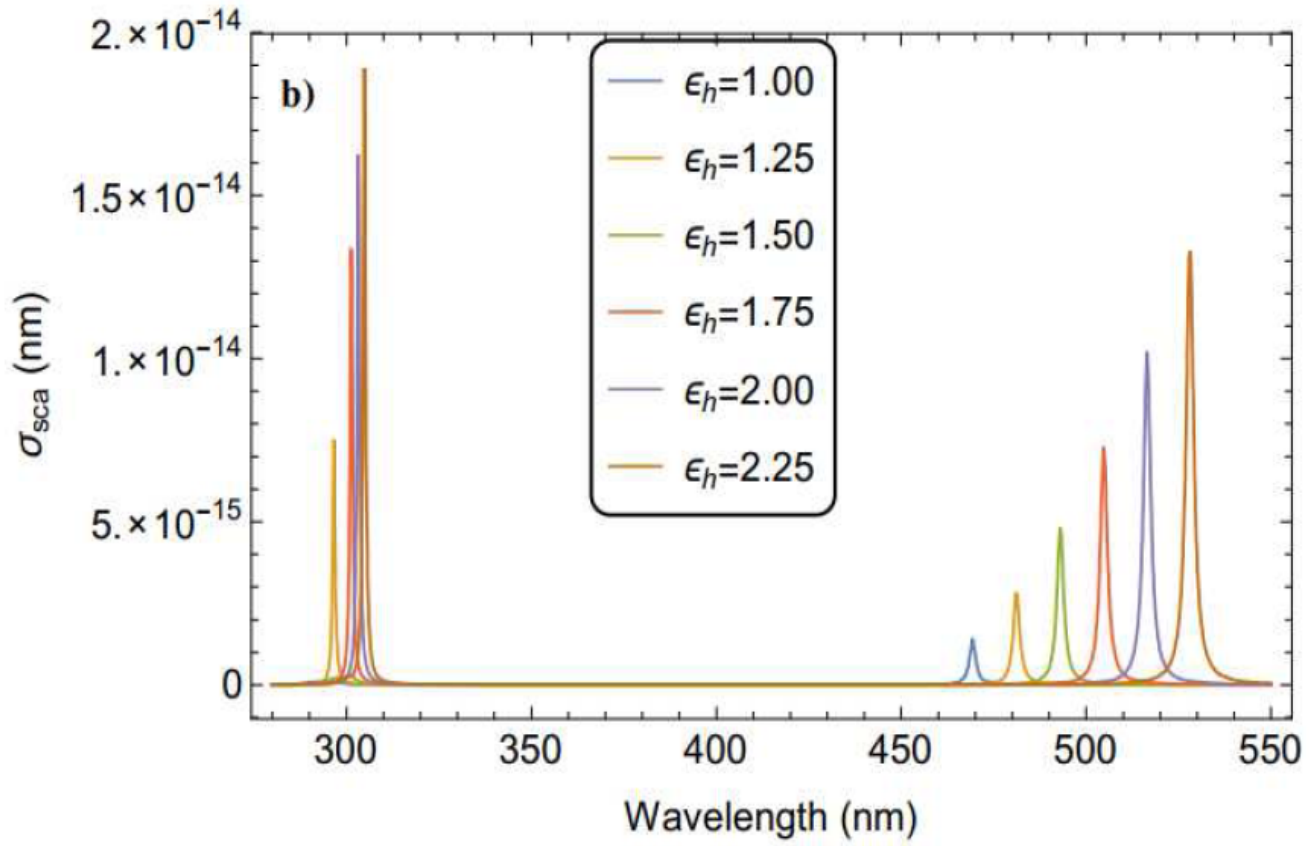
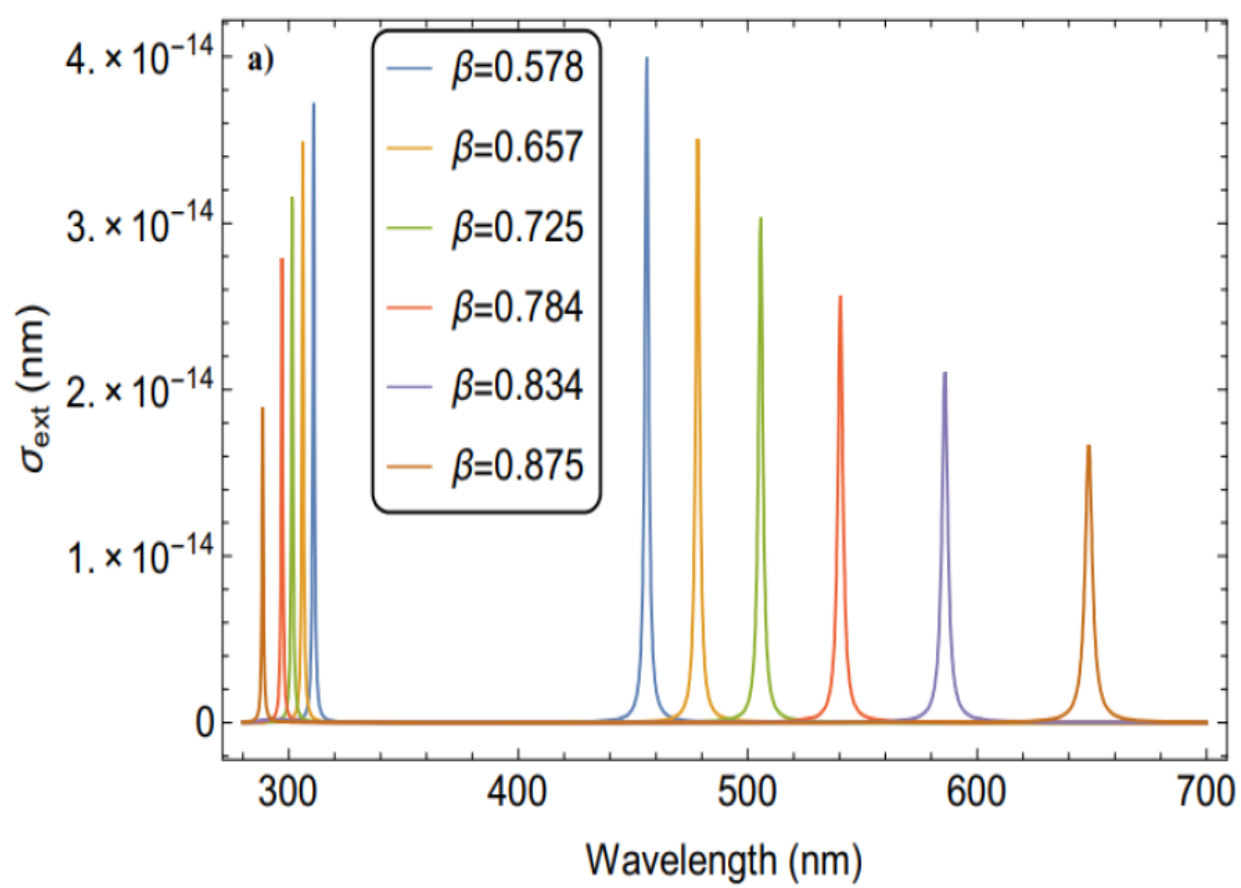


Figure 4.4: : The scattering cross section as a function of wave length a) for different value of β and b) for different values of ϵ_h with fixed value of $f=0.003$ and $\alpha_s = 10nm$



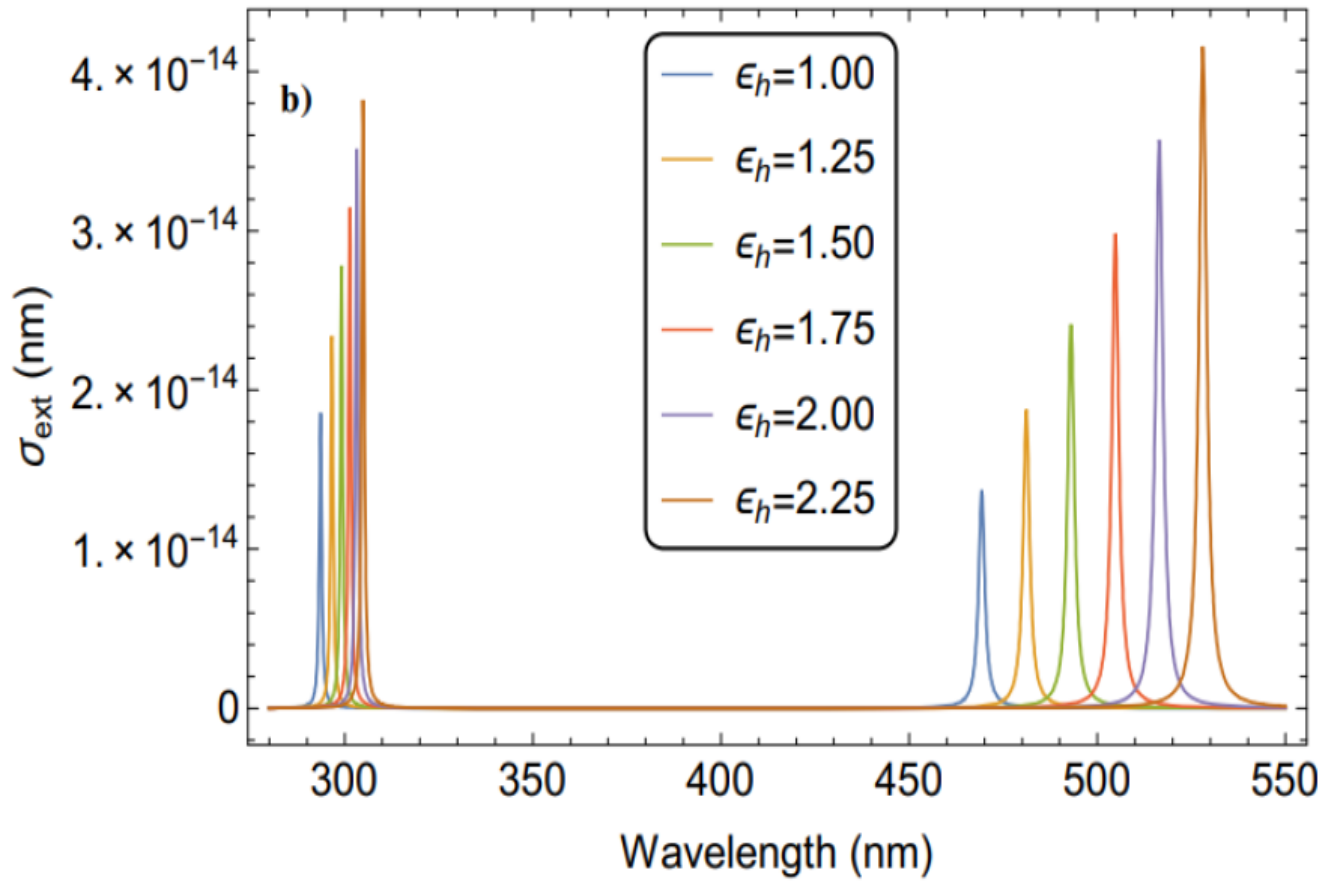


Figure 4.5: The extinction cross section versus wavelength for different values of a) β and b) ϵ_h ; with fixed values of $f=0.003$ and $a_s = 10\text{nm}$.

Chapter 5

Conclusion

In this study, we investigate the effect of varying parameters like the metal fraction and host matrix on the systems of spherical core/shell $Fe_3O_4@Au$ nanoparticles embedded in a dielectric host matrix. It is found that the real and imaginary parts of the polarizability, absorption cross section, scattering cross section as well as the extinction cross section of the system plotted for different value of β and ε_h as a function of wave length posses two sets of resonance peaks in the UV (in the vicinity of $\lambda \sim 300nm$) and visible (above $\lambda \sim 450nm$) spectral regions. These sets of peaks arise due to the coupling of the surface plasmon oscillations of gold with energy gap of the semiconducting core at the inner (Fe_3O_4/Au)interface and at the outer metal/dielectric(Au host matrix) interface. Moreover, when β is increased , the first set of peaks in the UV region are which is mainly attributed the decrease of the size of the semiconducting Fe_3O_4 core, while the second set of peaks are blue-shifted with an increase of β , due to an increase in the thickness of the metallic shell for the graph of the real and imaginary part of the polarizability. on the contrary, for absorption and scattering cross sections the resonance peaks are shifts towards higher frequencies in the first peaks and red shifts for the second set of peaks as β increases.

furthermore, the graphs of the real and imaginary parts of the polarizability as a function of wavelength for different values of the dielectric function of the host matrix (for fixed $\varepsilon_h = 1.77$) possess two set of peaks-the first in the UV (around $\lambda \sim 300nm$) and the second in the visible (above $\sim 420nm$) spectral regions. it is found that with an increase in the permittivity ε_h of the host, the resonance peaks of σ_{abs} , σ_{sc} and σ_{ext} are the enhanced accompanied with a red or blue shift. in this case, both set of peaks are shifted to higher wavelength with an increase in ε_h

finally, the enhancement of the optical properties of the system (spherical core/shell $Fe_3O_4@Au$ nanoparticles enhancement embedded in a dielectric host matrix) is because of the strong coupling of the surface plasma oscillations of the gold with energy gap of the magnetic semiconducting($Fe_3O_4@Au$) nano-core. it means that the gold nano-shell strongly modifies the optical properties of Fe_3O_4 nanoparticles which correspondingly modify its potential applications. The result obtained may be utilized in device fabrication and applications that integrates the plasmonic effects of noble metals with magnetic semiconductors such as Fe_3O_4 in core/shell nanostructures.

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