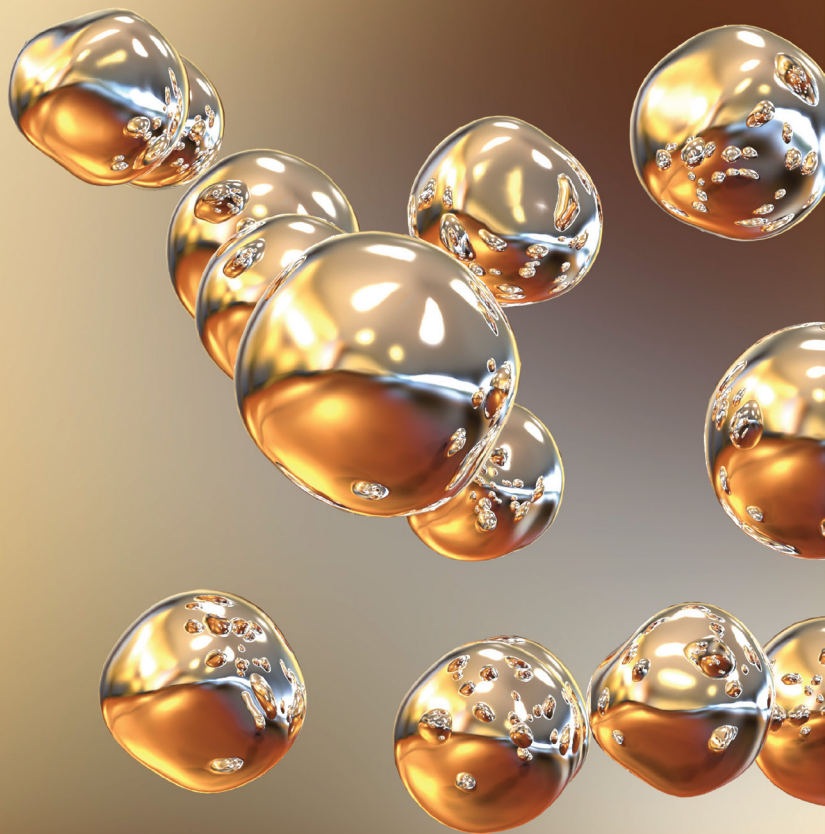


# THE GREAT WORLD OF NANOTECHNOLOGY



Marcos Augusto de Lima Nobre  
(Organizador)

VOL II

 EDITORA  
ARTEMIS  
2021

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## PREFACE

The insertion of new and enhanced materials based on materials belonging to the Nano scale in the day-by-day has growth up in a silent way. In part, a number of works in the nanotechnology stemming of theoretical research using Density Functional Theory (DFT) and sophisticated simulation methods; another part is associated to the protected technologies associated to the military and patented nanomaterial and its process. In this sense, open access to recent aspects on the nanostructures application and properties can be reached in this book. Here, an interesting set of chapters gives opportunity of access texts that reach process and processing of nanostructures, applications of nanotechnology, advanced techniques to theoretical development. A broad set of nanostructures are here covered such as, nanocrystal, superficial nanograins, inner microstructures with nanograins, nanoaggregates, nanoshells, nanotubes, nanoflowers, nanoroad, nanosheets, Also, reveals new investigations areas as grainboundary of nanograins in ceramics and metals. A great number of software has been used as a tool of development of Science and Technologies for nanotechnology COMSOL Multiphysics 5.2. Phenomena and properties has been investigated by recent or classical techniques of materials characterization as Localized Surface Plasmon Resonance (LSPR), X-ray photoelectron spectroscopy (XPS), Field Emission Gun Scanning Electron Microscopy (FEG-SEM) with Energy Dispersive Spectroscopy (EDS), Raman Scattering Spectroscopy (RSS), X ray diffraction (XRD), <sup>57</sup>Fe Mössbauer spectroscopy, UV-vis spectroscopy, dynamic light scattering (DLS), Atomic Force Microscopy (AFM), and Field Emission Gun Scanning Electron Microscopy (FEG-SEM). In this sense, collections of spectra from Mössbauer spectroscopy, UV-vis spectroscopy and Infrared spectroscopy can be found. As a matter of fact, some chapter's item can be seemed as specific protocols for synthesis, preparations and measurements in the nanotechnology.

I hope you enjoy your reading.

Prof. Dr. Marcos Augusto Lima Nobre

## TABLE OF CONTENTS

### CHAPTER 1..... 1

ROLLING OF 316L STAINLESS STEEL WITH ROUGH ROLLS: A POSSIBLE TECHNIQUE TO OBTAIN SUPERFICIAL NANOGRAINS

Carlos Camurri

Alejo Gallegos

DOI 10.37572/EdArt\_3006213611

### CHAPTER 2..... 11

EFFECTS OF DIFFERENT ASPECT RATIOS AND JUNCTION LENGTHS ON THE COUPLED PLASMON GOLD NANOROD DIMERS

Hafiz Zeeshan Mahmood

Umer Farooq

Usman Rasool

Noor ul Huda

Sana Gulzar

Mahmood Ali

Maryam Iftikhar

Yasir Javed

Sajid Farooq

DOI 10.37572/EdArt\_3006213612

### CHAPTER 3.....21

AB-INITIO STUDY OF ELECTRONIC AND MAGNETIC PROPERTIES OF ZnO NANOCRYSTALS CAPPED WITH ORGANIC MOLECULES

Aline L. Schoenhalz

Paulo Piquini

DOI 10.37572/EdArt\_3006213613

### CHAPTER 4 .....39

CONFINED WATER CHEMISTRY: THE CASE OF NANOCHANNELS GOLD OXIDATION

André Mourão Batista

Herculano da Silva Martinho

DOI 10.37572/EdArt\_3006213614

**CHAPTER 5..... 67**

PLASMONIC RESPONSE OF GOLD- SILICA AND SILVER- SILICA METAL CORE NANOSHHELLS BY OPTIMIZING THE FIGURE OF MERIT

Hafiz Zeeshan Mahmood

Zainab Shahid

Alina Talat

Imama Irfan

Bushra Arif

Sana Habib

Saba Munawar

Yasir Javed

Shaukat Ali Shahid

Sajid Farooq

**DOI 10.37572/EdArt\_3006213615**

**CHAPTER 6 ..... 76**

AMORPHOUS MICRO AND NANO SILICA EXTRACTED FROM RICE HUSKS AND OBTAINED BY ACIDIC PREHYDROLYSIS AND CALCINATION: PREPARATION ROUTE AND CHARACTERIZATION

Eduardo Roque Budenberg

Eilton Aparecido Prado dos Reis

Deuber Lincon da Silva Agostini

Renivaldo José dos Santos

Felipe Silva Bellucci

Aldo Eloizo Job

Daltro Garcia Pinatti

Rosa Ana Conte

**DOI 10.37572/EdArt\_3006213616**

**CHAPTER 7..... 92**

FORMATION OF METAL NANOPARTICLES BY SPUTTER DEPOSITION ON UNCD FILMS BY NPIII INSIDE CONDUCTIVE TUBES

Nazir Monteiro dos Santos

Divani Carvalho Barbosa

Evaldo José Corat

Mario Ueda

**DOI 10.37572/EdArt\_3006213617**

**CHAPTER 8 ..... 109**

X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) STUDY OF CONDUCTIVE TUBE AFTER NITROGEN PIII

Nazir Monteiro dos Santos  
Elver Juan de Dios Mitma Pillaca  
Mario Ueda  
Steven Frederick Durrant  
Pericles Lopes Sant'Ana

**DOI 10.37572/EdArt\_3006213618**

**CHAPTER 9 ..... 125**

APPLICATION OF CLAY-CARBOXIMETHYLCHITOSANE NANOCOMPOSITE-SILVER NANOPARTICLES IN FILTERS TO TREAT CONSUMPTION WATER IN RURAL AREAS OF CAMANA - AREQUIPA-PERU

Maria Elena Talavera Nuñez  
Irene Zea Apaza  
Corina Vera Gonzales  
Julia Zea Alvarez  
Luis Rodrigo Benavente Talavera

**DOI 10.37572/EdArt\_3006213619**

**CHAPTER 10..... 138**

NANOGRAIN BOUNDARY PHENOMENON IN CERAMIC NANOMETRIC MICROSTRUCTURE

Marcos Augusto Lima Nobre  
Silvania Lanfredi

**DOI 10.37572/EdArt\_30062136110**

**CHAPTER 11..... 150**

ON SPIN HAMILTONIAN FITS TO MÖSSBAUER SPECTRA OF NIFE<sub>2</sub>O<sub>4</sub> NANOPARTICLES SYNTHESIZED BY CO-PRECIPIATION

Jose Higinio Dias Filho  
Jorge Luis Lopez  
Adriana Silva de Albuquerque  
Renato Dourado Maia  
Wesley de Oliveira Barbosa  
Ernando Campos Ferreira  
Fellipe Silva Pereira  
Kátia Guimarães Benfica

**DOI 10.37572/EdArt\_30062136111**



**CHAPTER 12..... 162**

EFFECT OF GRAPHITE NANOSTRUTURES ON THE VISCOSITY PROPERTIES OF BLENDS DIESEL-S10 AND BIODIESEL

Túlio Begena Araújo

Marcos Augusto Lima Nobre

**DOI 10.37572/EdArt\_30062136112**

**CHAPTER 13..... 172**

REMOCIÓN DE ARSÉNICO DE EFLUENTES ACUOSOS EMPLEANDO COMO ADSORBENTE MAGNETITA NANOESTRUCTURADA

Orfelinda Avalo Cortez

Luis Jean Carlo Cisneros García

David Pedro Martínez Aguilar

**DOI 10.37572/EdArt\_30062136113**

**CHAPTER 14..... 182**

AVALIAÇÃO DA MICRODUREZA DE NANOCOMPÓSITOS DE MATRIZ DE ALUMÍNIO REFORÇADOS COM ÓXIDO DE GRAFENO REDUZIDO

Daniel Andrada Maria

Andreza de Sousa Andrada Jordânio

Samuel Siqueira

Adelina Pinheiro Santos

Clascídia Aparecida Furtado

**DOI 10.37572/EdArt\_30062136114**

**CHAPTER 15..... 197**

ROTA ECOLOGIA PARA SINTESE DE ELETRODO NANOESTRUTURADO DE ZnO PARA SUPERCAPACITOR

Eguiberto Galego

Marilene Morelli Serna

Tatiane Yumi Tatei

Bruna Rodrigues de Lima

Rubens Nunes de Faria Junior

**DOI 10.37572/EdArt\_30062136115**

<b>CHAPTER 16.....</b>	<b>212</b>
MORFOLOGIA DE FILMES FINOS NANOESTRUTURADOS DE ZnO PRODUZIDOS PELO MÉTODO SILAR	
Eguiberto Galego	
Marilene Morelli Serna	
Lalgudi Venkataraman Ramanathan	
Rubens Nunes de Faria Junior	
<b>DOI 10.37572/EdArt_30062136116</b>	
<b>CHAPTER 17.....</b>	<b>228</b>
OBTENÇÃO E CARACTERIZAÇÃO DE NANOCRISTAIS DE CELULOSE A PARTIR DE PAPEL RECICLADO VIRGEM E PÓS-CONSUMO	
Jean Brito Santos	
Emanoel Igor da Silva Oliveira	
Nádia Mamede José	
<b>DOI 10.37572/EdArt_30062136117</b>	
<b>ABOUT THE ORGANIZER.....</b>	<b>234</b>
<b>INDEX.....</b>	<b>236</b>

# CHAPTER 5

## PLASMONIC RESPONSE OF GOLD- SILICA AND SILVER- SILICA METAL CORE NANOSHELLS BY OPTIMIZING THE FIGURE OF MERIT

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**ABSTRACT:** Plasmonic nanoaggregates have great potential for sensing applications, due to their spectral sensitivity response to the surrounding environment of the nanostructure and efficient extinction efficiency. A novel refractive index (RI) based SPR nano scale sensor which composed of metallic (Au/Ag) core and silica shell has been analysed theoretically. To simulate the

proposed geometry in radio frequency module, 3-D finite element method (FEM), an efficient tool to investigate the electromagnetic properties and electric field distribution surrounding the nanoparticle surface, based on commercially available software COMSOL Multiphysics were utilized. In FEM simulation, to determine the scattered field distribution and extinction cross section the nanostructure surface was divided into extremely small mesh elements which lead to finer size. The background field amplitude was fixed  $1 \text{ Vm}^{-1}$  and to restrain the simulation from any reflection, a perfectly matched layer was created around the nanostructure. We found dielectric metal nanoshells to be more absorbing with gold core compared to silver core, leading to high figure of merit (FoM) for Ag nanoshell 3.0, having the same silica shell thickness 5 nm. This result points out that our proposed multilayer geometry can be extended to other systems, enabling the plasmonic sensors have a high FoM over wide spectral ranges with phenomenal accuracy).

**KEYWORDS:** RI. FEM. COMSOL. FoM.

## 1 INTRODUCTION

The plasmonic metallic nanostructures have been extensively investigated substantial subject which stimulated the interest of the researchers due to their fascinating optical characteristics, conspicuous features linked with geometric tunability (M. Alejandro-Arellano et al., 2000), as well as advancements in particle synthesis which makes them valuable in the fields of controlled drug delivery, imaging, nonlinear optics and various biosensing modalities (Yang, X et al., 2015). An interesting phenomenon provokes when light interacts with noble metals nanostructures (Au/Ag) known as Localized Surface Plasmon Resonance (LSPR), i.e., the collective oscillations of the conduction electrons (Non- Propagating) prompted by electromagnetic radiation having a pertinent wavelength. In nanoscale regime, the resonances for Au/Ag exhibits within the visible region i.e., 400-700 nm (A. Maier, 2007).

It has been studied that Refractive index (RI) based sensitivity and figure of merit, (defined as the ratio of sensitivity to the linewidth) (Jéssica et al 2021), depends on the geometry of the Au nanoparticles (Klantsataya. E et al., 2015; Z Yang et al., 2008). For single particle LSPR sensor, the fundamental principle utilizes the fact that LSPR spectrum position varies as a function of dielectric host medium (A.D. McFarland et al., 2003; Klantsataya et al., 2015) revealed the fact narrow full width at half maximum (FWHM) will result in the enhancement of LSPR sensing behavior.

In this study, we evaluate the Au/Ag nanoshell based on gold/silver core encapsulated by silica shell having nano scale varying thickness likewise their tune ability linked with surface plasmon resonance were also theoretically investigated. The simulations were carried out by Finite Element Method (FEM) based on partial differential equations commercially available software COMSOL Multiphysics 5.2, which is an

efficient tool to explore the electromagnetic properties as well as electric field distribution on the surface of nanostructures having various shapes to predict the unprecedented dependence of the plasmonic properties of core-shell nano scale structure (Du, C, M et al., 2014). The background field amplitude was fixed 1 Vm<sup>-1</sup> and to restrain the simulation from any reflection, a perfectly matched layer was created around the nanostructure.

## 2 LSPR MATERIAL DEPENDENCE

The fundamental optical characteristics of metal nanoparticles may be predicted calculating their size-dependent dielectric function. The dielectric function value of a metal is influenced by its structure. As the metallic nanoparticle becomes smaller, electron scattering on the NP surface becomes more pronounced, therefore affecting the dielectric function value of the material. The complex dielectric function  $\epsilon(\omega)$  can be described by Drude model, which also account for the conduction electrons scattered by the nanoparticle surface. Therefore, dielectric function can be written as [1]:

$$\epsilon(\omega) = \epsilon_{inter}(\omega) + \frac{\omega_p^2}{\omega(\omega + i\gamma)} \quad (1)$$

Where  $\epsilon_{inter}(\omega)$  depicts interband transitions,  $\omega_p$  represents plasmon frequency and  $\gamma$  is a phenomenological scattering parameter. The plasma frequency can be expressed for bulk metal by:

$$\omega_p = \left( \frac{N e^2}{\epsilon_0 m_e} \right)^{1/2} \quad (2)$$

Where  $m_e$  is the effective mass of an electron,  $N$  is the number density of free electrons,  $e$  is the charge of an electron and  $\epsilon_0$  dielectric function of free space (vacuum). For nanoparticles, the scattering parameter has inherent contributions of the intrinsic properties of the material as well as from interface scattering and therefore, it can be described as  $\gamma = \gamma_{bulk} + \gamma_{scat}$ .

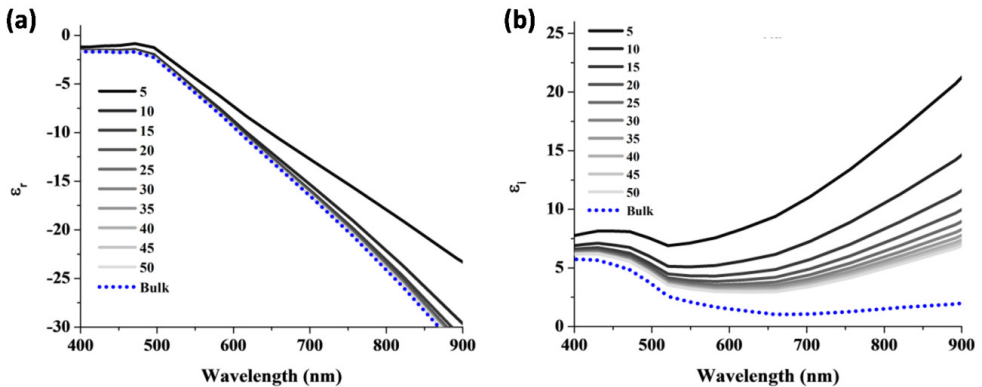
Interface scattering becomes significant when the effective electron path length  $L_{eff}$  is larger than to the nanoparticle itself (L.J. Mendoza et al 2014). The effective path length for convex shapes particles, for instance sphere, rods, cubes etc., is expressed as  $L_{eff} = 4V/S$  where  $V$  is the volume and  $S$  is the surface area (Ross et al. 2015). Thus, the scattering parameter is given by  $\gamma_{scat} = AV/L_{eff}$  where  $A$  is scattering efficiency (L.J. Mendoza et al 2014). For gold,  $\gamma_{bulk} = 1.07 \times 10^{14} \text{ s}^{-1}$ ,  $V_f = 1.40 \times 10^6 \text{ ms}^{-1}$ , while for silver  $\gamma_{bulk} = 3.22 \pm 1.22 \times 10^{13} \text{ s}^{-1}$ , and  $V_f = 1.39 \times 10^6 \text{ ms}^{-1}$  (P.B Johnson 1973). Table 1 depicts the radii of spheres and effective electron path lengths with respect to their sizes.

TABLE 1: NANOSPHERES RADII AND THEIR CORRESPONDING EFFECTIVE ELECTRON PATH LENGTHS ( $L_{eff}$ ).

Sphere Radius (nm)	$L_{eff}$
5.0	6.67 nm
10.0	13.34 nm
15.0	20.00 nm
20.0	26.67 nm
25.0	33.34 nm
30.0	40.00 nm
35.0	46.67 nm
40.0	53.34 nm
45.0	60.00 nm
50.0	66.67 nm

The figure 1 depicts the dielectric functions of Au materials, considering size correction, showing that decreasing the nanoparticle radius (effective path length) both real ( $\epsilon_r$ ) and imaginary parts ( $\epsilon_i$ ) of metallic dielectric changes. The real part of dielectric function depicts the pattern of electron polarization in the medium as a consequence of incident field and determines LSPR peak position.

Figure 1. Complex dielectric function based on surface scattering of real (a) and imaginary part (b) of gold materials with different radii (5, 10, 15, 20, 25, 30, 35, 40, 45, 50 nm).



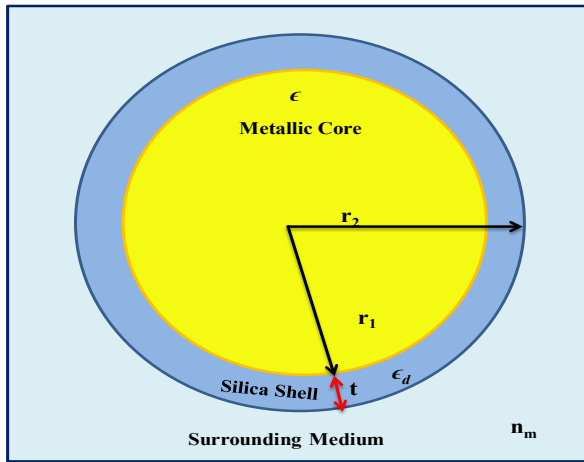
However, imaginary part  $\epsilon_i$  describes energy dissipation or loss in the materials. Decreasing of the nanoparticle size leads to a lower polarizability of the metal, while increases the magnitude of  $\epsilon_i$  Figure.1 (b). Therefore, higher loss is expected for metallic particle with 5nm radius than to 50 nm radius nanostructures due to surface scattering. One can notice that on decreasing effective path length (particle radius), both real and imaginary parts of  $\epsilon(\omega)$  are affected. Real part of  $\epsilon(\omega)$  Figure. 1(a) becomes less negative, showing that metals are less polarizable, while increase in magnitude of imaginary part

Figure.1 (b) of  $\epsilon(\omega)$  causing increase in overall losses in the NP. In particular, these effects yield overall poor plasmonic metal.

### 3 MODELLING AND CALCULATIONS

Figure 2 illustrates the schematic geometry of Au/Ag silica coated nanoshell being investigated in this work. The inner most region is attributed as core having radius and dielectric function  $r_1$  and  $\epsilon$  respectively. The second portion represents the shell with radius  $r_2$  and dielectric function  $\epsilon_d$ , where shell thickness is given by  $t = r_2 - r_1$ .

Figure. 2. Schematic model of the gold/silver silica coated nanoshell.



The interaction between core-shell based metallic nanostructures and electromagnetic radiation in this study was ascribed by Mie theory which elucidated well the solution of Maxwell's equation with appropriate boundary conditions. The general solution for the potion in each region ( $i= 1, 2, 3$ ) is expressed as in Eq. 3, (Erickson, T. A. and J. W. Tunnel, 2009):

$$V_i = \left[ L_i r + \left( \frac{M_i}{r^2} \right) \right] \cos(\theta) \quad (3)$$

Where radius  $r$ , angle  $\theta$  and coefficients  $L_i, M_i$  can be calculated by satisfying the boundary conditions (Averitt, R. D et al., 1999). When the dielectric function is geometrically tunable, the effect of electron scattering can be interpreted by practicing the modified bulk collision frequency as expressed in Eq. 4:

$$\Gamma = \Gamma_{bulk} + \frac{Av_f}{m_f} \quad (4)$$

Where  $\Gamma_{\text{bulk}}$ ,  $m_f$  and  $v_f$  are collision bulk frequency, electron mean free path and Fermi velocity respectively. In case of single refractive scattering and for simple Drude model  $A = 1$  (Averitt, R. D et al., 1999). For nanoshells, the bulk dielectric function can be modified to analyse the free electrons scattering, which is given by Eq. 5:

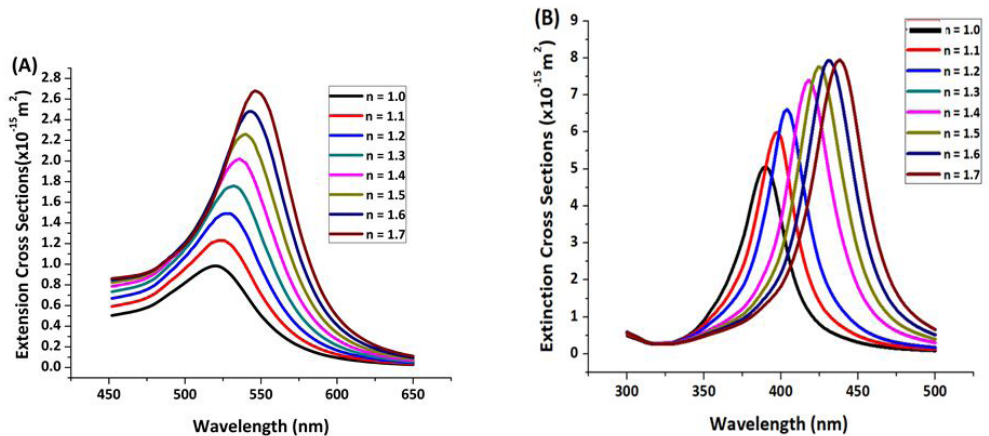
$$\epsilon(m_f, \omega) = \left(1 - \frac{\omega_{bp}^2}{\omega^2 + i\omega\Gamma}\right) + \epsilon(\omega)_{int} \quad (5)$$

Here, the second term represents the Interband transitions,  $\omega_{bp}$  bulk plasma frequency and  $\epsilon(m_f, \omega)$  is dielectric function (size dependent).

#### 4 RESULTS AND DISCUSSION

In this probed model, our focus is on the optimization of the figure of merit by varying the refractive index of the surrounding medium. Despite their simplest core-shell based structure, these metallic nanostructures can still display refractive index tunability based on their LSPR effect. Fig. 3 (A & B) depicts the response of the  $\lambda_{\text{LSPR}}$  and extinction spectra of Au/Ag@SiO<sub>2</sub> nanoshells to the refractive index of the neighbouring medium respectively. For both nanoparticles, by varying the RI the extinction varied significantly in the visible regime and exhibits red shifts which obviously results increase in the intensity of the extinction peak. In case of Au@SiO<sub>2</sub> shell, the extinction spectra continued to red shift in the visible region and the peak wavelength approaches 540 nm. On contrary, the extinction peak of Ag@SiO<sub>2</sub> shell initially blue shifted near UV regime and eventually the peak wavelength was recognizable around 430 nm in the visible region.

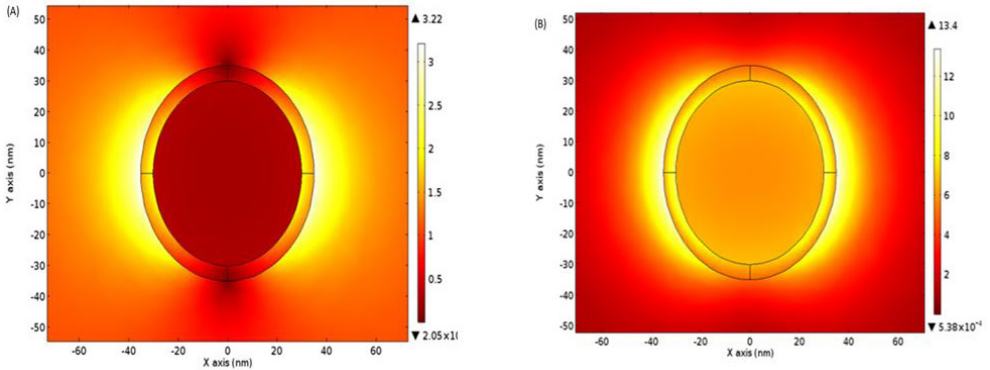
Figure. 3. The LSPR extinction for gold (A) and silver (B) nanoshells





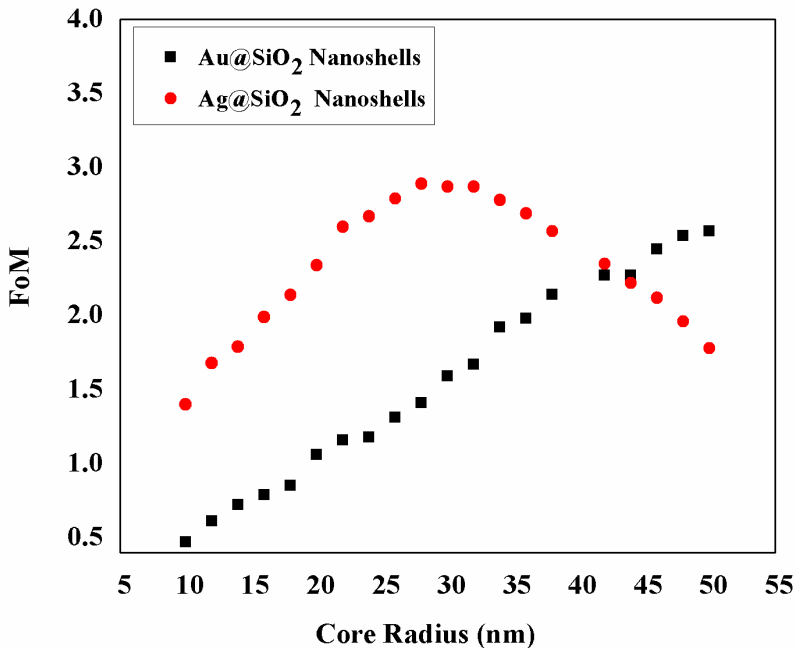
The E-field profile around the nanoshells for the dipole mode (gold and silver) can be observed in Figures 4 (A) and 4 (B) respectively. The changes in normalized electric field of nanoshells were compared at the LSPR wavelengths.

Figure. 4: Electric field profile for gold (A) and silver nanoshells (B).



For linear polarization, the electric field distribution is expressed by the two lobes which ensure the influence of plasmon dipole. LSPR peak position can be determined not only by the real part of nanostructure dielectric function, but also by the RI of the surrounding medium. In refractive index based LSPR sensors, bulk sensitivity reflects how LSPR peak position varies by changes in the RI of the local medium.

Figure. 5. Figure of merit for gold and silver nano shells



The effects of NP core radius on the FoM determining nanoparticle sensing efficiency with varying radii from 10 - 50 nm were theoretically analysed as depicted in figure 5. As the Ag nanosphere radius increases, the FWHM increase due to radiation damping factor (Hu, H., Novo et al., 2008). Therefore, FoM of Ag nanoshells decrease as the particle size grows, as shown in Figure 5. Albeit, the  $\epsilon_i$  value of Ag dielectric function is less than that of Au across visible region, therefore less damping occurs, resulting narrow FWHM (Figure 2(A) and Figure 2(B) and high values of FoM for silver particles. The calculated value of FoM (3.0) of silver nanoshells ( $r = 30$  nm) is higher than the reported values of more complex shapes, such as single Au nanorod (1.3) (Mayer, K.M et al., 2008), Au nanostar (1.9) (Nehl, C.L et al., 2006), Au pyramid (2.2) (Nehl, C.L et al., 2006) Ag nanocube (1.6) (Sherry, L.J et al., 2005).

## 5 CONCLUSION

The theoretical results indicated a nonlinear behavior of the bulk and refractive indexed based sensitivity as function of the varying shell thickness. Moreover, LSPR peak shift is also determined by changing surrounding medium and the shell thickness. Our results possess high figure of merit for silver nanoshell (3.0) as compared to gold nanoshell (2.50) having silica shell thickness 5 nm for each nanostructure. The proposed approached can be extended to engineer the efficiently use of different nanostructures on molecular biosensing.

## 6 ACKNOWLEDGEMENT

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## INDEX

### A

Adsorbente 172, 173, 179, 180

Alumínio 182, 183, 184, 186, 187, 189, 190, 191, 192, 193, 198, 200, 204, 205, 206, 208, 209, 210

Annealing 1, 2, 4, 5, 7, 9, 10, 227

Arsénico 172, 173, 174, 178, 179, 180, 181

AuNR dimer 12, 14, 16, 17, 18, 19

### B

Biodiesel 162, 164, 165, 168, 169, 171

Blends 162, 168, 169, 170, 171

Bulk sensitivity 12, 14, 15, 16, 17, 18, 19, 73

### C

Carboxymethylchitosan 125, 127, 128, 129, 132, 133, 136

Celulose 228, 229, 230, 231, 232, 233

Chemical composition of SS surface 109

Clay 125, 127, 128, 130, 131, 133, 136, 137

Comparison among Silica and reuse of waste 77

COMSOL 14, 15, 68

Conductive tubes 92, 93, 94, 95, 100, 102, 104, 106

Confined water 39, 40, 41, 42, 52, 55, 58, 59, 60, 61, 63, 65

### D

DFT 21, 23, 35, 36, 49, 50, 63

Diesel 162, 163, 164, 165, 168, 169, 171

DSSC 213, 214, 217

### E

Efluente 172, 173

Evolutionary strategies 151, 156

### F

FEM 14, 68

Figure of merit 11, 12, 14, 15, 16, 17, 67, 68, 72, 73, 74

Filmes finos 205, 212, 213  
Filter 125, 126, 127, 128, 131, 132, 134, 135, 136, 137  
Fits on Mössbauer spectra 151  
FoM 15, 16, 17, 18, 19, 68, 74

## G

Graphite nanostructures 162

## K

$\text{KSr}_2\text{Nb}_5\text{O}_{15}$  ceramic 138, 139, 141, 144, 146

## M

Magnetita nanoestruturada 172, 173  
Metalurgia do pó 182, 186, 191, 192  
Métodos químicos 198, 201, 205  
Micro and nano silica 76, 77, 78, 79, 84, 90

## N

Nanocomposite 36, 37, 91, 125, 126, 127, 128, 132, 133, 134, 135, 136, 137, 161, 182, 183, 194, 195, 196, 198, 211  
Nanocompósitos 182, 183, 185, 186, 193  
Nanocristais 228, 229, 230, 232, 233  
Nanoestruturas 182, 198, 200, 201, 202, 206, 210, 213, 217, 218, 219, 222, 223, 224, 226  
Nanograins 1, 2, 3, 9, 138  
Nanolithography 39, 40, 41, 42, 45, 50, 62, 64, 66  
Nanopartículas 151, 180, 212, 224, 228, 229, 231  
Nanostructures 2, 9, 12, 13, 14, 15, 17, 19, 21, 22, 23, 25, 38, 61, 68, 69, 70, 71, 72, 74, 138, 162, 170, 211, 213, 226, 227  
Nanostructures surface 21, 22, 23  
Nanotechnology 12, 20, 62, 66, 102, 106, 126, 138, 162, 183, 195, 213, 226  
Nanotecnologia 182, 212  
 $\text{NiFe}_2\text{O}_4$  nanoparticles 150, 151, 153

## O

Oxidation 39, 40, 41, 42, 53, 55, 59, 64, 65, 91, 109, 117, 118, 121  
Óxido de grafeno reduzido 182, 183, 186

Óxido de zinco 197, 213

## P

Papel reciclado 228, 229, 232, 233

Perfectly matched layer 11, 12, 15, 68, 69

PIII in magnetic field 109

Plasma immersion ion implantation 92, 93, 94, 107, 108, 109, 122, 123, 124

## R

RI 15, 16, 67, 68, 72, 73

Rice husk Silica 77

Rolling 1, 2, 3, 4, 5, 6, 7, 9

Rough rolls 1, 2, 3, 8, 9

## S

SILAR 198, 200, 201, 204, 205, 206, 210, 212, 213, 216, 217, 218, 219, 220, 221, 222, 223, 224, 226

Silica Morphology 77, 83

Silver nanoparticles 74, 125, 127, 128, 129, 130, 132, 133, 136, 137

Supercapacitores 197, 198, 199, 200, 202, 209, 210

Surface 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14, 19, 20, 21, 22, 23, 24, 27, 28, 29, 30, 31, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 44, 45, 50, 52, 53, 54, 55, 57, 58, 59, 60, 63, 64, 65, 66, 68, 69, 70, 75, 77, 79, 80, 81, 82, 84, 85, 88, 91, 92, 93, 94, 95, 96, 98, 99, 100, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 116, 117, 118, 119, 121, 122, 129, 152, 160, 161, 173, 211, 213, 226, 227

Surface modification 37, 38, 92, 93, 106, 109, 110

## U

Ultrananocrystalline Diamond Films 93, 108

## V

Viscosity 89, 162, 163, 165, 166, 167, 168, 169, 170, 171

## X

X-ray photoelectron spectroscopy 42, 92, 96, 103, 108, 109, 111, 123



## Z

ZnO 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 197, 198, 199, 200, 201, 202, 204, 205, 206, 207, 208, 209, 210, 211, 212, 213, 214, 215, 217, 218, 219, 220, 221, 222, 223, 224, 225, 226, 227

ZnO nanocrystals 21, 23, 25, 35



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