Revista Brasileira de Ensino de Física, vol. 46, e20240184 (2024)
www.scielo.br/rbef
DOI: https://doi.org/10.1590/1806-9126-RBEF-2024-0184

Study of the Role of the Size of Metallic Nanospheres in the Extinction of the Light Based on the Mie Theory Using Python

Estudo da Influência do Tamanho das Nanopartículas Metálicas Esféricas na Extinção da Luz Baseado na Teoria de Mie Usando Python

Lucas Johnny Monte Tamayo[1], Renan Tostes Couto[2], Núbia Monteiro Batista Pereira[1], Larissa dos Santos de Góes[2], Alexia Nogueira Rodrigues Alves[1], Zeila Virginia Torres Santos[3], Clara J. Pacheco[1], Larissa Maria Beserra Soares[1], Marcos Vinícius Colaço[1], Juliana Fonseca de Lima[2], Alexandre de Resende Camara[*1]

[1]Universidade do Estado Rio de Janeiro, Instituto de Física, Rio de Janeiro, RJ, Brasil.
[2]Universidade do Estado Rio de Janeiro, Instituto de Química, Rio de Janeiro, RJ, Brasil.
[3]Patrice Lumumba People's Friendship University of Russia, Moscow, Russia.

Received on May 23, 2024. Revised on August 19, 2024. Accepted on August 23, 2024.

The inclusion of nanoparticles in technological development increases every year. For example, metallic nanoparticles are applied in cosmetics, medicine, and sensing areas among others. When light interacts with metallic nanoparticles, the Localized Surface Plasmon Resonance (LSPR) can occur. LSPR is the subject of advanced courses in Physics and some of the students could have several difficulties in its comprehension. To benefit the students, it is proposed a very simple simulator built in Python to study the influence of the features of metallic spherical nanoparticles and of the host medium in the LSPR effect through the Mie Theory.
Keywords: Gold nanoparticles, LSPR, Mie Theory, Python.

A inclusão de nanopartículas no desenvolvimento da tecnologia se expande continuamente. Nanopartículas metálicas já são usadas em cosméticos, na área médica e em sensoriamento, dentre outras. Quando um feixe de luz interage com nanopartículas metálicas a Ressonância de Plasmons de Superfície Localizada (em inglês, LSPR) pode ocorrer. A LSPR é assunto de disciplinas avançadas em cursos de Física e alguns estudantes podem apresentar dificuldades em compreendê-la. Com o intuito de ajudar esses estudantes, é proposto um simulador simples, construído em Python para estudar a influência das características das nanopartículas metálicas e do meio que as circunda na LSPR através da Teoria de Mie.
Palavras-chave: Nanopartículas Metálicas, Teoria de Mie, RPSL, Python.

1. Introduction

Metals are very well-known elements whose main characteristic is to be a conductor of electricity and heat. When studying the physical properties of a conductive solid and even more, the interaction with electromagnetic radiation close to visible light, important fluctuation effects are defined to understand more thoroughly the behavior and function that it fulfills in nature.

Faraday prepared the first colloidal solution of gold nanoparticles in 1857. He studied a colloidal gold dispersion in a two-phase system consisting of an aqueous solution of gold salt and a solution of phosphorus in carbon disulfide. It probably was the first reported observation of nanoparticles (NPs). One important consequence of the use of nanoparticles is the high-volume density of NPs when they are deposited in a substrate. This surface area-to-volume ratio can lead to a highly significant influence of the atoms on the surface of a particle to determine the general properties of NP. The inorganic NP is seen as a building piece due to its optical, magnetic, and electronic properties. Such modulated properties vary based on NP surface size, shape, and functionalization, without changing material composition [2, 3].

In terms of the electronic features, the movement of electrons in a nanomaterial is very limited by the dimensions of the material itself. Therefore, if the dimensions were reduced, the properties are going to be modified. As a result, materials can be developed with the desired properties. When the particle size is close to the electron-free path (around 50 nm for Au), the dielectric function and the refractive indices become strongly dependent on size [4]. For example, the nanoclusters have sizes

*Correspondence email address: professoralexandrecamara@gmail.com

comparable to the Fermi wavelength of an electron, which shows optics, electronic, and chemical properties widely different from particles with diameter > 100 nm.

All the consequences of the interaction between light and metallic nanoparticles are treated by the Electromagnetic Theory [5, 6]. In particular, the theory of LSPR is a subject studied in advanced courses in Physics most commonly at the Graduation level. Since this theory has some complexities, some of the students can have difficulties in its comprehension. Thus, a very simple open code simulator built in Python is proposed as a new tool for learning the phenomenon of LSPR.

Python is an interpreted, interactive, object-oriented programming language that was implemented in 1989 by Guido van Rossum succeeding the ABC language and compatible with AMOEBA operational system [7]. Over the years Pyhton became relevant in many aspects and nowadays is considered the main programming language in multiple areas. With a high-level syntax, i.e. a very simple comprehension and intuitive language, Python has an important goal that resembles the usual human being language. When building code, Python tends to be shorter due to, e.g., the lack of need to declare variables, compared to C++ or Java.

Furthermore, Python is an open-source language that has a very active community and many libraries developed for different applications. These features made Python one of the most important programming languages in the academic area.

This work presents a Python code to study how the size of metallic nanoparticles influences the light extinction process, which can be explained from the point of view of a phenomenon called Surface Plasmon Resonance or LSPR to be used as a new didactic resource that can be useful in Graduation Courses as Nonlinear Optics or Plasmonics.

2. Theorectical Aspects

Metals are a class of materials that have a dielectric constant with a negative real part and a positive imaginary part. This feature allows the generation of linear and nonlinear effects where, among them, Surface Plasmon Resonance (SPR) attracts the attention of researchers worldwide. In a brief explanation, when light impinges in a metallic thin film deposited in a dielectric substrate, e.g. a prism, the light is partially absorbed and partially reflected by the film. The amount of light that will be reflected or absorbed by the film depends on the angle at which the light arrives at the film [8]. Due to the absorption of the light surface plasmons are generated. As metals are conductors most of their electrons are in the conduction band. The coherent oscillation of those electrons is known as surface plasmons. Moreover, in the case of thin films, the surface plasmons can propagate along the metal-dielectric interface called surface plasmon polaritons (SPPs). In the case where

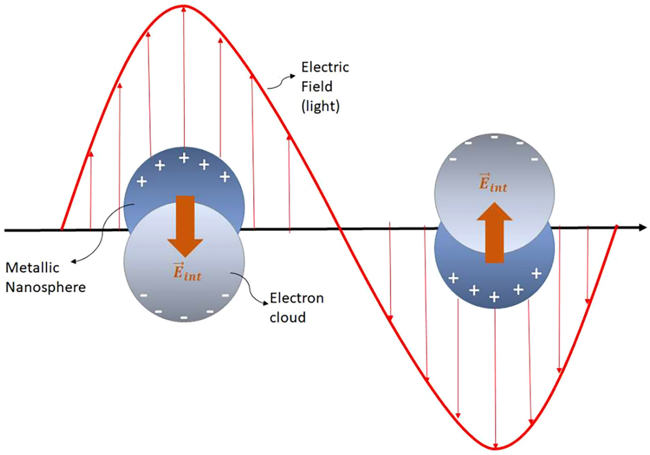

Figure 1: Schematic diagram of the generation of a localized surface plasmon in metallic spheres.

the metal is not in a thin film form but nanoparticles with radius, the coherent oscillation does not propagate but occurs locally around the nuclei of the NPs. The schematic of the interaction among light and spherical metallic particles is shown in Figure 1.

Figure 1 shows the schematic of the interaction of an incident electromagnetic field in spherical particles. When the nanoparticles are not in the presence of an external electric field, the electron clouds of the particles oscillate around the static positive nuclei with the natural frequency (also known as plasmonic frequency). If there is an external electromagnetic field, the oscillation of the electron clouds is dramatically affected. The general solution to this problem is given by the Mie Theory [9]. However, in a particular case, if the size of the particles is much smaller than the wavelength λ of the incident electromagnetic field (EMF), the quasi-static approximation can be used to study the problem. Here, the nanoparticles interact with an external EMF that can be considered uniform over the nanoparticle volume. Then, a force is exerted by the EMF on the electron clouds removing them from the equilibrium region. As a result, an electric dipole is induced and an electric field emerges inside the particles ($\vec{E}_{int}$) to restore the situation of equilibrium [10]. If the frequency of the external electric field is equal to ω_p, all energy of the incident photons is commuted to the LSPR mode. Noble metals such as gold, silver, copper, and aluminum exhibit the resonance for wavelengths in the visible range of the electromagnetic spectrum, which make them very interesting to the LSPR-sensing area. A way to study the interaction between the incident light and the metallic nanoparticles is through the scattering cross-section (σ_{scat}) and the absorption cross-section (σ_{abs}) of the NPs, as can be seen in Equations (1) and (2):

$$\sigma_{abs}(\lambda) = k(\lambda) \cdot Im[\alpha(\lambda)] \tag{1}$$

$$\sigma_{scat}(\lambda) = \frac{k(\lambda)^4}{6\ \pi} \cdot |\alpha(\lambda)|^2 \tag{2}$$

 DOI: https://doi.org/10.1590/1806-9126-RBEF-2024-0184

where $k(\lambda) = \frac{2\pi n}{\lambda}$ is the wavenumber, n is the refractive index of the medium that surrounds the NPs and $Im[\alpha(\lambda)]$ represents the imaginary part of the complex polarizability of the dipole $\alpha(\lambda)$ given by [11, 12]:

$$\alpha(\lambda) = \frac{V}{\left(L + \frac{\varepsilon_h}{\varepsilon_i(\lambda) - \varepsilon_h}\right) + A\varepsilon_h x^2 + B\varepsilon_h^2 x^4 - i\frac{4\pi^2\varepsilon_h^{1.5}}{3} \cdot \frac{V}{\lambda^3}} \tag{3}$$

where V is the volume of the NPs, ε_h is the dielectric constant of the host medium, $x = \frac{2\pi r n}{\lambda}$ is a scale factor, L is the depolarization factor ($L = \frac{1}{3}$ for spherical particles). A and B are, respectively, L-dependent empirical constants defined as:

$$A\,(L) = -0.4865L - 1.046L^2 + 0.8481L^3 \tag{4}$$

$$B\,(L) = 0.01909L + 0.1999L^2 + 0.6077L^3 \tag{5}$$

The last parameter of $\alpha(\lambda)$ is the dielectric constant of the metallic NPs $\varepsilon_i(\lambda)$, given by the Drude-Lorentz Model [13–17]:

$$\varepsilon(\lambda) = \varepsilon_b + 1 + \frac{\omega_p^2}{\omega(\lambda)^2 - i\omega(\lambda)\gamma_f} \tag{6}$$

Here, ε_b is the contribution of the electrons from the valence band to the dielectric constant, ω is the angular frequency of the incident EMF and ω_p is the plasma frequency of the NP. The parameter γ_f is the damping parameter and it is related to the collision time associated with the collective oscillation of the electrons. However, taking into account that the incident light is in the visible-near infrared range, if the NPs have radius smaller than 10 nm, γ_f is strongly dependent on the value of r [18]. The size dependence of γ_f is shown below:

$$\gamma_f = \frac{1}{\tau} + \frac{v_f}{r} \tag{7}$$

where τ the collision time associated with the collective oscillation of the free electrons and v_f is the Fermi velocity.

Thus, the total interaction between light and the metallic NPs is given by the extinction cross-section σ_{ext} [16, 17], defined as:

$$\sigma_{ext} = \sigma_{abs} + \sigma_{scat} \tag{8}$$

To improve the understanding of the interaction between electromagnetic waves and the metallic nanoparticles produced for this work as well as estimate the absorbance curve and the value of λ_{LSPR}, a Python code was created to estimate the extinction (absorption + scattering) of light by a metallic (gold or silver) nanoparticle.

3. The Python Code

The Python code, which will be shown in the Supplementary Material, simulates the extinction of the incident light due to the interaction with a spherical metallic nanoparticle. As mentioned in the previous section the type of metal is crucial in this process once the LSPR is highly dependent on the real and imaginary parts of the dielectric constant of the metal. This information is available in a refractive index database [19]. It is important to highlight that this code can simulate the extinction cross-section for other metals, e.g. silver [20]. The user only needs to download the information of the dielectric constant of the desired metal in a text file, with the columns tab-separated as shown in Figure 2.

The first column shown in Figure 2 has the wavelengths (wl) for which the real (n, second column) and

wl	n	k
0.1879	1.28	1.188
0.1916	1.32	1.203
0.1953	1.34	1.226
0.1993	1.33	1.251
0.2033	1.33	1.277
0.2073	1.30	1.304
0.2119	1.30	1.350
0.2164	1.30	1.387
0.2214	1.30	1.427
0.2262	1.31	1.460
0.2313	1.30	1.497
0.2371	1.32	1.536
0.2426	1.32	1.577
0.2490	1.33	1.631
0.2551	1.33	1.688
0.2616	1.35	1.749
0.2689	1.38	1.803
0.2761	1.43	1.847
0.2844	1.47	1.869
0.2924	1.49	1.878
0.3009	1.53	1.889
0.3107	1.53	1.893
0.3204	1.54	1.898
0.3315	1.48	1.883
0.3425	1.48	1.871
0.3542	1.50	1.866
0.3679	1.48	1.895
0.3815	1.46	1.933
0.3974	1.47	1.952
0.4133	1.46	1.958
0.4305	1.45	1.948
0.4509	1.38	1.914
0.4714	1.31	1.849
0.4959	1.04	1.833
0.5209	0.62	2.081
0.5486	0.43	2.455
0.5821	0.29	2.863
0.6168	0.21	3.272
0.6595	0.14	3.697
0.7045	0.13	4.103
0.7560	0.14	4.542
0.8211	0.16	5.083
0.8920	0.17	5.663
0.9840	0.22	6.350
10.880	0.27	7.150
12.160	0.35	8.145
13.930	0.43	9.519
16.100	0.56	11.21
19.370	0.92	13.78

Figure 2: Information of the real (n) and imaginary (k) parts of the refractive index of gold in function of the incident wavelength.

imaginary (k, third column) parts of the dielectric constant of the metal (gold in this case) were measured [21]. These values are important because the real part of the dielectric constant leads with the refraction/reflection of the light while the imaginary part of the dielectric constant is related to the absorption of the light by the metal that allows among other effects the Localized Surface Plasmon Resonance.

Taking into account the values shown in Figure 2, the first part of the proposed code leads with the libraries used to calculate the extinction of the light by the metallic nanospheres (Pandas and Numpy), plot the obtained results in a graphic showing the extinction of the light versus the incident wavelength (Matlibplot), and create an interactive interface where the user can change some parameters of the problem (Tkinter).

The Panda library was developed by Wes McKinney in 2008 and has as its initial goal to implement statistical improvements in Python to make this programming language more competitive when compared to relevant languages such as R, Matlab, STATA, and SAS [22]. Among its advantages is the introduction of an object called DataFrame, which is particularly relevant when dealing with large amounts of structured two-dimensional data (for example, a table). For example, you can import an external file in the format of a two-dimensional table into Python, which will be read as a DataFrame, an object that allows for simple manipulation in a variety of ways, such as reordering or grouping its items, mathematical and statistical treatment involving its data, among others [22].

Many of the features of this library have made the Python language even more relevant for data analysis and processing, and together with R, it has become the most widely used language in the field of Data Science.

The NumPy library was created by Travis Oliphant in 2005 to allow operations in multidimensional arrays such as data analysis, linear algebra, and Fourier Transform, among others, in a simpler way [23]. As a consequence, the results obtained using this library occupy less memory and can be processed 10 to 100 times faster than applications that use other Python structures.

The Matlibplot is a library originally created by John Hunter and heavily inspired by the graphical tools offered by Matlab, which initially aimed to generate various types of 2D graphs in the Python programming language [24].

Its development over the years has enabled the inclusion of new tools, such as the generation of 3D graphs. By combining its functionalities with those of other libraries such as Pandas or Numpy, it becomes an extremely useful tool in many areas of science.

Finally, the Tkinter is a library that comes with the Python language interpreter, originally developed by John Ousterhout [25], whose main motivation is to provide a graphical interface for programs, making them accessible to an end user without having to access the program's internal code.

Although simple, it is quite functional and fulfills its purpose by generating a simple design window whose content and possible interactions are up to the programmer, while the end user only uses the program.

Even though the complete code is available in the Supplementary Material, Figure 3 shows the flowchart of the code to improve the understanding of how the proposed code operates.

Firstly, the code calls the information contained in the .txt file downloaded from [19] and declares the variables corresponding to wavelength (wl) and real (n) and imaginary (k) parts of the dielectric constant columns and calculates the value of the Extinction Cross Section of the nanosphere. Furthermore, two other parameters are needed: the radius of the nanosphere and the dielectric constant of the medium that surrounds the nanoparticles. To make the user experience more interactive, the proposed code creates an interface (Figure 4) where the user can type the information to produce the "Extinction Cross Section versus Incident Wavelength" graphic.

Once all parameters are typed, the user just needs to press the button "Generate Graphic". If the user wants to generate a new graphic using other values for the radius of the nanoparticle and/or the dielectric constant of the host medium, one only needs to type the desirable value in the correct box and press again the button "Generate Graphic". Figure 3 also shows that is possible to generate three graphics at the same time, but if the user wants less than three curves, one shall let

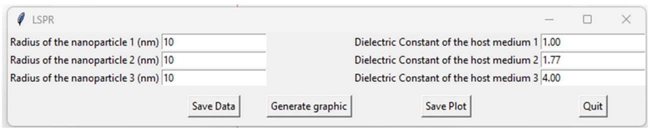

Figure 3: Flowchart of the purposed Python code.

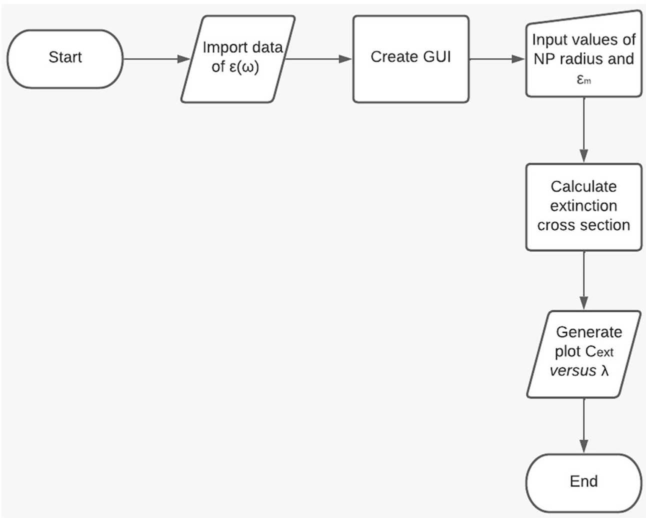

Figure 4: Interactive interface created by the proposed Python code.

the correspondent boxes empty. The other buttons are "save data", where the user can save the graphics data in a text file, "save plot", where the graphic is saved in a PNG file, and "Quit", to close the program.

4. Results and Discussion

4.1. Comparison with COMSOL multiphysics

As shown in Figure 5, the results obtained using this Python code allow the user to obtain for three different configurations simultaneously not only the λ_{LSPR} value but also how this value changes for the alteration of the host medium and the role of the size of the nanoparticles in the λ_{LSPR} value and in the full-width-half-maximum (FWHM) value of the LSPR band.

In the case presented in Figure 5, the obtained λ_{LSPR} values are respectively 495 nm (blue curve), 521 nm (orange curve), and 582 nm (green curve).

Every time that a model or a programming code is built to simulate a physical phenomenon, it is very important that a validation of the obtained results is done. In this work the validation was performed in two steps: comparing with the theoretical results obtained using the COMSOL Multiphysics platform (Figure 6), which is a software used in Physics, Engineering, and Chemistry among others to perform simulations in 0D, 1D, 2D, and 3D [26], and comparing with experimental data (Figure 6). As the AuNPs produced in by our research group have a size distribution centered in 8 nm, this value was used as a parameter in the simulations made in COMSOL and using the Python code.

As can be seen in Figure 6, using water ($\varepsilon = 1.7689$) as the host medium the COMSOL simulated data and the data produced using the proposed Python code fit almost perfectly indicating that the proposed Python code can be used to perform this study.

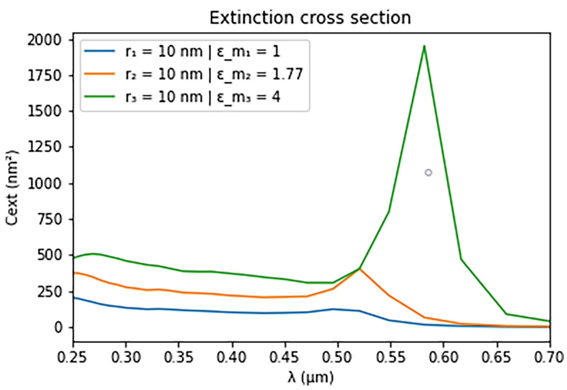

Figure 5: Extinction Cross Section versus incident wavelength of a 10 nm radius AuNP in three different host media using the default template of the function "mathplotlib" in Pyplot package.

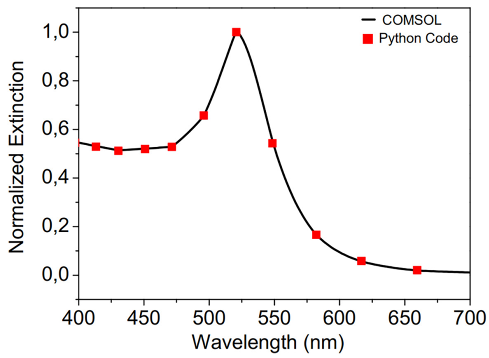

Figure 6: Normalized Extinction versus incident wavelength for a single AuNP with radius equal to 8 nm using COMSOL Multiphysics platform (black line) and the proposed Python code (red squares).

4.2. Experimental validation

As mentioned, the next step was to verify if these results were compatible with real situations, and an experimental validation was performed. The gold nanoparticles (AuNPs), in this case, with a radius equal to 8 nm, were produced using an adaptation of the well-known Turchevich Method [27, 28]. The experimental setup consists of depositing the AuNPs in a dielectric substrate (in this case, microscope slides). Then, the samples are placed in front of a UV-Vis spectrometer (FLAME S-XR1_ES, Ocean Insight, US) to measure the absorption of the incident white light (DH-2000-BAL, Ocean Insight, US) by the AuNPs as shown in Figure 7. The data is collected using proper software (SpectraSuite, Ocean Insight, US).

Figure 8 shows a comparison between the experimental (black curve) and simulated (red squares) normalized extinction of the incident light.

As can be seen, to AuNPs with a radius of 8 nm surrounded by water, the experimental and simulated λ_{LSPR} values were coincident, around 520 nm. This is very important because it shows the results obtained using the proposed LSPR simulator are valid. However, there is a considerable difference between the FWHM of the LSPR band in each case. The main reason for this

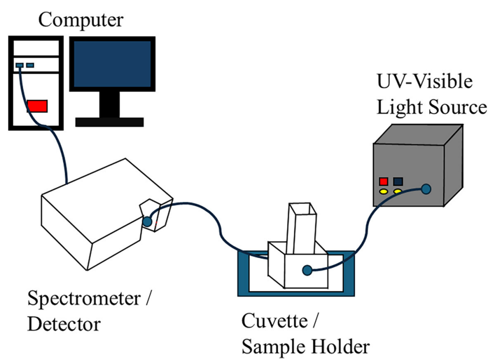

Figure 7: Experimental setup.

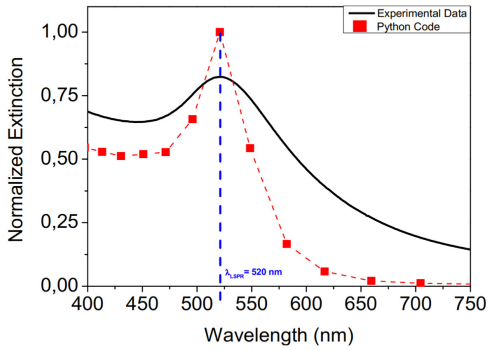

Figure 8: Normalized Extinction versus incident wavelength for a colloidal AuNPs solution with radius distribution centered in 8 nm (black line) and for a simulated AuNP with radius 8 nm using our proposed Python code (red squares).

difference is the fact that the experimental data were obtained from a colloidal solution of AuNPs that has many nanoparticles that present variation in their radius values [28] while the simulated data consider a single and perfectly spherical AuNP. It is very well established that the wider the curve that describes the size distribution of the nanoparticles, the wider the extinction band will be.

As demonstrated, the results obtained using the proposed Python code are in good agreement with the real cases. Thus, it is expected that if the students can use this program during the classes, their understanding of phenomena such as scattering of light, absorption of light, and resonance will be improved once they do not work only with the mathematical tools but also through playing with features as size, shape, type of metal, and refractive index of the surrounding medium evaluate in real time how each one contributes for the LSPR phenomenon.

5. Conclusions

To improve the understanding of the interaction among light and metallic nanoparticles given by the Mie Theory, it was proposed a simple Python code that can be used by teachers and students in courses such as Plasmonics or Advanced Electromagnetism. The interface is very clear and straightforward to the user and the proposed code produces results that are in according with the COMSOL simulated results and also in according with the experimental results obtained by our research group. Thus it is possible to say that the proposed code is a potential tool to be a free-of-cost alternative to simulate the LSPR band of metallic nanoparticles and aid the students to have a better understanding of this phenomenon.

Acknowledgments

All the authors would like to thank to Fundação de Amparo à Pesquisa do Estado do Rio de Janeiro (FAPERJ E_26/2021 Auxílio Básico à Pesquisa (APQ1) em ICTs Estaduais UERJ, – UENF e UEZO-2021) for the financial support. Alexandre Camara wants to thank Dr. Isabel Carvalho (Physics Department, PUC-Rio, Brazil) for allow the use of the COMSOL Multiphysics.

Supplementary material

The following online material is available for this article: The Python Code.

References

[1] T. Rahman and E.V. Rebrov, Processes **2**, 466 (2014).
[2] D.A. Pichugina, N.E. Kuzmenko and A.F. Shestakov, Russian Chemical Reviews **84**, 1114 (2015).
[3] K. Ariga and M. Anono, Supra-materials Nanoarchitectonics (Elsevier, Oxford, 2016).
[4] K.J. Prashant, S.L. Kyeong, I.H. El-Sayed and M.A. El-Sayed, J. Phys. Chem. B **110**, 7238 (2006).
[5] R.M. Wald, *Advanced Electromagnetism* (Princeton University Press, Oxford, 2022), v. 1.
[6] J.D. Jackson, *Classical Electrodynamics* (John Wiley and Sons, New York, 1998), 3 ed.
[7] L. Tulchak and A. Marchuk, *History of Python*, available in: https://ir.lib.vntu.edu.ua/bitstream/handle/123456789/10471/461.pdf, accessed in: 08/05/2024.
[8] Y. Chen, L. Chen, Y. Wu and J. Di, Microchemical J. **147**, 955 (2019).
[9] K.A. Willets and R.P. Van Duyne, Annu. Rev. Phys. Chem. **58**, 267 (2007).
[10] S.A. Maier, *Plasmonics: Fundamentals and Applications* (Springer, New York, 2007).
[11] S. Xiao, J. Lu, L. Sun and S. An, Spectrochim. Acta Part A Mol. Biomol. Spectrosc. **271**, 120924 (2022).
[12] M.R. Cunha, E.C. Lima, D.R. Lima, R.S. Silva, P.S. Thue, M.K. Seliem, F. Sher, G.S. Reis and S.H. Larsson, J. Environ. Chem. Eng. **8**, 104506 (2020).
[13] D. Dolar, M. Gros, S. Rodriguez-Mozaz, J. Moreno, J. Comas, I. Rodriguez-Roda and D. Barceló, J. Hazard. Mater. **239**, 64 (2012).
[14] N. Klamerth, S. Malato, A. Agüera and A. Fernández-Alba, Water Res. **47**, 833 (2013).
[15] R. Mailler, J. Gasperi, Y. Coquet, A. Buleté, E. Vulliet, S. Deshayes, S. Zedek, C. Mirande-Bret, V. Eudes, A. Bressy et al., Sci. Total Environ. **542**, 983 (2016).
[16] M.B. Ahmed, J.L. Zhou, H.H. Ngo, W. Guo, N.S. Thomaidis and J. Xu, J. Hazard. Mater. **323**, 274 (2017).
[17] P. Kar, K. Shukla, P. Jain, G. Sathiyan and R.K. Gupta, Nano Mater. Sci. **3**, 25 (2021).
[18] M.J.A. Cortes-Diaz, J. Rodríguez-Flores, G. Castañeda-Peñalvo, M. Galar-Martínez, H. Islas-Flores, O. Dublán-García and L.M. Gómez-Oliván, Sci. Total Environ. **605–606**, 811 (2017).
[19] RefractiveIndex.Info, available in: https://refractiveindex.info, accessed in 08/05/2024.
[20] L.J.M. Tamayo, *Desenvolvimento de um Simulador da Ressonância de Plasmons de Superfície Localizada Utilizando Python.* Trabalho de Conclusão de Curso,

Universidade do Estado do Rio de Janeiro, Rio de Janeiro (2021).

[21] P.B. Johnson and R.W. Christy, Phys. Rev. B **6**, 43706 (1972).

[22] W. McKinney, *pandas: a foundational python library for data analysis and statistics*, available in: https://www.researchgate.net/profile/Wes-Mckinney/publication/265194455_pandas_a_Foundational_Python_Library_for_Data_Analysis_and_Statistics/links/5670827c08ae0d8b0cc0f3cc/pandas-a-Foundational-Python-Library-for-Data-Analysis-and-Statistics.pdf, accessed in 08/05/2024.

[23] B. Mulinari, *Numpy Python: O que é, vantagens e tutorial inicial*, available in: https://harve.com.br/blog/programacao-python-blog/numpy-python-o-que-e-vantagens-e-tutorial-inicial/, accessed in 29/07/2024.

[24] J.D. Hunter, IEEE Computer Society **9**, 90 (2007).

[25] J.E. Grayson, *Python and Tkinter Programming* (Manning Publications, New York, 2000).

[26] COMSOL, *COMSOL Multiphysics® Simulation Software*, available in: https://www.comsol.com/comsol-multiphysics, accessed in: 08/05/2024.

[27] J. Turkevich, P.C. Stevenson and J. Hiller, Discuss. Faraday Soc. **11**, 55 (1951).

[28] R.T. Couto, *Síntese e Caracterização de Nanopartículas de Ouro para Sensoriamento*. Dissertação de Mestrado, Universidade do Estado do Rio de Janeiro, Rio de Janeiro (2020).