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# Effect of MoS<sub>2</sub> layer on the LSPR in periodic nanostructures

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In this work, we propose a new configuration of the localized surface plasmon resonance (LSPR), based on MoS<sub>2</sub> hybrid structures for ultrasensitive biosensing applications. The plasmonic resonances are widely used in bimolecular detection and continue to be an active network because of the rich variety of surface configurations and measurement donations. The present work studies the interaction of gold nanoparticles with a MoS<sub>2</sub> film. MoS<sub>2</sub> is used as a thin spacer between the gold nanoparticles and the dielectric medium used for detection. MoS<sub>2</sub> monolayers have emerged recently as promising nanostructures for various applications in both the optics and electronics. This paper gives an overview of the optical properties of 2D nanostructures based on this new class of materials. A stronger behavior of the resonance positions in the absorption spectrum exhibits a strong coupling between the LSPR on the gold nanoparticles and the MoS<sub>2</sub> coating film. Numerical simulations display a significant red shift of the plasmonic resonance ( $\lambda_{max}$ ) and the results show that using a 3.90 nm MoS<sub>2</sub> layer, the plasmon resonance wavelength is increased of 333.7 nm. We also study the performance of the proposed biosensors in terms of sensitivity using multilayers of MoS<sub>2</sub>, and normal incidence to the surface of SiO<sub>x</sub>/AuNPs/MoS<sub>2</sub>/water and SiO<sub>x</sub>/MoS<sub>2</sub>/AuNPs/water. We obtain a very high sensitivity of 297.62 nm/RIU corresponding to an increase of 26% compared to the results obtained on SiO<sub>x</sub>/AuNPs/water, with a location of the electric field on the gold nanoparticles and the covering MoS<sub>2</sub> layer. These characteristics should make these biosensors a preferred choice for detection applications.

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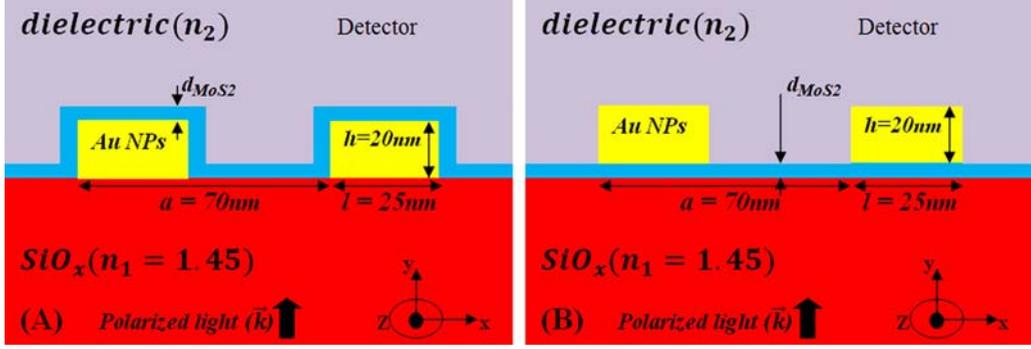
## 1. Introduction

Plasmonic response of the metal nanoparticles is highly dependent on their size [1–3], their form [4–6] and the material constituting the chemical 2D composition [7–9]. The understanding of their properties is even more complex when they are deposited on a substrate [1,10,11] or when they interact with each other [12–14]. It appears from the theoretical and the experimental studies already completed that there are many parameters governing their behavior [15]. As part of our study, we will investigate the influence of the MoS<sub>2</sub> layer on the LSPR. The complex refractive index of the MoS<sub>2</sub> monolayer obtained from the experimental measurement data by Castellanos-Gomez et al. [16] is  $n_{\text{MoS}_2} = 5.9 + 0.8i$  at 632.8 nm and the thickness of the MoS<sub>2</sub> layer is  $d_{\text{MoS}_2} = N \times 0.65$  nm [17,18], where  $N$  is the number of coatings of MoS<sub>2</sub> [19–22], deposited on the metal nanoparticles of gold. Molybdenum disulfide (MoS<sub>2</sub>) holds great promise for optical applications due to the variations of optical transition depending on the atomic thickness of the film [19]. A gradual red shift of the absorption bands the background absorption. Hence, Increasing MoS<sub>2</sub> film thickness is observed to allow tuning the absorption properties of such films. The optical processes in a low dimensional materials

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**Fig. 1.** Schematic representation of the plasmonic structures studied in this work. (A) Periodic gold nanoparticle (Au NPs) array on  $\text{SiO}_x$  ( $n_1 = 1.45$ ) and coated with a layer of  $\text{MoS}_2$  ( $\text{SiO}_x/\text{AuNPs}/\text{MoS}_2$ ); (B)  $\text{SiO}_x$  ( $n_1 = 1.45$ ) coated with a thin film of  $\text{MoS}_2$  onto which a periodic gold nanoparticle (Au NPs) was deposited ( $\text{SiO}_x/\text{MoS}_2/\text{Au NPs}$ ). The height ( $h = 20 \text{ nm}$ ), width ( $l = 25$ ) and lattice parameter ( $a = 70 \text{ nm}$ ) defined as the closest distance between two adjacent AuNPs is the same in both cases. The input source is placed in the substrate ( $\text{SiO}_x$ ) and the detector in the dielectric, being water ( $n_2 = 1.333$ ).

such as  $\text{MoS}_2$  can furthermore be changed by the presence of resonance cavities and plasmonic nanostructures [16]. In biosensing applications, the gold is not well adapted because of its poor absorption of biomolecules, causing limitations on the sensitivity of the biosensor [23]. As a solution to this limitations, the gold layer is substituted for the gold nanoparticles (AuNPs). Gold nanoparticles have a unique property called localized surface plasmon (LSPR). The AuNPs-based LSPR is widely used for the detection [24]. In addition, the dielectric environment of the Localized surface plasmons resonance (LSPR) has been extensively studied in recent years [25,26] 2D networks nanoparticles of gold (AuNPs). In this work, we theoretically study the impact of the  $\text{MoS}_2$  substrate thickness on the plasmonic signal of gold nanoparticle (AuNPs) arrays (Fig. 1B). Throughout this paper, the geometrical parameters of the AuNPs is fixed with  $l$  is the particles length,  $a$  is the lattice parameter (along  $x$ -axis), and  $h$  is the particles height. It is well established that AuNPs strongly absorb within narrow frequency bands in the visible range as their localized surface plasmon resonances get excited. Besides, the effect of the dielectric environment surrounding the AuNPs has been widely studied [27,28]. A part of this work consists of investigating numerically the influence of  $\text{MoS}_2$  coatings (0–7.15 nm) on the localized surface plasmon resonance signal of AuNPs arrays (Fig. 1A). In the first part, the idea is to highlight the role of a few layers of  $\text{MoS}_2$  as one of the finest collection thickness of layers deposited on  $\text{MoS}_2$  nanostructures. The considered range is from 0 nm to 3.90 nm (strong red shift of the resonance). The layers of the dielectric have been deposited on a substrate of  $\text{SiO}_x$  ( $n_1 = 1.45$ ) over which two types of nanostructures have been investigated. In the second part, numerical simulations of structures  $\text{SiO}_x/\text{AuNPs}/\text{MoS}_2/\text{water}$  and  $\text{SiO}_x/\text{MoS}_2/\text{AuNPs}/\text{water}$  with a normal bias following the  $z$ -axis, show significant sensitivity  $\sim 300$  ( $\text{nm RIU}^{-1}$ ) Fig. 1(A) and  $\sim 171$  ( $\text{nm RIU}^{-1}$ ) Fig. 1(B) for the eight layers  $\text{MoS}_2$  5.20 nm [29–34]. In addition, the plasmonic response of metal nanoparticles with various geometrical parameters gold nanoparticles  $l = 125 \text{ nm}$ ,  $a = 300 \text{ nm}$ , and  $h = 15 \text{ nm}$ . These results are consistent with other reports in the literature showing long row detecting refractive index on plasmonic nanostructures [15,20,22]. The distributions of the electric field structures excited to resonance at normal incidence and represented by the maps of the 2D and 3D electrical fields which indicate that this mode is a localized surface plasmon dipole whose hot spots (areas of high intensities field) are pushed to the top and bottom corners of AuNPs for the structure  $\text{SiO}_x/\text{AuNPs}/\text{MoS}_2/\text{water}$ , and top corners of AuNPs to layer  $\text{MoS}_2$  under the nanoparticles to the structure  $\text{SiO}_x/\text{MoS}_2/\text{AuNPs}/\text{water}$  to the lengths wave resonances ( $\lambda_{max}$ ).

One observes a significant enhancement of the sensitivity of localized surface plasmon resonances of coated AuNPs with layers of  $\text{MoS}_2$  to the surrounding environment as compared to bare nanoparticles. Hence, the design of Au nanoparticles/ $\text{MoS}_2$  based-plasmonic bio-sensors with more sensitive could be reached. Indeed, we show that AuNPs coating with few layers of  $\text{MoS}_2$  leads to approximately a 26% higher sensitivity. The optimal thickness of  $\text{MoS}_2$  layers is numerically investigated to achieve a high LSPR sensitive system.

## 2. Theoretical methods

The optical properties of gold nanoparticles are solved numerically, in the frequency domain, using the scattered field formulation. Field analysis was performed using a commercially available Finite Elements Method (FEM) method package (COMSOL Multiphysics 4.4) [35,36]. The simulation method has been well documented [37–39]. A layer of gold nanoparticles of diameter ( $l$ ), height ( $h$ ) and interparticle distance ( $a$ ), is coated with a  $\text{MoS}_2$  thin-layer and immersed in a homogeneous matrix. A transparent glass of  $\text{SiO}_x$  (refractive index  $n_1 = 1.45$ ) is used as a substrate. The frequency-dependent complex permittivity of metal (gold) is described by the Lorentz–Drude model (Eq. (1)) [40,41].

$$\varepsilon(\omega) = \varepsilon_{r,\infty} + \sum_{m=0}^M \frac{f_m \omega_p^2}{\omega_m^2 - \omega^2 + j\omega\Gamma_m} \quad (1)$$

where  $\varepsilon_{r,\infty}$  is the relative permittivity at infinite frequency,  $\omega_p$  the plasma frequency, and  $\omega_m$ ,  $f_m$  and  $\Gamma_m$  the resonance frequency,

**Table 1**

Gold (Au) Lorentz–Drude model parameters.

Term	$f_m$ (rad/s)	$\omega_p$ (rad/s)	$\omega_m$ (rad/s)	$\Gamma_m$ (rad/s)
$m = 0$	0.760	$13.72 \times 10^{15}$	0.00	$0.08052 \times 10^{15}$
$m = 1$	0.024	$13.72 \times 10^{15}$	$0.6305 \times 10^{15}$	$0.3661 \times 10^{15}$
$m = 2$	0.010	$13.72 \times 10^{15}$	$1.261 \times 10^{15}$	$0.5241 \times 10^{15}$
$m = 3$	0.071	$13.72 \times 10^{15}$	$4.511 \times 10^{15}$	$1.322 \times 10^{15}$
$m = 4$	0.601	$13.72 \times 10^{15}$	$6.538 \times 10^{15}$	$3.789 \times 10^{15}$
$m = 5$	4.384	$13.72 \times 10^{15}$	$20.24 \times 10^{15}$	$3.364 \times 10^{15}$

strength and damping frequency, respectively, of  $m$ th oscillators. The Lorentz–Drude model uses  $M$  damped harmonic oscillators to describe the small resonances observed in the metals frequency response. The values of the constants in Eq. (1) are taken from reference [40], with the value of the dielectric constant of infinite frequencies being  $\epsilon_\infty = 1$ . The values of the other parameters are listed in Table 1:

### 3. Results and discussion

#### 3.1. Localized surface plasmon for periodic nanostructures

The evolution of the localized surface plasmon modes in 2D periodic nanostructures on two different surface architectures are investigated (Fig. 1). The morphology of the periodic gold nanoparticle such as particle diameter ( $D$ ), height ( $h$ ), and period ( $a$ ) is kept the same. The difference between the two structures is the position of the dielectric MoS<sub>2</sub> layer, being either around the Au NPs (Fig. 1A) or below the Au NPs (Fig. 1B). A transparent glass substrate SiO<sub>x</sub> with  $n_1 = 1.45$  is used in both cases and the assembly immersed in a non-absorbing medium such as water ( $n_2 = 1.333$ ).

For the refractive index of MoS<sub>2</sub>, we have used a constant value  $n_{\text{MoS}_2} = 5.9 + i 0.8$  (at 632.8 nm) [16,17], the thickness of the MoS<sub>2</sub> layer being estimated by  $d_{\text{MoS}_2} = N \times 0.65$  nm, where  $N$  is the number of MoS<sub>2</sub> layers, and we have not used the function of the wavelength  $n_{\text{MoS}_2} = \sqrt{\epsilon(\omega)}$  [42], because in our nanostructures the absorption spectra either varies in the thickness of the MoS<sub>2</sub> layer or in the detection refractive index medium. This simulation demonstrates a single peak that varies and the two skins remain fixed. So, in our work we focus on the plasmon resonance of localized surface which changes according to the parameters of nanostructures. In other different computational checks we have noticed that we are using a fixed value of  $n_{\text{MoS}_2}$ .

The LSPR spectrum of a glass/AuNPs interface where the AuNPs parameters were set to a length of 25 nm, a height of 20 nm and a period of 70 nm, shows a plasmon resonance at 525 nm Fig. 2(A). As expected, an increase in the thickness of MoS<sub>2</sub> shifts the peak wavelength maximum  $\lambda_{\text{max}}$  to the red, from  $\lambda_{\text{max}} = 538$  nm for  $d_{\text{MoS}_2} = 0.65$  nm (monolayer) to  $\lambda_{\text{max}} = 611$  nm for  $d_{\text{MoS}_2} = 3.90$  nm (six layers). In addition, the presence of MoS<sub>2</sub> results in a considerable increase in the overall absorption intensity in the near-infrared Fig. 2(B). It also seems that some additional badly defined bands are occurring in the presence of MoS<sub>2</sub> thicknesses above 1.3 nm.

In Fig. 2B, we have plotted the evolution of the plasmon resonance wavelength in relation to the thickness of the dielectric layer MoS<sub>2</sub> calculated for interfaces SiO<sub>2</sub>/AuNPs/MoS<sub>2</sub>/water. Was found that an increase in the thickness of MoS<sub>2</sub> ( $d_{\text{MoS}_2}$ ) shifts the peak wavelength ( $\lambda_{\text{max}}$ ) to red almost linearly from  $\lambda_{\text{max}} = 538.21$  nm for  $d_{\text{MoS}_2} = 0.65$  nm up to  $\lambda_{\text{max}} = 611.25$  nm for  $d_{\text{MoS}_2} = 3.90$  nm, due to the interaction of AuNPs/MoS<sub>2</sub> with a normal incident light pulse.

In the case of MoS<sub>2</sub> present on the glass interface rather than the Au NPs (Fig. 1(B)), the plasmonic behavior is rather different. With increasing MoS<sub>2</sub> thickness, next to a band at 525 nm, a second strongly absorbing plasmon band is observed and shifts to higher wavelength with increase of the thickness of MoS<sub>2</sub> Fig. 2(C).

For the structure SiO<sub>x</sub>/MoS<sub>2</sub>/AuNPs Fig. 2(C), we observe that we add the MoS<sub>2</sub> layer between the substrate and the AuNPs, the refractive index of medium under the nanoparticles increase SiO<sub>x</sub> ( $n_1 = 1.45$ ) <  $n_2$  to SiO<sub>x</sub>/MoS<sub>2</sub> ( $n_{\text{MoS}_2} = 5.9 + 0.8i$ ) >  $n_2$  leads to an increase in the resonant wavelength rapidly, an enlargement of the plasmon band, as well as the appearance of a multimodal response [43]. The evolution of the amplitude of the oscillations thus seems to result from the competition between several phenomena. Two of them help to reduce the amplitude of the oscillations when  $n_1/n_{\text{MoS}_2}$  becomes larger than the detection medium refractive index. This is the decrease in the contrast of the standing wave system inside the cavity on the AuNPs, and the appearance of a second peak plasmonic response (multimodal). The last phenomenon is the increase of the spectral width of the main plasmonic mode with the increase in the thickness of the MoS<sub>2</sub> layer, which tends to increase the amplitude of surface plasmon oscillations.

The position of the resonant wavelength plasmon  $\lambda_{\text{max}}$  shifts almost linearly with the increase of MoS<sub>2</sub> thickness to  $\lambda_{\text{max}} = 865$  nm for ( $d_{\text{MoS}_2}$ ) = 3.90 nm Fig. 2(D). In contrast to glass/AuNPs/MoS<sub>2</sub>, the position of  $\lambda_{\text{max}}$  is unchanged for glass/MoS<sub>2</sub>/AuNPs interface when changing the refractive index of the immersion medium (from  $n_2 = 1$  to  $n_2 = 1.45$ ) Fig. 3. In the case of glass/AuNPs/MoS<sub>2</sub>, a shift is observed for all thicknesses of MoS<sub>2</sub>.

The influence of refractive index at the interface of the structure SiO<sub>x</sub>/AuNPs/MoS<sub>2</sub> was investigated by recording the wavelength shift when it is changed. In different proportions giving refractive indices ( $n_2 = 1.333$  for water, 1 for air and 1.45 SiO<sub>x</sub>), the response of the absorption spectrum of LSPR is generally described in Fig. 3(A). It shows that the position of  $\lambda_{\text{max}}$  moves the higher wavelength 530 nm (air) 542 nm (SiO<sub>x</sub>) to a layer of MoS<sub>2</sub> (0.65 nm) while increasing the refractive index of the detection medium [44,45]. For the SiO<sub>x</sub>/MoS<sub>2</sub>/AuNPs structure, conservation  $\lambda_{\text{max}}$  has been observed for the change in refractive index ( $n_2 = 1, 1.333$  and 1.45) Fig. 3(B), followed by a very large red shift of the length wave between  $0.65 \text{ nm} \leq d_{\text{MoS}_2} \leq 3.90$  nm.

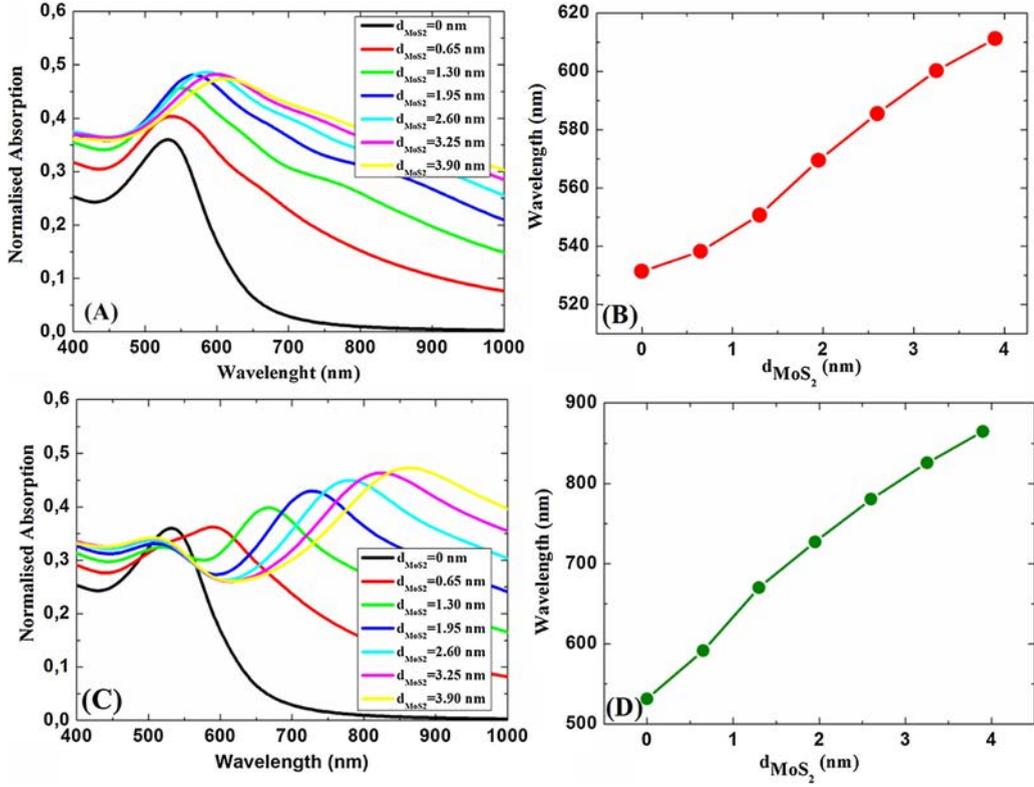


Fig. 2. (A) Variation in of absorption spectrum of the glass/Au NPs/MoS<sub>2</sub> interface (Fig. 1A) as a function of the thickness of MoS<sub>2</sub> ( $d_{\text{MoS}_2} = 0\text{--}3.9\text{ nm}$ ) when immersed in water. (B) Evolution of the position of the LSPR band as a function of the thickness of the MoS<sub>2</sub> coating; (C) Variation in of absorption spectrum of a glass/MoS<sub>2</sub>/Au NPs interface (Fig. 1B) as a function of the thickness of MoS<sub>2</sub> ( $d_{\text{MoS}_2} = 0\text{--}3.9\text{ nm}$ ) when immersed in water; (D) Evolution of the position of the LSPR band as a function of the thickness of the MoS<sub>2</sub> underlying coating.

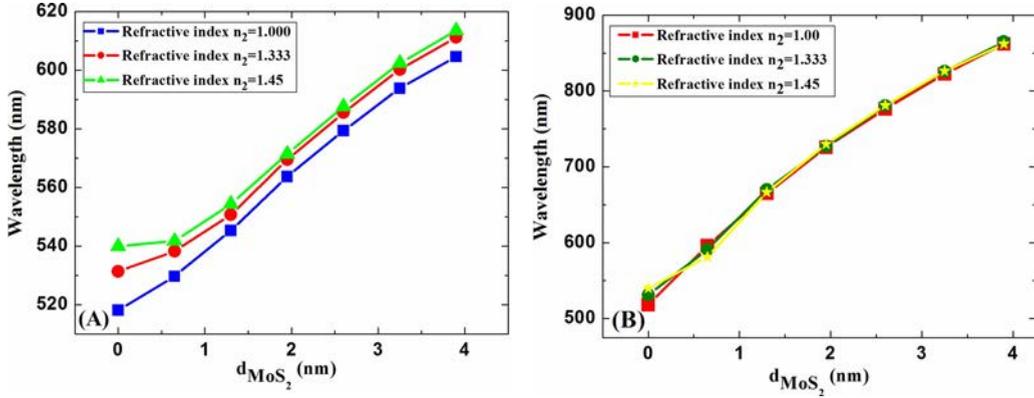
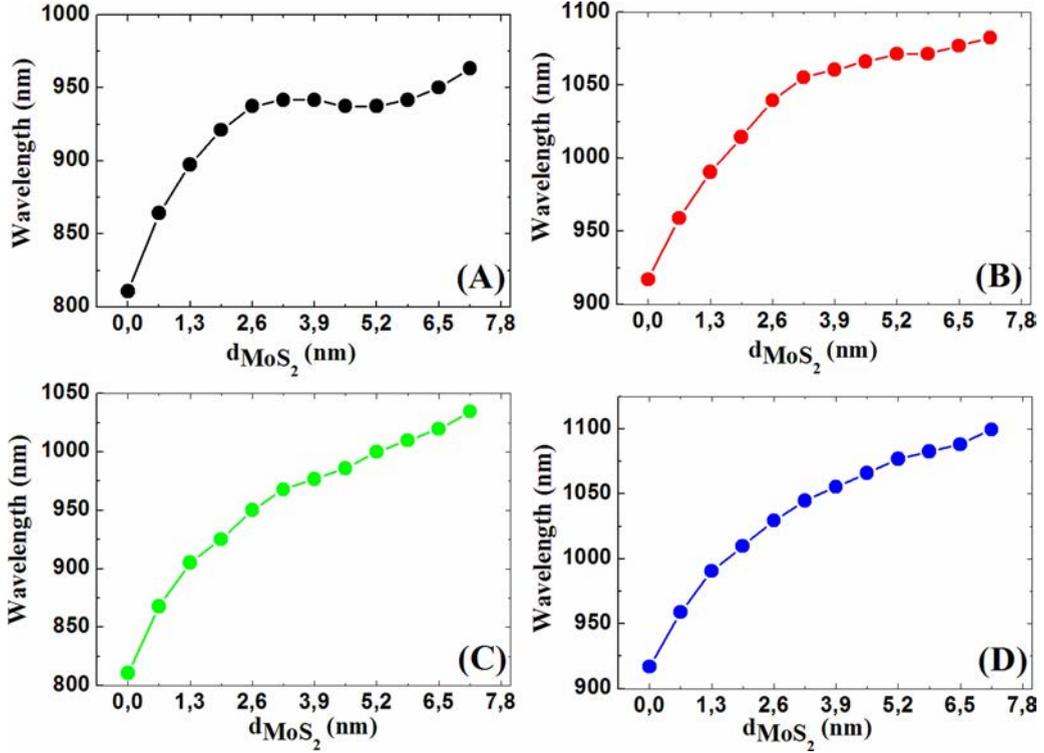


Fig. 3. Evolution of  $\lambda_{\text{max}}$  with the thickness of the overcoat MoS<sub>2</sub>, comparison upon change of the refractive index of the surrounding medium: (A) for structure "Fig. 1(A)", air (blue square), water (red circle) and SiO<sub>x</sub>(green triangle). (B) for structure "Fig. 1(B)", air (red square), water (olive circle) and SiO<sub>x</sub> (yellow star). The nanoparticles are characterized by  $l = 25\text{ nm}$ ,  $h = 20\text{ nm}$  and  $a = 70\text{ nm}$ . The refractive index of the substrate on which they are deposited is  $n_1 = 1.45$ . (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

In the purpose of comparing the absorption spectrum of results calculated with the model of L–D by the FEM method (for  $0.65\text{ nm} \leq d_{\text{MoS}_2} \leq 3.90\text{ nm}$  thickness of MoS<sub>2</sub> layer) are structures that were studied in Fig. 2. Which shows the evolution of the normalized absorption resonance wavelength of the two structures according thick MoS<sub>2</sub>, after the interaction of the studs with a light pulse incident [400–1000 nm]. The parameter values selected structures are:  $l = 25\text{ nm}$ ,  $a = 70\text{ nm}$  and  $h = 20\text{ nm}$ . Giving the structure SiO<sub>x</sub>/MoS<sub>2</sub>/AuNPs/water a very significant growth of the resonance wavelength of 333.7 nm plasmon which passes from 531.35 nm to 865.05 nm (Fig. 2B). Relative that obtained in the structure SiO<sub>x</sub>/AuNPs/MoS<sub>2</sub>/water we see dramatic growth of the



**Fig. 4.** Evolution of  $\lambda_{max}$  with the thickness of the overcoat  $\text{MoS}_2$  comparison of different refractive index of the medium surrounding structure (Fig. 1(A)), (A) air  $n_2 = 1.000$  and (B)  $\text{SiO}_x$   $n_2 = 1.45$ . Comparison with the structure (Fig. 1(B)), (C) air  $n_2 = 1.000$ ), and (D) and  $\text{SiO}_x$   $n_2 = 1.45$ . The nanoparticles are characterized by  $l = 125$  nm,  $h = 15$  nm and  $a = 300$  nm. The refractive index of the substrate on which they are deposited is  $n_1 = 1.45$ .

resonance wavelength of the plasmon studs which pass 538.21–611.25 nm (Fig. 2D), with an offset of 73.04 nm to the red. The change in position of  $\lambda_{max}$ , shows a linear dependence as a function of the thickness of the surrounding environment. Fig. 3(B) shows the influence of the refractive index of the detection medium on the plasmon response of the system studied. Contrary to what has been observed in Fig. 3(A),  $\lambda_{max}$  presents a spectral shift to red when the nanoparticles are started to be covered for deferments  $n_2$  media.

It was investigated by recording that the wavelength shifts when it is changed, in small proportions giving 518.13 nm for air, 531.35 nm for water and 539.96 nm for  $\text{SiO}_x$  at  $d_{\text{MoS}_2} = 0$  nm, with the sensitivity of  $S = 39.68$  nm/RIU, and 776.40 nm for air, 780.49 nm for water and 781.25 nm for  $\text{SiO}_x$  at  $d_{\text{MoS}_2} = 2.60$  nm with the sensitivity  $S = 12.28$  nm/RIU. It is found that the sensitivity, like the resonance wavelength, shows a weak oscillation when  $n_2$  increases. The studied system thus has a non-zero sensitivity, but this is small and always less than the sensitivity of the nanoparticles covered by  $\text{MoS}_2$ , for the  $n_2$  values to be considered. Indeed, for  $n_2 = 1.000$ , 1.333 and 1.45, Almost a small variation of the resonance wavelength is observed. Moreover, for the thickness of  $\text{MoS}_2$  increases, the resonance wavelength is shifted towards the red as Fig. 3B. These behavioral differences are simply due to the way the refractive index ( $n_2$ ) by the nanoparticles varies and geometrical parameters Au nanoparticles. Fig. 4, it is deduced that whatever the value of  $n_2$ , and for large geometrical parameters of the structure  $l = 125$  nm  $a = 300$  nm and  $h = 15$  nm, the sensitivity and the resonance wavelength of the structures studied are presented extremely for the same thicknesses of  $d_{\text{MoS}_2}$ . Note also that the sensitivity and the resonance wavelength oscillate as a function of  $d_{\text{MoS}_2}$ . However, it is now known that the value of the refractive index of the detection medium ( $n_2$ ) and the geometric characteristics of the nanoparticles have an impact on the displacement of LSPR and the sensitivity. Moreover, it can be deduced that the sensitivity is oscillated for two reasons. On the one hand, the fact of depositing the layer of  $\text{MoS}_2$  under the nanoparticles is detrimental to the sensitivity, and causes a decrease in the latter for the thicknesses of  $d_{\text{MoS}_2}$  (0.65–7.15 nm). On the other hand, the refractive index of the dielectric covering the nanoparticles ( $n_2$ ) is lower than the refractive index of the medium which deposits the AuNPs ( $n_1 = 1.45/n_{\text{MoS}_2} = 5.9 + 0.8i$ ), and the geometric parameters of system, that's what we can check in Fig. 4 and Table 2.

This variation in the effect of geometric parameters of gold nanoparticles leads to the increase of detection optic properties. Increasing the geometric parameters of the AuNPs first generates an increase in the wavelength of plasmon resonance. The increase in  $\lambda_{max}$  is consistent with the evolution of the electric field contact within the gold nanoparticles. These results are consistent with other reports in the literature showing long row detecting refractive index on the plasmonic nanostructures [46] have studied these effects, which show a linear dependence as a function of the refractive index of the surrounding medium.

The refractive index sensitivity, defined as the ratio of the variation of the position of the plasmon band during the variation of the

**Table 2**

Comparison of the evolution of sensitivity acquired theoretically for glass/AuNPs/MoS<sub>2</sub> and glass/MoS<sub>2</sub>/AuNPs. The nanoparticles are characterized by  $l = 125$  nm,  $h = 15$  nm and  $\alpha = 300$  nm. The refractive index of the substrate on which they are deposited is  $n_1 = 1.45$ .

	MoS <sub>2</sub>	Thickness (nm)	Sensitivity (nm/RIU)
Glass/AuNPs/MoS <sub>2</sub>	0	–	236.04
	1	0.65	210.46
	2	1.30	206.95
	3	1.95	207.64
	4	2.60	226.90
	5	3.25	252.38
	6	3.90	264.23
	7	4.55	285.53
	8	5.20	297.62
	9	5.85	288.28
	10	6.50	281.55
Glass/MoS <sub>2</sub> /AuNPs	11	7.15	264.82
	0	–	236.04
	1	0.65	202.52
	2	1.30	189.76
	3	1.95	187.79
	4	2.60	175.97
	5	3.25	171.19
	6	3.90	174.51
	7	4.55	177.94
	8	5.20	170.94
	9	5.85	161.91
10	6.50	152.59	
11	7.15	144.43	

refractive index (Eq. (2)) and determinable from the slop of a quasi-linear plot of  $\lambda_{max}$  vs.  $n_2$  [47].

$$S = \frac{\Delta\lambda_{max}}{\Delta n_2} \text{ (nm RIU}^{-1}\text{)} \quad (2)$$

Of both interfaces us shown in Table 2. Two circles used to determine the sensitivity for the same interface indexes in the  $n_2 = 1.45$  material and air  $n_2 = 1$  ( $\Delta n_2 = 0.45$ ).

Fig. 4, shows the change of  $\lambda_{max}$  with the refractive index of different dielectrics used to put some dielectric layers (MoS<sub>2</sub>) and gold nanostructures.

Several numerical simulations were done to find out how changing the sensitivity depend on the thickness of MoS<sub>2</sub> filed on nanoparticles (AuNPs/MoS<sub>2</sub>) or between the substrate and the nanoparticles (MoS<sub>2</sub>/AuNPs).

These results are in agreement with other reports, in the field of study, showing long rank refractive index of detection of plasmonic nanostructures [46] Table 1, exposes this evolution of sensitivity according to the layer thickness of MoS<sub>2</sub>.

We have initially determined the sensitivity of the system described in Fig. 1, without the thickness of MoS<sub>2</sub> ( $d_{MoS_2} = 0$  nm) above or below the gold nanoparticles. The wavelength of resonance of such a system is  $\lambda_{max} = 810.81$  nm for  $n_2 = 1.000$  and  $\lambda_{max} = 917.03$  nm for  $n_2 = 1.45$ , we find  $S = 236.04$  nm/RIU.

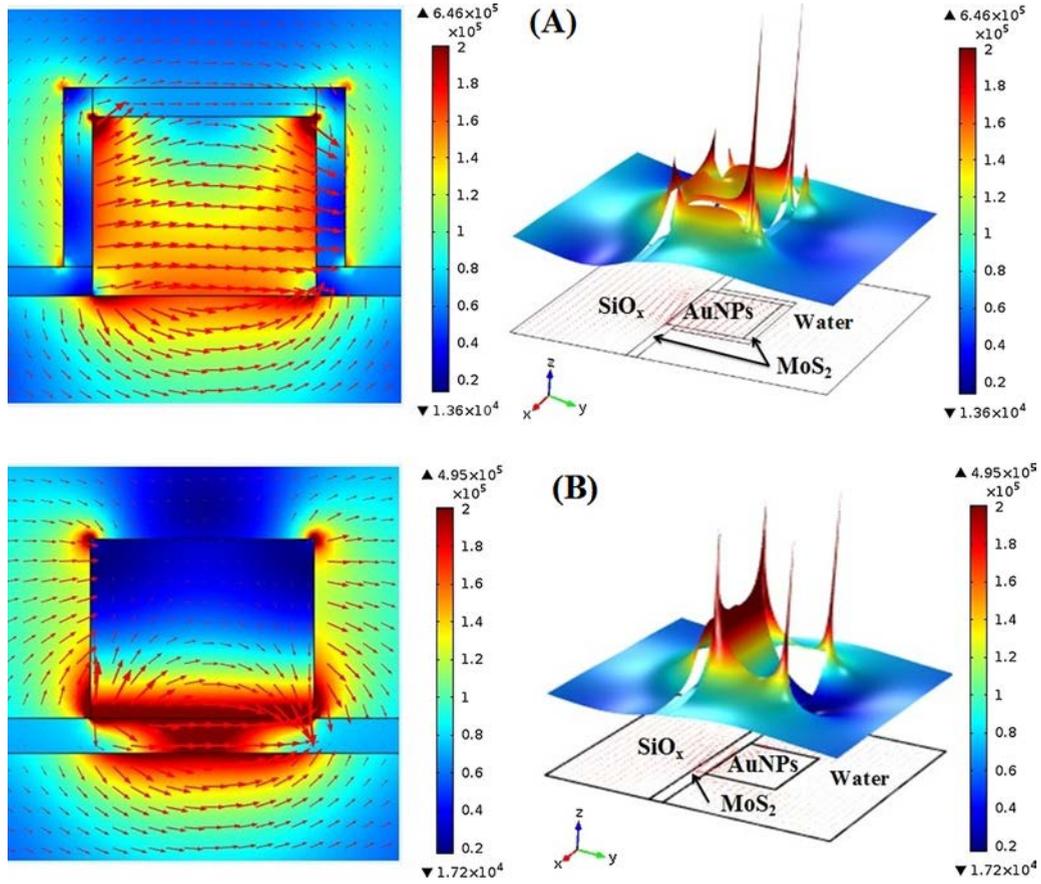
On the other hand, for ( $d_{MoS_2}$ ), either when the nanoparticles are covered by different MoS<sub>2</sub> slips or when the nanoparticles are covered with 8 layers of MoS<sub>2</sub> ( $d_{MoS_2} = 5.20$  nm), the resonance wavelength is  $\lambda_{max} = 937.5$  nm for  $n_2 = 1.000$  and  $\lambda_{max} = 1071.43$  nm for  $n_2 = 1.45$ , which corresponds to a sensitivity of  $S = 297.62$  nm/RIU.

For a thickness of MoS<sub>2</sub> (from 0.65 to 7.15 nm) we vary in sensitivity by changing the thickness of MoS<sub>2</sub>. We find that the sensitivity is proportional to the thickness of MoS<sub>2</sub>. First of all, there has been an increase in sensitivity (glass/AuNPs/MoS<sub>2</sub>) for thicknesses of MoS<sub>2</sub> between 1.95 and 5.20 nm. Indeed,  $S = 206.95$  nm/RIU for 2 layers (1.30 nm) and  $S = 297.62$  nm/RIU to 5.20 nm, after we noticed a decrease in sensitivity from thickness 9 layers (5.85 nm).

Indeed, the sensitivity that corresponds to the structure (Fig. 1B) is decreasing when the thickness of the layer of MoS<sub>2</sub> diminished,  $S = 202.52$  nm/RIU for  $d_{MoS_2} = 0.65$  nm at  $S = 144.43$  nm/RIU for  $d_{MoS_2} = 7.15$  nm [20,22,48,49]. The enhancement of sensitivity for the AuNPs/MoS<sub>2</sub> based LSPR biosensor is calculated to have more than 26% of when compared the sensors LSPR conventional without the layer of MoS<sub>2</sub>, with the same parameters of AuNPs. These characteristics should make these biosensors a preferred choice for bio-detection applications, compared to other contemporary biosensors.

### 3.2. Influence of dielectric MoS<sub>2</sub> on the distribution of electric field

The sensitivity of the interface can be understood from the electrical field maps in Fig. 5 shows the distribution of the electric field to the resonance near nanoparticles. It can be seen by comparing Fig. 5(A) that when the nanoparticles (Au NPs) are covered with MoS<sub>2</sub> a substantial part of the field is found inside of the latter. In the case of MoS<sub>2</sub> coated glass Fig. 5(B) that when the nanoparticles covered with a non-absorbing dielectric (water) the field spreads out more and more deeply into the substrate as that its refractive



**Fig. 5.** Electric field maps on (A) glass/AuNPs/MoS<sub>2</sub> for  $d_{\text{MoS}_2} = 2.60$  nm under monochromatic incident radiation at 585 nm; (B) glass/MoS<sub>2</sub>/AuNPs for  $d_{\text{MoS}_2} = 3.90$  nm under monochromatic incident radiation at 865 nm.

index increases (MoS<sub>2</sub>).

Maps of calculated electric field Fig. 5(A) to the resonance wavelength plasmon  $\lambda_{\text{max}} = 585.48$  nm for  $d_{\text{MoS}_2} = 2.60$  nm show a strong improvement of the field located on the four corners of the nanoparticles within the confined field. The corners of AuNPs with strong localization at the upper corners of AuNPs compared to the structure of Fig. 5(B) calculated at the resonant wavelength plasmon  $\lambda_{\text{max}} = 865.05$  nm  $d_{\text{MoS}_2} = 3.90$  nm a strong localization is observed at the upper corners and at the lower surface of the AuNPs in contact with the layer of MoS<sub>2</sub> [50–52]. It is thus seen in Fig. 5(B), that in the MoS<sub>2</sub> nanoparticles, the present two hotspots electric field at the upper corners of AuNPs and the surface in contact with the substrate. In addition, Fig. 5(A) shows that the nanoparticles coated with 2.60 nm of MoS<sub>2</sub> have hot spots in each of their corners, and the two hot spots in contact with the substrate have spread spatially. Furthermore, the addition of MoS<sub>2</sub> led to an increase of the amplitude of the electric field in both sides of AuNPs in contact with this medium recouvrement.

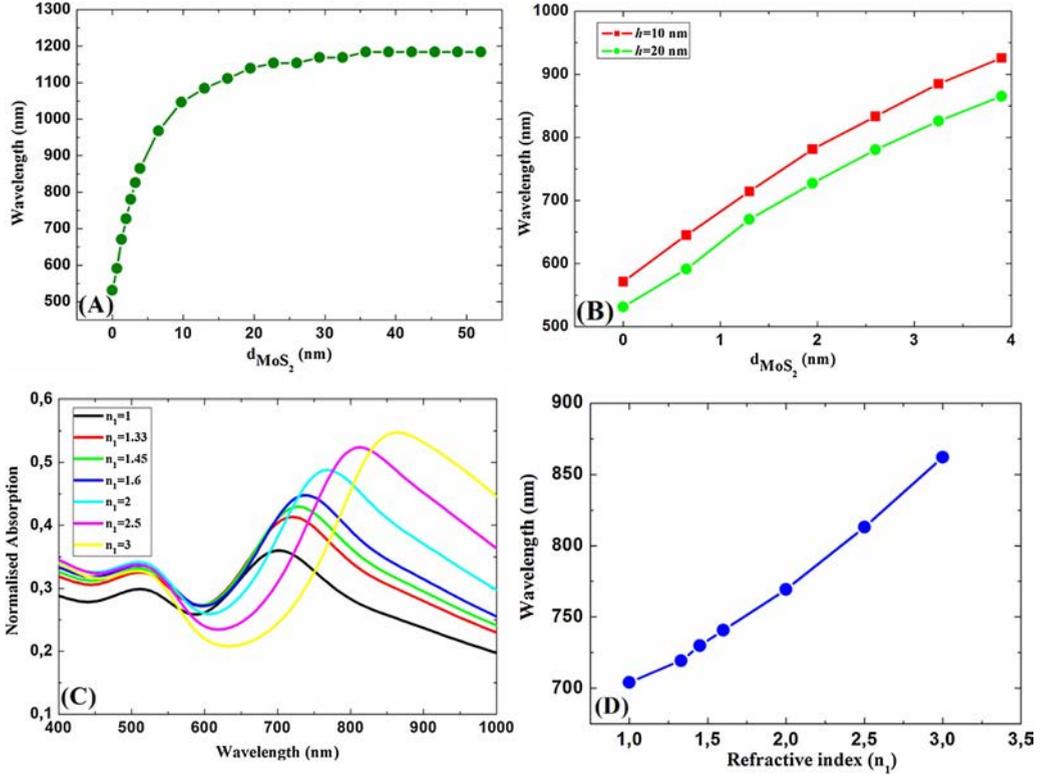
Fig. 6 shows the change in the resonance wavelength depending on the thickness of  $d_{\text{MoS}_2}$  MoS<sub>2</sub> layers deposited below the gold nanoparticles to study the structure SiO<sub>x</sub>/MoS<sub>2</sub>/AuNPs/water, The effect of the allowance index of dielectric substrate.

Fig. 6(A) shows the change in resonance wavelength as a function of the thickness  $d_{\text{MoS}_2}$ , studied for the structure SiO<sub>x</sub>/MoS<sub>2</sub>/AuNPs/water. It is found that the  $\lambda_{\text{max}}$  of shift for the same detection medium is different  $d_{\text{MoS}_2}$  value from 0 to 50 nm. Fig. 6(A) shows the influence of the thickness of the dielectric layer on the plasmonic response of the system studied SiO<sub>x</sub>/MoS<sub>2</sub>/AuNPs/water. Indeed, the resonant wavelength is not shifted towards the red but remains constant. It is recalled that the refractive index of the substrate is  $n_1 = 1.45$  (SiO<sub>x</sub>), and which covers the nanoparticles with a dielectric having a refractive index  $n_2 = 1$  (water). For the variation of the thickness of MoS<sub>2</sub> from 0 to 19.25 nm resonance wavelength plasmon red-shifted from 531.35 nm to 1168.83 nm. Then from  $d_{\text{MoS}_2} = 29.25$  nm, there is almost no variation observed in the resonant wavelength LSPR.

Fig. 6(B) shows that the resonant wavelength plasmon increases when the height decreases,  $\lambda_{\text{max}} = 531.3$  nm for  $h = 20$  nm and  $\lambda_{\text{max}} = 571.4$  nm for  $h = 10$  nm to  $d_{\text{MoS}_2} = 0$  nm, and  $\lambda_{\text{max}} = 865$  nm for  $h = 20$  nm and  $\lambda_{\text{max}} = 926$  nm for  $h = 10$  nm to six layers of MoS<sub>2</sub>  $d_{\text{MoS}_2} = 3.90$  nm. This red shift of LSPR when the height ( $h$ ) decreases when  $d_{\text{MoS}_2}$  remains constant increases, is varied from 40 to 60 nm.

This is what highlights Fig. 6. We can see the evolution of the position of resonance, when the dielectric substrate of refractive index changes to the value of  $d_{\text{MoS}_2} = 1.95$  nm distinct.

As before, we mapped the absorption spectra of the studied MoS<sub>2</sub>/AuNPs system for  $d_{\text{MoS}_2} = 1.95$  nm (3 layers of MoS<sub>2</sub>), in order



**Fig. 6.** (A) Evolution of LSPR peak with change in thickness of the layer of  $\text{MoS}_2$  ( $d_{\text{MoS}_2}$ ) of the structure (Fig. 1B)  $\text{SiO}_x/\text{MoS}_2/\text{AuNPs}/\text{water}$ , for  $a = 70$  nm,  $l = 25$  nm and  $h = 20$  nm. (B) Evolution of  $\lambda_{\text{max}}$  with the thickness of the overlay  $\text{MoS}_2$  ( $\text{SiO}_x/\text{MoS}_2/\text{AuNPs}/\text{water}$ ) to compare two values of the height ( $h$ ) of gold nanoparticles ( $h = 10$  nm red square) and ( $h = 20$  nm green circle), the other parameters are  $a = 70$  nm,  $l = 25$  nm. (C) Absorption spectrum corresponding to the structure substrate/ $\text{MoS}_2/\text{AuNPs}/\text{water}$  for defeated refractive index of the substrate. (D) Change in the resonant wavelength in plasmon function of refractive index of the dielectric substrate. The geometric parameters of the gold nanoparticles are:  $l = 25$  nm,  $h = 20$  nm,  $a = 70$  nm and  $d_{\text{MoS}_2} = 1.95$  nm. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

to analyze the influence of  $n_1$  on the plasmonic response of the nanoparticles (see Fig. 6(C)). It appears, similar to what was found for Fig. 2(C), that the growth of the amplitude of absorption spectra when  $n_1$  increases, coincides with the appearance of new modes of plasmonic resonance in addition to the main mode [21,43]. This is what highlights Fig. 6. We can see the evolution of the position of resonance, when the dielectric substrate of refractive index changes to the value of  $d_{\text{MoS}_2} = 1.95$  nm distinct. In Fig. 6(C), one can verify that  $\lambda_{\text{max}}$  is red-shifted when the substrate refractive index increases, it therefore becomes independent from you the value of the refractive index of the substrate.

Moreover, Fig. 6(D) depicts the change in the localised surface plasmonic resonance ( $\lambda_{\text{max}}$ ) with the substrate refractive index, there is a very significant linear increase  $\lambda_{\text{max}} = 704.23$  nm to  $\lambda_{\text{max}} = 862$  nm, with an amplitude of 0.36–0.55 calculated for the substrate refractive index increases from  $n_1 = 1$  to  $n_1 = 3$ . This observation is important to search for a plasmonic sensor to optimal properties.

#### 4. Conclusion

We have theoretically studied the optical properties of the influence of the dielectric film with  $\text{MoS}_2$  nanoparticles of gold structure on plasmonic properties and sensitivity. The Lorentz–Drude model was used to calculate the optical signal of localized surface plasmon resonance (LSPR) gold nanostructures  $\text{SiO}_x/\text{AuNPs}/\text{MoS}_2/\text{water}$  and  $\text{SiO}_x/\text{MoS}_2/\text{AuNPs}/\text{water}$ ; this study provides a better understanding resonance coupled to systems based on gold nanoparticles and  $\text{MoS}_2$  layers. Due to this research put into the development of the surface plasmon functionalization of hybrid interfaces applications. Developing several sensing components, the offset to the wavelength of red, localization of the electric field and sensitivity of the interface hybrid of the LSPR depends on thickness of the  $\text{MoS}_2$  layer. A general conclusion can be drawn that the interest in these multilayer interfaces is the possibility of sensitive long detection range with important implications for biological detection studies.

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