

# Refractometric sensing with plasmon resonances in dimer, trimer and quadrumer ensembles of gold nanoparticles

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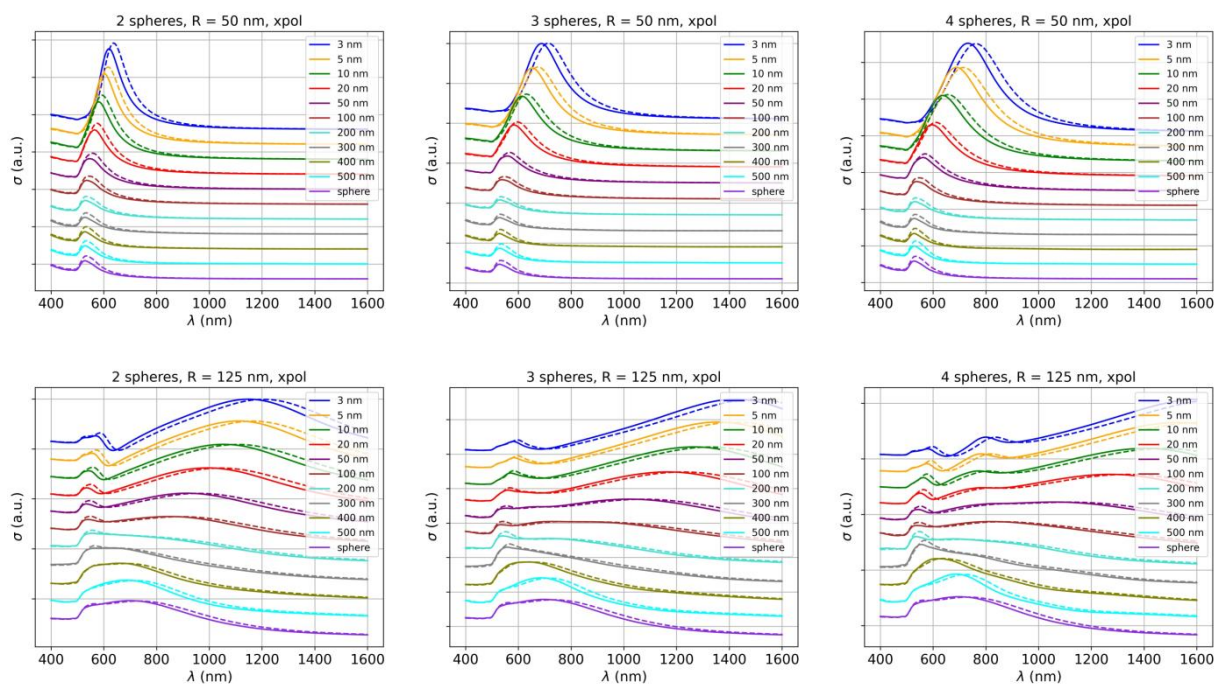
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**Abstract.** We studied by FDTD computer simulations the dependence of the surface plasmon resonances in linearly arranged gold nanospheres on incident light polarization, spheres number and diameter, and interparticle gap. The observed scattering spectra of large particles show a particularly interesting behaviour, with coupled plasmon resonances that can be either red or blue shifting with the modification of the interparticle gap. The sensitivity of the various observed coupled plasmon modes to refractive index variations is then evaluated.

## 1 Introduction

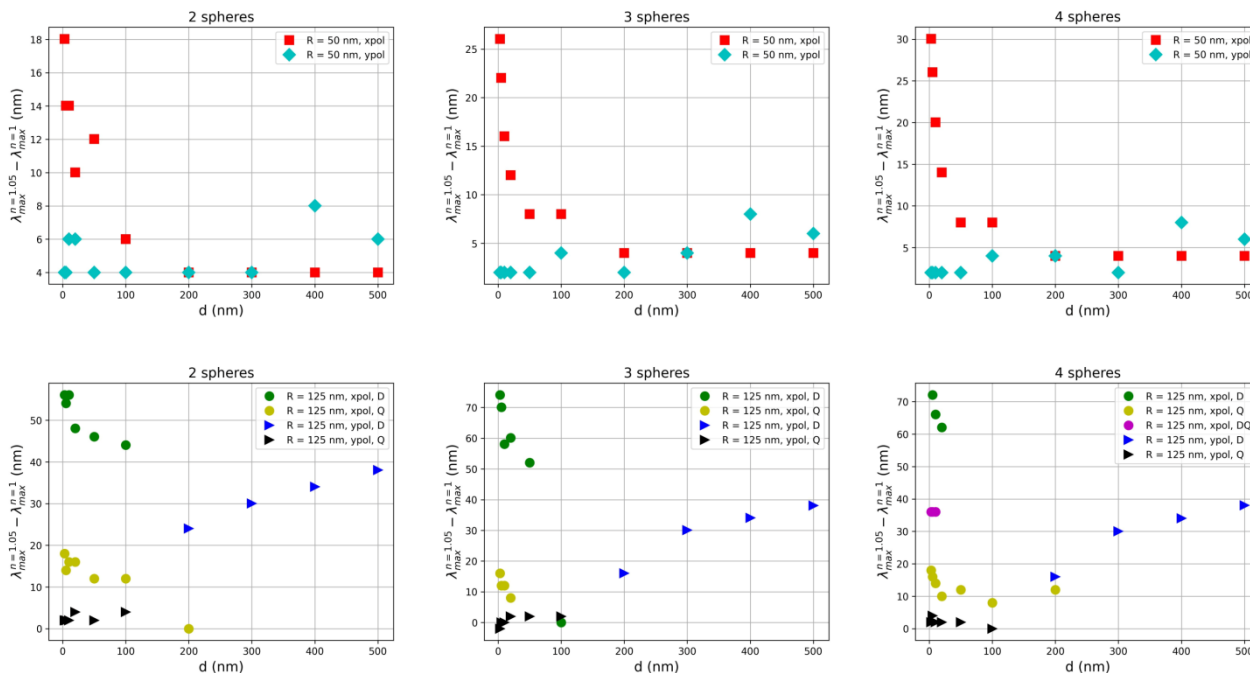
Local plasmon resonances are the result of the interaction between electromagnetic radiation and free conduction electrons in a nanoparticle (NP), which results in plasmonic oscillations at a frequency dependent on the composition, size, geometry, dielectric environment and interparticle gaps between NPs [1]. In this work we analyzed the optical response of dimers, trimers and quadrumer of gold nanospheres arranged in a linear fashion for different polarization of the incident

light, for different sized NPs with varied interparticle distance and for different refractive index of the surrounding medium. Our final goal is to develop potential new plasmon enhanced optical spectroscopy applications based on the active tuning of plasmonic resonances by mechanically actuating the interparticle distance for example. Active tuning of plasmonic resonances, by altering one or more of the parameters mentioned above, remains of great interest [2-4] in the view of developing potential new



**Fig. 1** Scattering spectra of gold single spheres, dimers, trimers and quadrumer for an incoming radiation polarized along the x direction and for medium-sized ( $R = 50$  nm) and large ( $R = 125$  nm) nanospheres. The solid lines correspond to a medium with a refractive index 1.00, while the dashed lines to a medium of refractive index 1.05. The legend shows the interparticle gap corresponding to each spectrum and the spectra for a single sphere, respectively.

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**Fig. 2** Difference of the maxima of the scattering spectra for different refractive indices. The results are shown for  $R = 50, 125$  nm and for x and y polarization of the incident radiation and for dipole (D) and quadrupole (Q) interactions.

sensing applications.

## 2 Methods and results

We performed Finite Difference Time Domain (FDTD) simulations in Ansys Lumerical software, for dimers, trimers and quadrumers aligned along the x direction of the simulation box. We analyzed the scattering spectra for linearly polarized light along the x and y directions, respectively, using a Total Field-Scattered Field method. The optical response was analyzed for three different sized particles with radii  $R = 10, 50$  and  $125$  nm, respectively. The interparticle distance was varied in the 3-500 nm range and the optical response was recorded for two, slightly different refractive indices of the surrounding medium:  $n = 1$  and  $1.05$ . In Fig. 1 we show partial results for x polarized light and only for  $R = 50$  and  $125$  nm radius and ensembles of two, three and four nanospheres. For smaller spheres we observe a dipole mode interaction (D) and a corresponding resonance maximum, which red-shifts for decreasing interparticle distance. As the number of spheres increases, this shift becomes more pronounced. We also observe an important shift due to the change in the refractive index of the medium. Although the difference in the refractive index amounts only to  $0.05$ , the observed difference between the maxima corresponding to different refractive indices effect is clearly observable and it increases with the number of spheres involved. For larger spheres, beside the dipole interaction, which again red-shifts, we observe maxima at shorter wavelengths corresponding to a quadrupole (Q) interaction and in the case of quadrumers there is also an intermediate maximum (DQ) at small interparticle gaps. In Fig. 2 we show the shift of the maxima induced by the refractive

index change as a function of the interparticle gap. Here we also plotted the results for an incident radiation polarized along the y direction. These results show that for larger spheres there is a strong coupling between the spheres also for y polarized light at large and intermediate distances, where the resonance maxima blue shifts and the difference between the maxima in different refractive index media is also decreasing with smaller interparticle gaps.

## Acknowledgements

This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS-UEFISCDI, project number PN-III-P4-ID-PCE-2020-1607, within PNCIDI III. I.T acknowledges support from MCID through the "Nucleu" Program within the National Plan for Research, Development and Innovation 2022-2027, project PN 23 24 01 02.

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