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# A numerical study of plasmon-induced enhancement of dipole emission by arrays of silver nanospheres and nanoprisms

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**Abstract.** Plasmon-induced enhancement of the photoluminescence (PL) intensity of quantum emitters by plasmon nanoparticles (PNPs) is a promising approach for the design and fabrication of PL hybrid materials with improved properties for biosensing and optoelectronics applications. This enhancement can be achieved through careful selection of such parameters as the PNP's shape, material, size, the type of the medium around them, as well as the excitation and emission wavelengths of the emitter. Here, we simulated the nano-hybrid materials based on arrays of silver nanospheres, nanoprisms, and their combinations, located on polymer films with embedded dipole emitters. For these systems, the Purcell effect, as well as the excitation enhancement, transmittance, and absorption were evaluated. The results show the way to improve the PL properties of thin hybrid films by careful design of their composition using developed models.

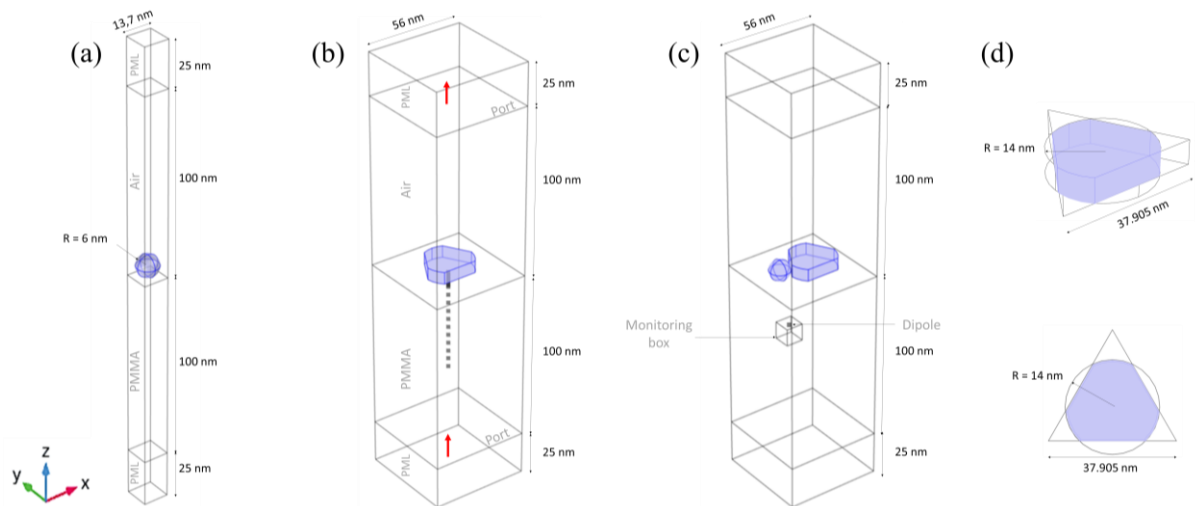
## 1. Introduction

Plasmon metal nanoparticles (PNPs) have been demonstrated to enhance the photoluminescence (PL) of fluorophores due to the effects of light-matter coupling [1]. Under the interaction with electromagnetic radiation at the PNP resonance frequency, the localized electromagnetic field is enhanced specifically in the vicinity of the PNP surface, in so-called "hot spots" [2]. However, the local PL enhancement is limited by the losses inherent to the high nonradiative relaxation rates for plasmons, which leads to a reduction in the PL quantum yield (QY) of the plasmon-emitter system. Therefore, to achieve a large PL QY enhancement, local field and radiative rate enhancements need to be optimized while minimizing non-radiative losses. One of the ways to improve the PL QY is the realization of the Purcell effect when the emission wavelength of an emitter is in resonance with the plasmon band of PNPs. This effect leads to an increase in the radiative rate of the emitter and a corresponding increase in the PL QY. Thus, a plasmon-induced enhancement of a dipole could be maximized when the nanoparticle should be able to couple with the emitter at both excitation and emission wavelength. Numerical studies are important to optimize designs and understand what properties and arrangements are optimal for the enhancement [3]. Here we presented a set of simulations of dipole emission enhancement induced by PNP arrays of silver nanospheres and/or nanoprisms. The PL properties were evaluated for each PNP type and for their combinations to show the contribution of both nanoparticles in the dipole emission enhancement.



## 2. Finite element simulation

Infinite arrays were simulated with silver nanospheres and nanoprisms using the COMSOL Multiphysics software package using the Radio Frequency module. The dimensions of each PNP were verified by calculating the extinction spectrum in water using a spherical perfect matching layer (PML). The radius of the nanosphere was chosen in concordance with the calculations made for the diameter distribution of nanospheres reported previously [2, 4]. Afterward, the PNPs were simulated inside a unit cell with dimensions shown in Figure 1. These dimensions were established by calculating the transmittance for each nanoparticle. The materials used for the models were silver, air, and polymethyl methacrylate (PMMA). Refractive indexes of the silver and PMMA were taken from the references [5] and [6], respectively.



**Figure 1.** The geometries of the calculation models. (a) The unit cell for the array of the nanospheres; (b) the unit cell for the array of the nanoprisms showing the points of the intensity measurements; (c) the unit cell for a combination of the nanosphere and nanoprism showing the “monitoring” box for measuring the dipole intensity; (d) geometry of the nanoprism.

### 2.1. Interaction of emitter with an external electric field

In order to analyze the plasmon-induced enhancement of a dipole, measurements were made during and after the interaction of an external electric field (EEF) polarized in the x-axis, with an electric field amplitude defined as 1[V/m]. For the calculation during the interaction with EEF, the ports and Floquet periodicity were defined with periodicity conditions in the x and y-axis. The electric field dependence on the distance (in the range of 1 to 60 nm along the z-axis) with and without nanoparticles was calculated under a specific excitation wavelength at 485 nm (Figure 1b).

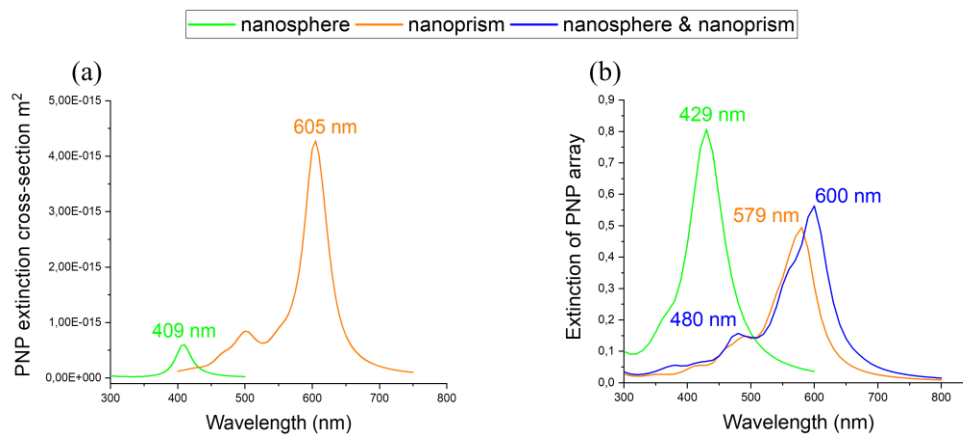
### 2.2. Interaction of emitter with a dipole

After the simulations of the interaction with the EEF, the ports were disabled and only the fluorophore was defined as a light emitter. The fluorophore was simulated as a dipole source with an emission wavelength  $\lambda=570$  nm and an electric current dipole moment of  $p(x) = 33.3 \cdot 10^{-15}$  [A·m]. Measurements were made at different distances of the nanoparticles (along the z-axis) using monitoring cubic boxes with 10 nm face length. The surface of the box was used for the field integration to find the emitting power of the dipole. In the case of silver nanospheres or nanoprisms separately, the monitoring box was

placed in the center of the XY plane while, in the case of their combination the monitoring box was placed just below the interparticle gap. The excitation enhancement, Purcell effect, PNP absorption rate, and the overall PL enhancement were calculated for each dipole separation distance in the range of 2 nm to 80 nm.

### 3. Results

The dimensions of the simulated nanoparticles were chosen in such a way as to match the experimental data. Thus, the positions of extinction peaks of PNPs in water (Figure 2a) were in agreement with experimental results [4]. Once the PNPs arrays were simulated on PMMA, the extinction peaks in the nanospheres or nanoprisms arrays extinction spectra [4] also match with the experimental results (Figure 2b).



**Figure 2.** (a) Extinction cross-section spectra of plasmonic nanosphere (green) and nanoprism (orange) in water. (b) Extinction spectra of the arrays of PNPs on PMMA: nanosphere (green), nanoprism (orange), and their combination (blue).

The dependence of the PL enhancement of the emitter  $F(d)$  on the distance between dipole and PNP array  $d$  could be affected both by the enhancement of the excitation rate, related to the electric field before ( $E_0$ ) and after ( $E$ ) the deposition of the nanoparticles, and the amplification of the PL QY:

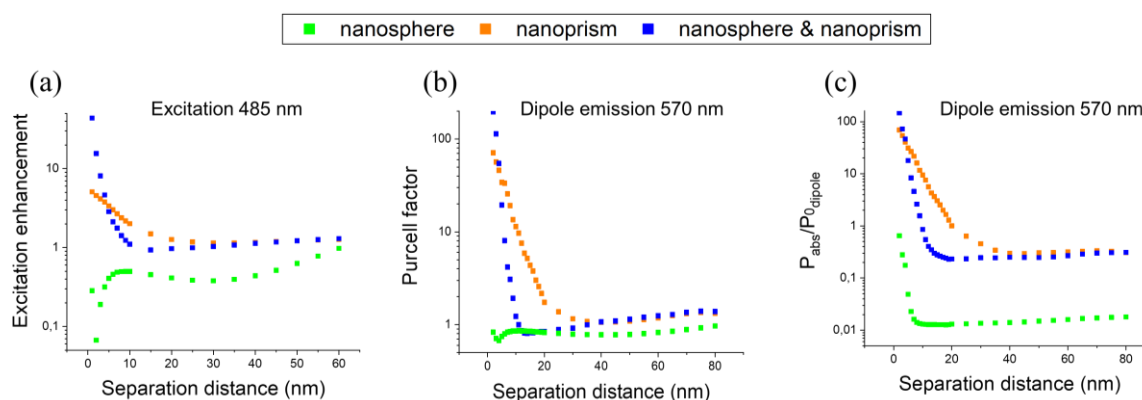
$$F(d) = \frac{|E(d)|^2}{|E_0|^2} \cdot \frac{QY(d)}{QY_0}, \quad (1)$$

where  $QY_0$  and  $QY$  are PL QY before and after adding of PNPs. Calculated variations of the local field enhancement across the separation distance  $d$  at  $\lambda_{exc} = 485$  nm (corresponding to the experimental conditions in reference [4]) are presented in figure 3a. According to the measurements made along the z-axis, the highest field in the three cases is located within 10 nm. In turn, the PL QY is affected by the change in radiative and nonradiative rates of the dipole:

$$QY(d) = \frac{\Gamma_r(d)}{\Gamma_r(d) + \Gamma_{nr-in} + \Gamma_{nr-PNP}(d)} = \frac{\beta(d) \cdot \Gamma_{r0}}{\beta(d) \cdot \Gamma_{r0} + \Gamma_{nr-in} + \Gamma_{nr-PNP}(d)}, \quad (2)$$

where  $\Gamma_{r0}$  and  $\Gamma_r$  are emitter radiative rate before and after interaction with PNP respectively,  $\beta$  is a Purcell factor,  $\Gamma_{nr-in}$  is an intrinsic nonradiative rate of the emitter, and  $\Gamma_{nr-PNP}$  is a plasmon-induced nonradiative rate. In our model, we calculated  $\Gamma_r$  as a power emitted by a dipole separately from PNP since the integration surface was only around the dipole without the PNP (figure 3b). We also calculated the ratio  $\Gamma_{nr-PNP}/\Gamma_{r0}$  as a ratio of the power absorbed by PNP to the power emitted by the dipole in the absence of PNP (figure 3c). The calculation of the overall change of the PL QY is a complicated task that depends on the  $\Gamma_{nr-in}$  value. For the low-QY limit ( $\Gamma_{nr-in} \gg \Gamma_r$ ) the PL QY amplification is

almost equal to the Purcell factor, while in the limit of the 100% initial QY ( $\Gamma_{nr-in} = 0$ ), it may be calculated using calculated values of the emitted (figure 3b) and absorbed (figure 3c) powers instead  $\Gamma_r(d)$  and  $\Gamma_{nr-PNP}(d)$ . As one can see from figure 3, for a dipole located near the “hot spot” region, the enhanced local electric field boosts the excitation rate of the dipole source, to enhance the emission intensity as in the case of the combination of one nanosphere and one nanoprism which show the greatest enhancement although it decreases quickly with the distance.



**Figure 3.** Interaction with the external electric field: (a) Plasmon-induced excitation enhancement at the 485 nm wavelength. Interaction with the dipole: (b) Purcell factor and (c) ratio of absorbed power by PNPs to initial dipole power.

#### 4. Conclusion

In this study, we have simulated arrays of silver PNPs (nanospheres or nanoprisms, or their combination) to find the effect of the PNPs of different geometries on the enhancement of the PL of quantum emitters. It was found that the local electric field in the vicinity of the silver nanoprisms will contribute to both the enhancement of the excitation efficiency and the radiative rate enhancement (Purcell effect) of the emitter located near the PNPs. Moreover, we found that the highest PL enhancement was achieved by the combination of silver nanospheres and nanoprisms. These results show the way to the maximizing of the PNP-induced enhancement of the PL of quantum emitters by an optimization of the size, shape, and interparticle distance of PNPs in arrays and also spacing between emitters and PNP arrays.

#### Acknowledgements

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