# Plasmonic Properties of Au@graphene Core-shell Nano-sphere

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## Abstract

Plasmonic signatures of graphene coated gold nano sphere has been studied numerically in term of backward and forward scattering efficiencies using Discrete Dipole Approximation (DDA) beyond the electro-static approximation.

## 1. Introduction

Core@shell nano-geometry provides a great strategy to tune localized surface plasmon resonances (LSPRs) in red domain instead of uncoated metal nano-particles (MNPs) [1-3].

In present study, we have analyzed backward ( $Q_{Bscat}$ ) and forward scattering ( $Q_{Fscat}$ ) efficiencies of graphene coated Au NPs by DDA techniques. LSPR tailoring is studied as a function of size embedded in air where core radius ( $R_1$ ) of Au NP is modified from 60nm to 140nm with fixed shell thickness of graphene mono layer ( $T_{GML}=0.1$ nm). The optical parameters of Au and graphene materials have been taken from the literature[1, 2].

### 2. Theory

DDA is the suitable numerical technique to calculate optical responses: forward and backward scattering, absorption and extinction efficiencies of core@shell NPs[4].

The schematic diagram of the proposed NP is shown in Fig. 1. Plasmonic coupling between inner and outer interfaces of core and shell of the NP is significantly explained by the hybridization theory [2]. According to this theory the mode lies in the higher and lower wavelength limit stand for the bonding ( $B_M$ ) and the anti-bonding ( $A_M$ ) modes, respectively.



Fig. 1. Schematic diagram of Graphene coated Spherical Au NP. R1 and R2 are the core and total radii of the core@shell NP where graphene shell thickness TGML = R2- R1.

## 3. Results and Discussion

Size effect on LSPR tailoring of the Au@GML has been depicted in Fig. 2. Figure 2a presents wavelength dependent Q<sub>Bscat</sub> of the Au@GML NPs with four different R<sub>1</sub>, varies from 60nm to 140nm. As R<sub>1</sub> increases, resonance peak of both the bonding (lies from 590nm to 980nm) and anti-bonding modes (lies below 590nm) are red shifted with the appropriate tunability  $\Delta\lambda_B \sim 381.2$ nm and  $\Delta\lambda_A \sim$ 

311.4nm, respectively. LSPR tailoring of  $Q_{Fscat}$  for  $B_M$  and  $A_M$  modes also follow the similar trend as Fig. 2a with high amplitude efficiencies having the tunability  $\Delta\lambda_B \sim 370.4$ nm and  $\Delta\lambda_M \sim 16.1$ nm, respectively, as shown in Fig. 2b. Hence, it can be observed that bonding modes of Au@GML exhibits higher LSPR tunability than antibonding mode for both  $Q_{Fscat}$  and  $Q_{Bscat}$ .



**Fig. 2.** Scattering efficiency spectrum of graphene coated spherical Au NPs (a)  $Q_{Bscat}$  and (b)  $Q_{Fscat}$  efficiencies by varying core radii (R<sub>1</sub>) from 60nm to 140nm with fixed shell thickness T<sub>GML</sub> =0.1nm in the surrounding environment of air.

Further, Table I provides the numerical values of Fig. 2 in term of  $\lambda_{SPR}$  (nm) and their corresponding amplitude (Amp.) for bonding modes only.

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R <sub>1</sub> (nm)	Bonding mode (B <sub>M</sub> )			
	Q <sub>Bscat</sub>		Q <sub>Fscat</sub>	
	$\lambda_{\text{SPR}}(nm)$	Amp.	$\lambda_{\text{SPR}}(nm)$	Amp.
60	611.4	0.1066	600.7	0.6952
80	681.2	0.2178	675.8	1.433
100	783.2	0.3	767.1	2.108
140	992.5	0.3748	971.1	2.85

#### 4. Conclusion

From this study it has been observed that  $Q_{Fscat}$  is significantly efficient for proposed geometry due to its higher amplitude ~7 times than  $Q_{Bscat}$ .  $Q_{Fscat}$  also shows board resonant spectrum owing to the excitation of red shifted higher order modes as  $R_1$  increases instead of  $Q_{Bscat}$ .

#### Acknowledgements

The author is thankful to MNRE, India for providing the financial support for this research.

#### References

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