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Extreme blueshift of surface plasmon resonance frequency in graphene nanodisk stacks

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ABSTRACT

The extraordinary properties of graphene surface plasmons like strong field confinement, long propagation distance and tunability have made graphene an attractive alternative to noble metals. However, it is still experimentally challenging to increase the resonance frequency in graphene nanostructures beyond the mid-IR limit. In this work, we investigate the blueshift of surface plasmon resonance frequency via plasmon hybridization in graphene disk stacks. Based on a nonretarded approach, we study the plasmon hybrid modes in graphene disk stack structures, considering the optical coupling between the uncouple eigenmodes of each disk. Through this methodology we were also able to extract the scattered and absorbed fields. We find that due to plasmon hybridization in an *N*-disk stack, each uncoupled mode splits into *N* hybrid modes. When the distance between disks is close to the strong coupling limit, we observe that for each uncoupled mode there is only one hybrid mode that is blue-shifted compared with the resonance frequency of its respective uncoupled mode. Analysis of the hybridization by reducing the distance between disks shows that in the transition between the weak and strong coupling regimes the interaction is mainly driven by the coupling of edge plasmons. For a stack with 25 graphene disks having a Fermi level of 1.0 eV and a 50 nm disk diameter, we observe that surface plasmon hybridization can effectively blueshift the resonance frequency up to 0.69 eV (1.8 μm). In addition, compared to a single graphene disk with the same diameter, the 25-disk stack can increase the peak of absorption and scattering cross sections by 12 and 38 times, respectively, opening up a wide range of applications for graphene surface plasmons in the near-infrared regime.

1. Introduction

Surface plasmons on doped graphene have attracted significant interest due to their extraordinary properties, like strong field confinement, long propagation distance and tunability, making them an attractive alternative to surface plasmons on noble metals [1,2]. A number of experiments have demonstrated that localized surface plasmons can be effectively excited by free space photons in graphene nanostructures like nanodisks or nanoribbons [1,2], which offers the possibility to control the resonance frequency not only by chemical doping or gate voltage, but also by adjusting the nanostructure size [2]. However, graphene surface plasmons normally exist in the mid-infrared (IR) and terahertz range, due to the low carrier concentration attainable in graphene in comparison with noble metals [1,3]. While the resonance frequency of graphene nanostructures can be blueshifted in theory by increasing their carrier concentration or reducing their size [4,5], it is still experimentally challenging to push the resonance frequency significantly beyond the mid-IR range.

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An alternative method to increase the resonance frequency of graphene surface plasmons beyond the mid-IR range is by critical coupling of surface plasmons in single-layer graphene with wave guided modes [6]. Through this method it has been proven it is possible to achieve a strong optical response at a wavelength of 1.5 μm. However, since the physical mechanism used by this approach is based on the absorption properties of graphene beyond the plasmonic response, some interesting features of surface plasmons like electrical tunability or field enhancement cannot be explored. Another feasible method for increasing surface plasmon resonance frequency in graphene is via surface plasmon hybridization [1,7]. Due to the quantum nature of Dirac fermions, plasmon hybridization by using graphene stacks can efficiently increase the resonance frequency and the amplitude of surface plasmon modes [3,8].

In this work we investigate the extreme blueshift of the surface plasmon resonance frequency by plasmon hybridization in graphene disk stacks. We begin with an analysis of the hybridization of surface plasmon modes by reducing the distance between disks. Then we focus on hybrid modes whose resonance frequencies are blueshifted with respect to their original uncoupled modes, and study the physical mechanism involved in the hybridization process. In the last section, we explore some extreme cases, regarding the maximum gap between disks for strong coupling between surface plasmons, maximum blueshift of resonance frequency physically attainable through hybridization in a stack configuration, and the absorption and scattering spectra for an extreme blueshift case. Our work is focused on dipolar plasmons, since these modes can be easily excited by plane waves.

The study is based on semi-analytical expressions obtained from the problem of graphene disk stacks under a non-retarded approach, which has been proved to accurately represent the interaction between electromagnetic waves and localized surface plasmons on graphene nanostructures at long wavelengths [9–12]. Our method is a combination of the work done by Fetter [13], to extract the eigenmodes of the uncoupled surface plasmons for disk geometry, and the optical coupling theory [14], which considers the effects of interparticle coupling. Through the optical coupling theory, we construct an eigenvalue equation, from which the coupled or hybrid modes are extracted. Unlike the coupled dipole theory [11], whose formulation is restricted to the cases where the distance between bodies is larger than their characteristic dimensions, the optical coupling theory has the advantage of providing enough accuracy even at small distances, since its fundamentals consider the multiple interactions between all the eigenmodes.

By using the direct implementation of the optical coupling theory to the analysis of coupling between graphene nanostructures, we develop a complete and robust methodology to analyze the interactions between graphene nanostructures and an external field, which is simple and accurate. Some important results can be easily extracted, like interaction between eigenmodes and between nanostructures, as well as scattered or absorbed power. This methodology can also be extended to other graphene nanostructures like semi-infinite sheets and nanorings, whose analytical solutions for a quasi-static field have been derived previously [9,12].

Though the fundamentals of this method rely on the electrostatic approximation, we confirm through comparison with numerical simulations based on the Boundary Element Method (BEM) that our results remain fairly accurate for a broad spectrum.

2. General formulation

2.1. Surface plasmon modes for one disk

Analysis of surface plasmons in confined geometries whose dimensions are smaller than the wavelength of the external field can be simplified by the electrostatic approximation [15]. Under this approach, the incident field is assumed to be quasi-static, and the general problem involving a solution of the Maxwell equations is reduced to solving a single Poisson equation. In the particular case of graphene nanoparticles, it is reasonable to approximate the electric charge density as a surface charge distribution ρ_{2D}. This representation is valid when the thickness of graphene is negligible compared with the overall dimensions considered in the analysis. Thus, surface plasmon modes in graphene nanoparticles are found by solving the following equation:

$$\varepsilon_0\varepsilon_h\nabla^2\Phi_{sur} = \rho_{2D}(r)\delta(z_0 - z), \tag{1}$$

where Φ_{sur} and ε_h are the electrostatic potential and the dielectric permittivity at the surroundings, respectively. In this expression, we consider that the surface charge distribution is located at z_0 on a plane perpendicular to z.

In the case of disk shape, the solution of Eq. (1) is [13,16]

$$\Phi_{sur} = \frac{R}{\varepsilon_0\varepsilon_h}\sum_l e^{il\phi}\int_0^1 K_l(r,r';z)\rho_{2D}(r')r'\,dr', \tag{2}$$

$$K_l(r,r';z) = \frac{1}{2}\int_0^\infty J_l(pr)e^{-\frac{p|z-z_0|}{R}}J_l(pr')dp, \tag{3}$$

where $J_l(pr)$ is the Bessel Function of the first kind.

The second equation for ρ_{2D} is given by the charge conservation law, which in the case of a uniform surface charge distribution is expressed by [9,13]

$$\sigma_\parallel\left[\nabla_\parallel^2 + \frac{\partial}{\partial r}\delta(r-R)\right]\Phi_{ind} = -i\omega\rho_{2D}, \tag{4}$$

where $\nabla_\parallel^2$ is the 2D Laplace operator, $\sigma_\parallel$ is a 2D conductivity, R represents the radius of the disk, and Φ_{ind} is the induced electrostatic potential.

In the process to derive Eq. (4), we considered the following relation between the induced conductivity and the electrostatic potential:

$$\vec{J}_{ind} = -\sigma_\parallel(\omega)\nabla\Phi_{ind} \tag{5}$$

The solution of Eq. (2) (4) is given by [13]

$$\Phi_{ind} = \frac{i\omega R^2}{\sigma(\omega)}\sum_l e^{il\phi}\int_0^1 G_l(r,r')\rho_{2D}(r')r'\,dr', \tag{6}$$