Absorption tunability of asymmetric and bridged graphene dimers

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Graphene's plasmonic properties in the infrared are under extensive investigation for various applications. In this communication we take advantage of its tunability to numerically design asymmetrically doped graphene nano-disk dimers. These structures show a complicated absorption pattern of anti-crossing bands arising from mode hybridization: modes originally invisible or dark for a single nano-disk become bright upon coupling, and vice versa. Additionally, we consider a connected dimer with a tunable graphene junction. Such a bridged dimer creates new resonances at smaller energies known as charge transfer plasmons. These modes are stronger and narrower than in the non-bridged case, and could lead to molecular junction conduction measurements or to tunable sensors.

Introduction

Although Mie described resonances of metallic nanoparticules in 1908, their resonant properties are still under strong investigation nowadays. These particules show a strong interaction with light, promising a wide range of applications such as biosensing [1], nonlinear optics [2], nanocircuits [3], optoelectronics [4] and transparent displays [5]. In the meantime, graphene enjoys a tremendous interest for its plasmon resonance tunability [6]. Single disks were theoretically described, focusing on the fundamental mode, and also dimers were considered, for their field enhancement at the edges [7, 8].

However, higher order modes have never been investigated. Here we show that new resonances appear for two graphene nanodisks with different doping: the asymmetry of the dimer converts dark or subradiant higher order modes into visible, relatively narrow resonances.

Additionally, dimers can be connected by a conductive junction, allowing the charges to oscillate in between the two metallic particles [9, 10]. This creates a new low energy resonance called a charge transfer plasmon. Here we apply this principle with graphene dimers connected by a graphene ribbon. The tunable, conductive junction creates a narrow and enhanced new resonance.

In this work the two-dimensional simulations are performed with COMSOL Multiphysics, a commercial finite element based software package. Graphene is modelled as a boundary condition with optical surface conductivity $\sigma(\omega, E_F)$ computed by the Kubo-Greenwood formula[11] with ω the angular frequency and E_F the Fermi level.

Asymmetric dimers

In this section, we investigate the absorption cross-section of a free-standing graphene nano-disk dimer, excited with polarization along the disks' axis (x-directed), see Fig. 1a.

The two disks of diameter $D = 60$ nm are separated by 5 nm. One of them is 0.4eV doped and the other varies from 0 to 1 eV doping. Note that the scattering is negligible (by three orders of magnitude) since the nanodisk is small in comparison to the wavelength ($D \ll \lambda_0$). The absorption efficiency is given by the absorption normalized with the irradiance and the surface area.

The logarithm of absorption efficiency of the graphene dimer is plotted as a function of doping and wavelength in Fig. 1b. We observe two main patterns: one curved (with stronger absorption for the top-curved line) and one vertical. The straight vertical resonances are from the fixed 0.4 eV doped graphene disk with the first dipolar mode resonating at 6.3 μm and the higher order modes appearing at higher frequencies. On the other hand, the curved pattern comes from the disk with varying doping. The continuous (dashed) black lines represent the 6 first modes of the varying (0.4 eV) doping graphene disk and were computed using a theoretical model from [7].

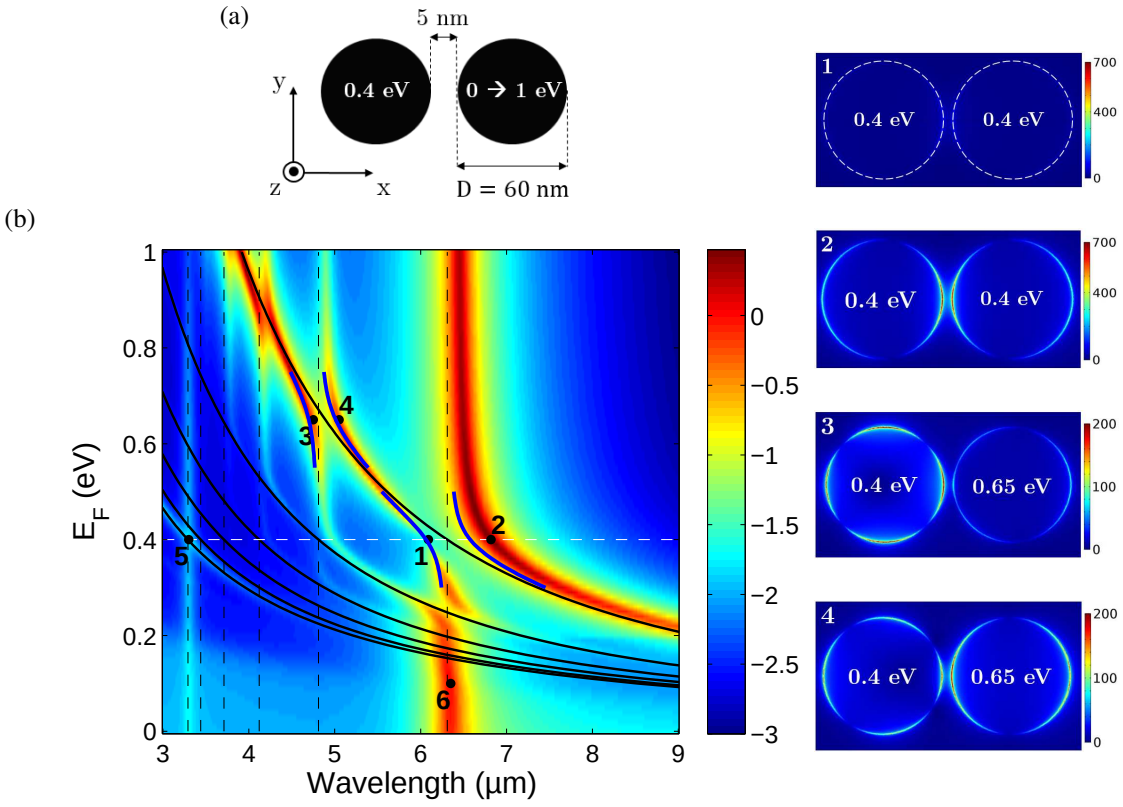

Figure 1: (a) Graphene dimer with one disk of 0.4 eV doping and the other of varying doping. Normal incidence along z-direction. (b) Logarithm of the absorption efficiency of a graphene dimer with a fixed 0.4 eV disk and a varyingly doped disk (from 0 to 1 eV) as a function of the wavelength for x-polarization. Continuous black lines represent the first six modes with varying doping, the vertical dashed lines for 0.4 eV. The horizontal white dashed line indicates equally doped disks. Blue lines are from perturbation theory. (1-4) Enhancement of the electric field (total electric field over incident electric field: $|E|/|E_0|$) for particular points of Fig. 1b.

When the resonance patterns (curved and straight) interact, the modes hybridize and give rise to two anti-crossing resonances. This is observed in point 1 and 2 or in points 3 and 4

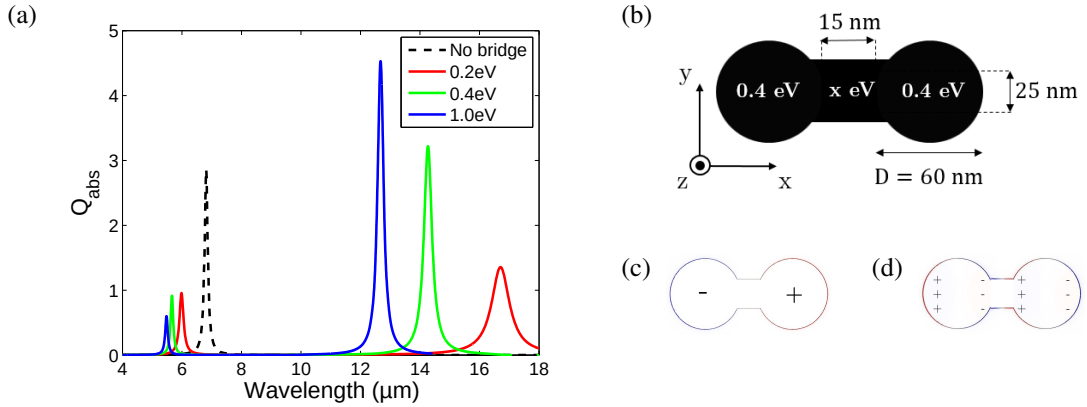

Figure 2: (a) Absorption efficiency of a graphene charge transfer dimer with varying bridge doping. The non-bridged dipolar-dipolar resonance is plotted in black dashed line for comparison. (b) Scheme of the studied structure. (c) Charge densities of the charge transfer plasmon resonance and (d) the screened bonding dipolar plasmon.

in Fig. 1b. Blue lines stand for a simple Hamiltonian model and emphasize this behaviour: the crossing point of dashed and continuous black lines is in between resonances, whereas the two blue curves follow the hybridized resonances.
The hybridization of two dipolar modes lead to a dark mode (no excitation in point 1) and a bright mode in point 2. This is explained by examining the possible combinations of the two identical dipolar modes (0.4 eV doping for both). Either the dipolar modes oscillate in opposition and the total dipolar moment is zero: that results in a dark mode. Or the dipolar modes sum up and create a stronger resonance, and thus a bright mode (point 2). The resulting plots of the enhanced electric fields are in Fig. 1.1 for point 1, where the mode is clearly dark, and in Fig. 1.2 for point 2, where an enhanced field is visible at the edge.
Finally, the line crossing around points 3 and 4 is investigated: the normally dark quadrupolar mode becomes bright over a large E_F range thanks to the evanescent field of the neighbouring dipolar mode. The crossing point splits in two modes: the point 3 in Fig. 1b is the quadrupolar mode with the enhancement of the electric field represented on Fig. 1.3 and the point 4 in Fig. 1b is the dipolar mode with the field represented on Fig. 1.4.

Charge transfer plasmons

In this section, we introduce a graphene ribbon connecting the two disks as a charge transfer component. This allows electric charges to oscillate from one disk to the other: the charge tranfer plasmon. Here, we examine two graphene disks (diameter $D = 60$ nm) separated by a distance of 15 nm and with the same doping (0.4 eV). We add a charge transfer junction of 25 nm wide, see Fig. 2b.
In this system we vary the junction conductance via the graphene doping, from 0.2 eV to 1 eV. The absorption is plotted in Fig. 2a for the wavelength range 4-18 μm. The hybridized non-bridged dipolar-dipolar resonance around $\lambda_0 = 6.5$ μm is also shown for comparison (dashed line). Two groups of resonances are distinguished: one is redshifted, while the other group appears at smaller wavelengths.
The redshifted resonances are the charge transfer plasmons[9], the particular oscillation

of the electrons between the disks is presented on Fig. 2c: one disk is a positive pole and the other a negative one. This is completely different from the previous section where the charges oscillate separately on each disk (Fig. 1.2). With the junction the dimer acts as a continuous particle of larger length, which consequently induces a redshift.
The blueshifted family of resonances is called the screened bonding dipolar plasmon[10]. The non-bridged dipolar-dipolar resonance, which is a capacitive coupling over the dimer gap, is screened by the charge transfer, inducing a blueshift and a weaker absorption efficiency. The charge densities are plotted in Fig. 2d for 0.4 eV doping throughout. The dipolar modes of the two nanodisks are still visible, as charge also appears on the edge of the junction.

Conclusion

In conclusion, we simulate the infrared response of asymmetric graphene dimers, induced by different doping levels, leading to an intricate and tunable absorption spectrum. We demonstrate mode hybridization with dark modes becoming bright, and vice versa.
Finally, we demonstrate strong and tunable absorption efficiencies with charge transfer plasmon resonances, when the graphene disks are coupled via a bridge of varying doping. These numerical considerations of junctions show their interest for the ease of tunability: with conventional metals the optical properties are only adjusted when the metal of the junction is exchanged for another metal. Our findings could lead to molecular junction conduction measurements or to tunable sensors.

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