

PhD Thesis Defense JOSE RAMON MARTINEZ SAAVEDRA 'Classical and Quantum Aspects of the Optical Response at the Nanoscale'

JOSE RAMON MARTINEZ

December 10, 2018

Monday December 10, 11:00 h. ICFO Auditorium

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Nanophotonics Theory

ICFO-The Institute of Photonic Sciences

Nanophotonics is one of today?s basic sciences and technologies: an in-depth understanding of the interaction between light and matter on the nano-scale, besides its intrinsic associated scientific interest, enables the precise control of light, that is relevant for technology in

diverse applications such as telecommunications, energy and medicine.

Plasmonics --the study of the collective oscillations of conduction electrons in materials with a metallic behaviour-- has become one of its most important sub-branches in recent years: the strong confinement of the electromagnetic energy density and its high sensitivity to the environment render plasmons as a key tool for the control of light at the nanoscale.
In this thesis, we explore several new paths that open up to Nanophotonics in general, and Plasmonics in particular, with the appearance on stage of materials such as graphene, which host optical excitations of increasingly smaller wavelengths, therefore requiring increasingly more compact structures. This new scenario demands new theoretical models that capture the structure of matter on an atomic scale.

After introducing the necessary fundamental concepts in Chapter 1, the thesis proceeds by exploring processes that can still be treated in terms of classical models for the optical response, such as geometrical plasmon focusing. Specifically, we apply this idea in Chapter 2 to graphene nanostructures, proposing a lens design capable of focusing plasmons and enhancing the third-order nonlinear response of this material.

We then move to more microscopic models of light-matter interaction: the description of the optical response of a nanoparticle from the individual response of its electrons allows us to explore in Chapter 3 the plasmon decay into hot-electron distributions, as well as the subsequent relaxation of these electrons back to their equilibrium state, thus presenting a complete picture of ultrafast plasmon and hot electron dynamics in nanoparticles.

From here on, we explore collective oscillations in molecular-sized structures, which demand the use of microscopic models incorporating many-body electronic response by massively demanding numerical solution of Schrodinger?s equations including the interaction with incident light. In particular, in Chapter 4 we have applied time-dependent density-functional theory (TD-DFT) to model the optical response of DNA that, besides being ubiquitous in biological organisms, we claim it to have some potential uses in nanotechnology.

Finally, we study light-matter interactions associated with ionic displacements of structures, quantized as phonons. In Chapter 5, we study the coupling between these excitations and plasmons supported in 2D materials: the distortions introduced into the electronic structure by ionic vibrations allow us to explain recent experiments in which the plasmonic dispersion is modified by the presence of vibrational modes. We also studied, in Chapter 6, the possibility of directly exciting and analyzing these vibrational modes, not by optical methods, but rather with electron beams, in clear analogy with plasmonic modes in nanostructures.
To summarise, this thesis explores the use of different theoretical models in Plasmonics,

covering a wide gap between fully classical macroscopic descriptions and quantum-mechanical atomic modeling, which we hope will contribute to a deeper understanding of optical phenomena at the nanoscale.

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