

Project B1: Electromagnetic simulation of optical response of metal nanoparticles (using COMSOL Multiphysics)

Introduction. Nowadays photonic devices mainly composed of dielectric materials with positive dielectric permittivity. However, dielectric media are diffraction limited and do not allow the localization of electromagnetic fields into nanoscale regions. By contrast, the collective excitations of conduction band electrons in a metal-like materials with negative dielectric permittivity, also known as *surface plasmons*, allow to achieve localization of electromagnetic energy into nanoscale regions [1-5]. For instance, the excitation of the surface plasmons leads to extreme localization of the electromagnetic field (near-field and far-field) with resonances that happen to be in optical range from ultraviolet over the visible to the near-infrared. A great advantage of the plasmonic materials is due to their *tunable* optical properties meaning that their electromagnetic response can be controlled through their shape, size, composition and type of the applied source of excitation [6]. In this contest the metal nanoparticles are very attractive as they can be used for applications in optics, solar cells, bio-sensing for detecting biological molecules, magneto-optical data storage, and information processing.

Objective: Calculation of optical response of metal nanoparticles by using the numerical Finite Element Method (Comsol Multiphysics). In particular, students will simulate the interaction of the specially designed metal nanostructures with external sources of light (electromagnetic wave and dipole emitters) on nanometer scale.

Tasks:

- Read articles related to the subject. Study the basic of the Finite Element Method and the electromagnetic module of the commercial software COMSOL Multiphysics.
- Simulate the interaction of metal nanoparticles with *plane wave* and *point dipole*. Calculate their optical response (optical cross sections, near- and far-fields, and photonic local density of state) and compare the obtained results with other methods (Mie theory, Boundary Element Method).
- Calculate the optical response of specially designed nanoparticles on a dielectric substrate.

References:

- [1] W. L. Barnes, A. Dereux, T. W. Ebbesen, Surface plasmon subwavelength optics, *Nature* **424**, 824 (2003).
- [2] W. A. Murray, W. L. Barnes, Plasmonic materials , *Adv. Mater.* **19**, 3771-3782 (2007).
- [3] J. Schuller, E. Barnard, W. Cai, Y. C. Jun, J. White, M. Brongersma, Plasmonics for Extreme Light Concentration and Manipulation, *Nature Materials* **9**, 193 (2010).
- [4] S.A. Maier, M. L. Brongersma, P.G. Kik, S. Meltzer, A. A.G. Requicha, H. A. Atwater, Plasmonics - A route to nanoscale optical devices, *Adv. Mater.* **13**, 1501-1505 (2001).
- [5] J. B. Pendry, D. Schurig, D. R. Smith, Controlling electromagnetic fields, *Science* **312**, 1780-1782 (2006).
- [6] V. Myroshnychenko, J. Rodríguez-Fernández, I. Pastoriza-Santos, A. M. Funston, C. Novo, P. Mulvaney, L. M. Liz-Marzán and F. J. García de Abajo, Modelling the optical response of gold nanoparticles, *Chem. Soc. Rev.* **37**, 1792 – 1805 (2008).