Spécialité de Master « Optique, Matière, Plasmas »

Stage de recherche (4 mois minimum, à partir de début mars)

Proposition de stage

Date de la proposition : 30/10/2014

Responsable du stage */ internship supervisor*:

Nom / *name*: RAYNAUD Prénom/ *first name* : Michèle

Tél : 01 69 33 45 20 Fax :

Courriel */ mail*: michele.raynaud-brun@polytechnique.edu

Nom du Laboratoire / *laboratory name*:

Code d'identification : LSI Organisme : CEA/CNRS/Ecole Polytechnique

Site Internet / *web site*: http://www.lsi.polytechnique.fr/

Adresse / *address:* Ecole Polytechnique, route de Saclay, 91128 Palaiseau

Lieu du stage / *internship place*: Ecole Polytechnique

Ab initio study of surface plasmons

Surface plasmons are coherent collective electron oscillations that develop at the solid-vacuum interface where the sign of the real part of the dielectric function changes. These oscillations can be resonantly laser excited and yield increased light absorption and electron emission. This is especially the case in metallic nanoparticle arrays, where interactions between nanoparticles change the plasmon properties and open the possibility of light confinement with possible applications in photonics and nano-optics. Despite the tremendous interest developed by the physicist community in this field, questions about the conditions of existence of these oscillations together with the mechanism of local electro-magnetic field amplification on the nanometer scale still remain, where quantum effects play an essential role.

Recently, a new method based on the density functional theory has been developed in our team 'Théorie des Sciences des Matériaux' (TSM) in the Laboratoire des Solides Irradiés (LSI), in collaboration with the International School for Advanced Studies at Trieste (SISSA) and the International Center of Theoretical Physics at Trieste (ICTP). It uses the Lanczos recursion method and allows the *ab initio* calculation of the electronic susceptibility of a periodic system at a given wavelength, without the requirement of calculating any unoccupied Khon-Sham states. This new approach, Turbo-EELS, has been implemented in the QUANTUM ESPRESSO package and opens the way to the study of systems which are too large to be treated with conventional *ab initio* approaches. In particular it gives new perspectives about the calculation on the quantum scale of surface plasmons without any fitting parameter for complex surfaces or nanoparticle systems. Thus we have developed in the TSM team a research program on surface plasmons in noble metals such as gold, coper and silver with the aim of investigating the relationships between the surface plasmon dispersion and the modification of the surface symmetry, taking into account spin-orbit coupling.

The goal of this internship, which will last between 4 and 6 months, and which may ideally continue with a PhD contract, is first to model a gold surface with high Miller indices, and calculate its ground state together with its band structure. The student will then study the surface plasmon of the system, calculating its electron energy loss spectra using the Turbo-EELS code. The different parameters which influence the surface plasmon dispersion will be searched for. This internship, and the PhD work that might follow, will be done in the frame work of a strong collaboration with the TSM group and with the International School for Advanced Studies (SISSA) and the International Center of Theoretical Physics (ICTP) at Trieste.

The proposed internship subject requires an understanding of quantum mechanics and solid state physics. It will involve theoretical as well as computational work, so some ability and willingness to program is essential. Some experience in computers with linux operating system is a plus, as well as some notions in Fortran. Experience in density functional theory is not mandatory.

Ce stage pourra-t-il se prolonger en thèse ? *Possibility of a PhD* **? : oui**

Si oui, financement de thèse envisagé/ *financial support for the PhD***: CNRS/CEA/X**

Lasers, Optique, Matière		Lumière, Matière, Interactions	**x**
Plasmas : de l'espace au laboratoire			