MASTER DE PHYSIQUE ET APPLICATIONS - 2ème année
Spécialité Sciences des Matériaux et Nano-objets
International Nanomat Master Program

Internship proposal 2009-2010

Laboratory : Institut des NanoSciences de Paris
Address : Campus Boucicaut, 140 rue de Lourmel
75015, Paris, FRANCE
Laboratory director : Bernard PERRIN

Internship supervisor : Jean Pierre ROZET, Emily LAMOUR and Dominique VERNHET
Phone : +33 (0)1 44 27 84 16 or 23 55 or 45 18

e-mail: rozet@insp.jussieu.fr

Title for the scientific project
Ab initio calculations to predict charge state distributions of heavy ions in matter

Scientific project :

The main driving topic of our research group is the study of interaction dynamics when matter (i.e. atoms, ions, nano clusters, surfaces or solid bulk) is submitted to strong perturbations induced either by the impact of highly charged ions or by the irradiation of femtosecond laser pulses of high intensity. Fast heavy ions going through matter induces material modifications, and in turn, their stopping power and charge state depends upon the material encountered. The continuous modification of the ion charge state during its transport through the material comes from competing processes which either excite or ionize the projectile electrons, from those which lead to a gain of electrons, and from other relaxation mechanisms like the radiative and autoinisation deexcitation of the projectile excited states. In this context, we developed a model allowing *ab initio* predictions of the evolution of the charge state distribution of fast heavy ions in matter. This model accounts for all the mechanisms that lead to a change of the projectile charge solving a system of coupled differential equations, including calculation of cross sections of all the processes which govern the temporal evolution of the ion charge state.

Besides tests of the fundamental processes involved in ion-matter interaction that can be provided by comparing model predictions with experimental measurements of ion charge state distributions, this model is also a tool of general interest for physicists from other fields (such as in nuclear physics or materials sciences) and for accelerators engineers as well. Indeed, experiments in which observed phenomena are related to the projectile charge state variations may need input from our model to complete the understanding of their data. On the other hand, our model is already widely used by people running large scale accelerator facilities around the world in order to optimize the beam production of fast heavy ions, and the software presently available for the users is called “ETACHA”.

Currently, we have to take up a new challenge coming from the advent of novel large scale accelerator facilities, such as FAIR in Germany or SPIRAL2 in France, or even from new phenomena that have been recently discovered in materials sciences. Both require widening the validity of the ETACHA code towards collisonal systems for which the projectile velocity is much lower and the initial number of electrons much larger. In principle, we have all the necessary data, but their integration in the present version of the code will need a certain investment which will be the main object of the internship. These corrections being incorporated into the code, we want also to be able to put a downloadable modern version on the web site of our laboratory. More precisely, this work will include several of the following aspects:

- test of the code routines used to calculate the cross sections and the resolution of the coupled differential equations
- comparison with experimental data available in the literature
- development of a convivial interface for users and implementation of the new version of the code on the website

During this internship, the student will have also the opportunity to become more familiar with the different topics of research driven by our team and could participate to experiments coupled either with a laser facility we will use in Saclay or with our ECR ion source located in Jussieu.

Techniques in use : Programmation FORTRAN ou C, théorie des collisions.

Applicant skills : Basic knowledge on atomic physics and/or material sciences.

Granted internship : yes (398 €/month)
C'nano IdF laboratory (France only) : yes
Possibility for a thesis : yes (type of grant : to be defined)