


Internship proposal 2011-2012

<p>Laboratory : IMPMC</p> <p>Address : 4 Place Jussieu, 75005 Paris</p> <p>Laboratory director : Bernard Capelle</p>	
<p>Internship supervisor : Michele Casula</p> <p>Internship co-advisor: Frédéric Decremps</p> <p>Phone : 01 44 27 43 60</p> <p>e-mail: michele.casula@impmc.upmc.fr</p>	

Title for the scientific project

New phases of Cerium: a step towards new plastic and metallic materials

Scientific project :

In general, polymeric glasses and metallic alloys show contrasting behaviors. The former have excellent molding properties at low temperature, the latter have great mechanical properties like high elastic strain and large compressive strength. Combining these two paradigms will result in a material with appealing capabilities and unique applications in micro- and nano- manufacture.

Cerium alloys, studied in our laboratory, seem to open a route to realize in practice such a material. Ternary compounds with Aluminium, Cobalt and a high concentration of Cerium show stable polyamorphic phases and metallic behavior. The high-density-to-low-density (HD-LD) amorphous transition is particularly interesting in Cerium based glasses, as it could be characterized by a reversible change in the nearest-neighbors distance associated with the same coordination number (a highly non trivial behavior for a glass).

The goal of this master internship is to shed light on the HD-LD transition in polyamorphic Cerium alloys by studying it with first-principles theoretical approaches, in close relation with the experimental group in our laboratory. The first step is to understand the properties of pure Cerium, which has never been explained consistently and quantitatively by any first-principle method. To address this issue, we are going to apply the variational quantum Monte Carlo method to this problem, an approach that will subsequently allow us to clarify both qualitatively and quantitatively the physical origin of the HD-LD transition in metallic glasses.

Techniques in use :

First-principles calculations based on Density Functional Theory and Quantum Monte Carlo

Applicant skills :

Condensed matter theory, quantum mechanics

Granted internship : yes (398.32 €/month)

C'nano IdF laboratory (France only) : yes

Possibility for a thesis : yes (type of grant : Ecole doctorale UPMC, Labex Matisse)