


Internship proposal 2009-2010

Laboratory : Institut de Minéralogie et de Physique des Milieux Condensés	
Address : 140, rue de Lourmel, 75015 Paris	
Laboratory director : Bernard Capelle	
Internship supervisor : Marc Blanchard	
Phone : +33 (0)1 44 27 98 22	
e-mail: marc.blanchard@impmc.upmc.fr	

Effect of cationic substitutions on the structure and isotopic composition of siderite (FeCO₃)

Scientific project :

The effect of impurities on the isotopic composition of minerals is an important question of isotopic geochemistry. The essential condition for the interpretation of isotopic measurements is to know the equilibrium isotopic fractionation factors. Most of the time, these fractionation factors are determined experimentally using pure phases while in nature, minerals contain many impurities.

Siderite is an iron carbonate (FeCO₃) that can incorporate within its crystal structure a large number of elements (Mg, Mn, Ca,...), up to the formation, for instance, of ankerite (CaFe(CO₃)₂). In particular, these minerals are present in Banded Iron Formations (i.e. Archean sedimentary rocks, -2.5 Ga) where the iron stable isotopes are used to track the paleo-environmental conditions.

Equilibrium isotopic fractionation factor is a thermodynamical property, which can be determined from the vibrational properties of the system. During this internship, a series of siderite with different chemical compositions will be simulated using a computational method based on the density functional theory. This will allow us to analyse the effect of cationic substitutions on the structural, vibrational and isotopic properties of siderite.

Techniques in use :

Ab initio calculations based on the density functional theory (DFT)

Applicant skills :

An experience in Unix and Fortran languages would be appreciated but is not mandatory

Granted internship : yes (398,13 €/month)

C'nano IdF laboratory (France only) : yes

Possibility for a thesis : yes (type of grant : Doctorate school)