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

Internship proposal 2011-2012

Laboratory : Institut de Minéralogie et de Physique des Milieux Condensés

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Ab initio calculation of vibrational and isotopic properties of iron-bearing minerals

Scientific project :

In soils and sediments, chemical reactions at the interfaces between iron oxyhydroxides and water play an important role in numerous natural processes, from controlling the fate and transport of environmental contaminants to the biological availability and geochemical cycling of iron. Moreover these mineral phases are widely used for paleoenvironmental reconstructions from their crystal-chemical and isotopic properties.

Infrared vibrational spectroscopy is a powerful technique for the characterization and investigation of finely divided minerals found in soils. It allows probing directly the organisation state and the presence of impurities in substitution within the crystal structure. However, it is often delicate to establish unambiguous relations between vibrational spectra and the microscopic mineral structure. The proposing group has successfully developed a theoretical approach, based on density functional theory, which allows to model infrared spectra of finely-divided minerals from their crystallographic structure. Moreover, it is now possible to use these theoretical vibrational properties for quantifying how the isotopes of a chemical element partition between two phases in thermodynamical equilibrium. The knowledge of these equilibrium isotopic fractionation factors is essential because it supports the interpretation of isotopic compositions measured in natural materials.

This project is a continuation of our work on pyrite, siderite and hematite (e.g. Blanchard *et al*. 2009, *GCA*, 73, 6565), and will focus on other minerals like goethite, ferrihydrite and magnetite. Beyond their strong environmental implications, the accurate modelling of the electronic properties of such phases is already challenging. The comparison of measured and calculated infrared spectra will improve the interpretation of the spectral signatures. This work will then lead to the determination of the equilibrium isotopic fractionation factors.

Techniques in use : *ab initio* calculations based on density functional theory

Applicant skills : Strong background in solid-state physics, and knowledge in quantum molecular computer simulations.

Granted internship : yes (~ 400 €/month)
C'nano IdF laboratory (France only) : yes
Possibility for a thesis : yes (type of grant : Ecole doctorale)