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

Internship proposal 2009-2010

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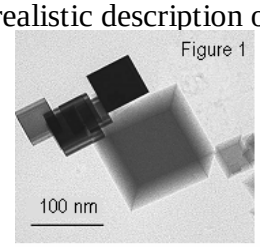
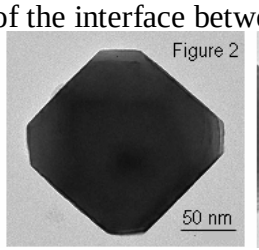
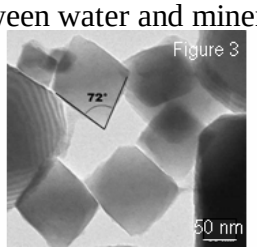
The interaction between water and oxide surfaces at the nano-meter scale

Scientific project: The behaviour of materials (either from the natural environment or manufactured) in contact with water is a key question. For instance, the kinetic rate of dissolution is often known but the process at the atomic scale is still poorly known, even for the most simple minerals. However, much progress is expected by the use of near-field microscopies, such as AFM, and numerical simulations.
At INSP, we study magnesium oxide (MgO) in contact with water by a joint experimental and theoretical approach. MgO crystallises in the NaCl system and theory predicts that its stable form in dry environment is a cube, which exposes (100) faces, as it can be seen on MgO smokes that are produced by burning Mg in dry atmosphere (Fig.1). Upon hydration, the most stable surface orientation becomes the (111), which was recently confirmed by an experimental study through transmission electron microscopy (TEM). However, during the transformation, truncated cubes along (110) faces have been also observed (Fig.2) and only after a certain time the hydrated MgO nano-crystals show octahedral shapes (Fig.3), which are indeed terminated by (111) faces. Understanding the precise sequence of transformations needs a better description of the influence of kinetics along the dissolution process, as well as a realistic description of the interface between water and minerals.







Images de microscopie en transmission de poudres nanométriques de MgO

To this end, we propose to employ semi-empirical and first-principles simulations of water/mineral interfaces. The focus is on the structure of water layer close to the interface, as a function of the presence of solvated species and of the morphology of the solid surface. An important result is to understand whether the surface energy may show big variations as a function of the hydration conditions. The applicant will profit of the experience that has been recently gained: at the INSP, on the water adsorption at the surfaces of MgO and brucite Mg(OH)2; at the IMPMC, on the structure of water in presence of solvated species like salts.
This proposal is part of a long-term project and it should be followed by a Ph.D. thesis.

Techniques in use : Molecular Dynamics simulations using semi-empirical inter-atomic potentials, on one side, and density functional theory, on the other side.

Applicant skills : The applicant should know the basics of the Linux operating system, be interested in numerical simulation and ready to write a few lines of computer codes for data analysis. The knowledge of chemical physics is a plus.
Granted internship : yes (398.32 €/month)
C'nano IdF laboratory (France only) : yes
Possibility for a thesis : yes (type of grant : Ministère)