Subject offered for a contract starting october 2015

SUBJECT TITTLE: Fate and transport of nanoparticles in soils

Advisor: **BENEDETTI Marc (Pr,), benedetti@ipgp.fr**
Second Advisor/ Supervisor:
GELABERT Alexandre, (MCF), gelabert@ipgp.fr
Host lab/ Team : **IPGP- Aquatic Geochemistry Team (LGE) – UMR7154**

Financing: Doctoral contract with or without assignment

For more information go to http://ed560.ipgp.fr, section: Offres de these (PhD offer), You must apply on the Doctoral School website

Presentation of the subject: (1 or 2 pages)

Recent progress in nanotechnology has led to the development of functional nanoparticles (NPs). Given their size, NPs can interact with living organisms by crossing cell membranes, and they have strong redox properties, raising concerns about the potential impact of their release in natural environments (water and soils). Whereas many studies have recently focused on the direct exposure of model organisms to NPs, only few of them have investigated their transfer to aquatic systems and their fate in soils. NPs released in soils will be transported by advection and diffusion, and their reactivity will depend on the presence of organic ligands (*i.e.* humic substances) that can stabilize the particles, the existence of bacteria that can complex, breakdown or uptake them, and the abundance of sorption sites available on mineral surfaces. Hence, critical information regarding the physico-chemical processes controlling the NPs distribution, transformation and toxicity are still missing and, more particularly, a molecular-scale characterization to accurately predict their fate in the environment.

The overarching goal of this project is to decipher how molecular-scale physico-chemical processes, promoted by mineral surfaces, microorganisms and organic ligands, affect NPs transport, reactivity and dissolution in soils.

We propose an innovative approach combining process-based laboratory experiments with microscopic, spectroscopic analyses and thermodynamic modeling. Our study will progress from simplified ferrihydrite coated sand columns, to systems integrating substances commonly found in soils such as mono-specific bacterial biofilms, EPS or humic substances. Microscopy (TEM, SEM) will be used to monitor changes in NPs morphology during their transport in soil columns and to detect aggregate formation. The role of organic ligands (*i.e.* humic substances or exudates from bacterial biofilms) in the NPs aggregation will be investigated. NPs size, surface properties and association with organic ligands will be investigated in the outflow samples using Field Flow Fractionation technique (FIFFF). Extended X-ray Absorption Fine Structure (EXAFS) will resolve their speciation, with a specific emphasis on the bacteria and organic ligands impact. Particularly, the bacteria biofilm reactivity, the NPs diffusion rates within it, and the changes in NPs chemistry and stability imposed by these biological structures will be investigated. To do so, *in situ* X-ray Standing Waves Fluorescence Yield (XSW-FY) will be performed. This synchrotron related technique provides quantitative *in situ* analysis of spatial distributions of various ions in the complex biofilm/mineral system. Associated to Grazing Incidence–Extended X-ray Absorption Fine structure (GI-EXAFS), it provides specific information on ion speciation and local coordination environment specifically in the biofilm or on the mineral surface.

The increasing complexity of the systems used will allow to discriminate the biological, geochemical and physical parameters controlling the fate of NPs in soils.

These results will improve our understanding of the mechanisms that attenuate or transport NPs in soils and will ultimately provide the predictive framework needed to assess NPs fate in soils, with important implications for the evaluation of nanotoxicity and maintenance of groundwater quality.

This PhD will be part of the QUADOS (Elucidating the Effects of Molecular-Scale Physico-Chemical Processes on the Fate and Transport of Quantum Dots in Soils) ANR project (collaboration between IPGP –Univ. Pau – Univ. Poitiers).