**Project title**: Structural investigation of carbo-silicate hydroxyapatites - Application to bone tissue engineering

**Project Description (~4000 characters, font 11 min):**

Biomaterials dedicated to therapeutic bone tissue engineering are intended to provide a temporary support for bone growth while stimulating this process. Calcium phosphate materials such as hydroxyapatite (HA, Ca10(PO4)6(OH)2) are commonly used in reconstructive surgery because of their chemical composition close to that of the mineral part of bone. Nevertheless, these biomaterials have a limited ability to stimulate the development of new bone tissue and inadequate in vivo biodegradation. The substitution of ions in the structure of HA will improve their bioactivity, namely all the interactions between the implant and the tissues (biocompatibility, bioabsorbability). The incorporation of carbonate ions (CO32-) into the HA structure allows to modulate the resorption and dissolution properties of the material(1), which are key factors in the successful repair of bone defects. On the other hand, the literature reports a beneficial influence of "soluble silicon" on the formation and calcification of bone tissue. Thus, hypothetically, the simultaneous incorporation of CO32- and SiO44- ions into the apatite structure (CSiHA) would allow coupling the resorption and dissolution properties of carbonatedapatites with the important metabolic role of silicon in the connective tissue. The control of the biological properties of these bioceramics necessarily involves the control of their purity and their composition which remains particularly challenging. The project aims to take up this challenge by coupling the Nuclear Magnetic Resonance with other physico-chemical characterization methods and ab initio structural modelling. In collaboration with the Centre d'Ingénierie et Santé (CIS) (Saint Etienne), which has developed methods for the preparation of these substituted hydroxyapatites(2,3) and the Laboratory Bioingénierie et Bioimagerie Ostéo - Articulaire (B2OA) (Paris Diderot), we have started a study on characterization and biological evaluation of these compounds. The project implements : (i) original and reliable preparation methods of CSiHA enriched in 13C and 29Si isotopes, (ii) detailed physicochemical analyses of CSiHA by X-ray diffraction, vibrational spectroscopies (Infrared, RAMAN) and high-resolution solid-state NMR and Dynamic Nuclear Polarization, (iii) ab initio structural modelling of substituted hydroxyapatites and subsequent calculations of spectroscopic properties.

**References**