**RESEARCH FIELD:**

Mineralogy

**RESEARCH TOPIC:**

CAP-TO - Crystal-chemical and structural investigations on the bulk and surfaces of carbonated-apatites along with amorphous-nanocrystal transit

**PARTICIPANTS:**

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**INTERNATIONAL COLLABORATION:**

Cristiano FERRARIS (Muséum National d'Histoire Naturelle, Paris – France)

**RESEARCH DESCRIPTION:**

This project is instrumental in finding the mechanisms ruling the transition from hydroxyapatite (HAP) to carbonated-apatite (CAP) in order to improve its quality as biomaterial for bones and teeth.

Three steps characterize our research:

1) Crystallization. HAP and CAP will be obtained controlling T, P and solution composition, in a new way with respect to the State of Art.
2) Characterization. The amorphous-crystal transition kinetics is followed under the Synchrotron Light; structural data is acquired through XRPD and single crystal analyses, along with the complementary information coming from TEM imaging, IR and Raman spectra (both for bulk and surface). Morphological data on the crystal aggregation and shape is obtained from SEM observations and AFM patterns.
3) Interpretation. Interface processes ruling crystal growth kinetics in solution are studied by managing: a) the crystallization patterns forming during the mineral reactions; b) the data analysis needed to calculate the end-members of the solid solutions; c) the morphology of the crystals; d) interface phenomena such as the growth twinning and the epitaxy. This done through prediction of several quantities, either to be compared with the experimental ones, or to be evaluated when they are not experimentally accessible. As a matter of fact, semi-empirical and ab initio methods are employed: i) - to find the defect structures due to the lattice replacement of phosphate or OH groups by the carbonate ions; ii) - to calculate the surface and the attachment energy of the HAP and CAP {hkl} forms, in order to predict the equilibrium and growth morphology of these phases and to manage the most stable interfaces playing a strategic role in the phase transformations.

**LABORATORIES OF THE DST IN USE:**

Laboratorio di diffrazione raggi X su cristallo singolo, laboratorio di crescita cristallina, laboratorio di microscopia di forza atomica, Centro Interdipartimentale di Ricerca per lo Sviluppo della Cristallografia Diffrattometrica (CRISDI), SEM-EDS, TEM-EDS, MicroRaman (Centro Scansetti)

**GROUP CONTACT:** Fernando CAMARA