DOCTORAL SCHOOL " MATERIALS, RADIATION AND ENVIRONMENTAL SCIENCES " (ED 104)

UNIVERSITY: University of Lille, Sciences and Technologies
PhD. programme: Molecules and Condensed matter
Title of the thesis: Conception of Functional Materials using Topotactic Chemistry Methods
Supervisors: Olivier MENTRE, Houria KABBOUR
Laboratory: UCCS – UMR CNRS 8181

THESIS PROJECT

New Materials: The search of new functional materials constitutes an important topic in the actual energy context. In that purpose, academic research toward innovative compounds is essential to allow the anticipation of the future energy transitions. The *OXYD* (Oxides and Advanced Diffraction) group at *UCCS* has developed a good expertise in the rational design and crystallochemistry of new inorganic phases with striking properties. Numerous new materials have been synthesized and studied for applications such as fuel cell electrodes[1,2] or for heterogeneous catalysis[3] for example, which represent key areas related to renewable energies. We have access to a large toolbox of chemical reactions, characterizations and calculations/simulation tools for the conception of such materials with targeted properties. Our methodology involves a modular approach of inorganic compounds structures (oxides or related phases), i.e. their description into "autonomous" blocks, each one bringing its own specificities. This makes possible the targeted modification of specific secondary building units and their assembly into original intergrowths. In the framework of this PhD thesis project, we target the stacking of blocks, in particular in transition metal based compounds, with non-conventional anionic sub-arrays (e.g. non stœchiometric oxides, oxy-halides, oxy-hydrides etc…), that will allow modulating the valence states of the cationic sub-arrays (Mn, Fe, Co, Ni…). The synthesis methods will be as various as solid state synthesis, crystalline growth, hydrothermal routes, high pressure, extreme redox conditions, topotactic routes *etc* …

Topotactic Chemistry: Concerning the so-called *topotactic* synthesis techniques, the central part of this thesis, the project will take advantage of the skills gained by our group[4] and of leading groups. These methods rely on the non-destructive modification of phases exhibiting a capacity for oxygen removal/insertion (*topotactic* reduction/oxidation) for example or more generally for the modification of the anionic sub-lattice, including by incorporation of other anions (→ oxy-hydrides, oxy-sulfides, oxy-nitrides…). It is possible in this way to tune the electronic structure around the Fermi level (valence band, conduction band, gap) which dictates the potentialities for energy, optics, magnetism, electronic transport and catalysis; properties that will be studied in this project.

Ph.D. thesis starts october 2015

Financial support : Université Lille 1

Contacts : olivier.mentre@ensc-lille.fr **;** houria.kabbour@univ-lille1.fr

---

[1] Ehora, G. et al. *Chemistry of Materials* **20**, p7425-7433 **(2008)**
[2] Rolle, A. et al. *Solid State Ionics* **184**, p31-34 **(2011)**
[3] Perillat-Merceroz, C. *Chemistry of Materials* **23**, p1539-1550 **(2011)**
[4] David, R. et al. Angewandte Chemie - International Edition **53**, p13365-13370 **(2014)**