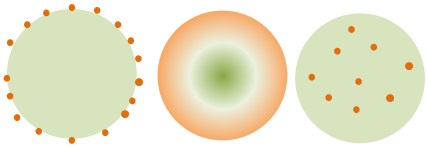
Internship 2018/19

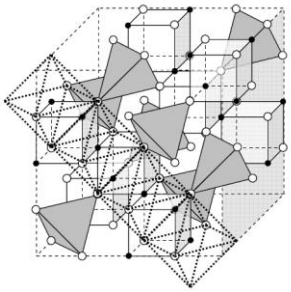
	Nanoparticles of mixed oxides and strain engineering for high-performace electrodes and saving applications
Location :	Laboratoire PMC - Ecole polytechnique, Route de Saclay – 91128 Palaiseau
Supervisor :	Isabelle MAURIN
e-mail/ telephone :	isabelle.maurin@polytechnique.edu, 01 69 33 47 31
	Details / short literature survey here – website of the group : here
Techniques :	Colloidal chemistry, dynamic light scattering, STEM coupled to EDX, powder x-ray diffraction possibly as a function of temperature (100-1400°C)
background :	Strong interest in materials science, study of the relationships between structure and properties. The student will be trained to the different techniques. A background in crystallography and diffraction techniques will be highly welcome.
Funding – Possibility to pursue the project as PhD :	yes

Our team is interested in mixed oxides with spinel crystal structure, which are extensively studied because of their wide range of properties: dielectric, magnetic, or low-cost alternative for the oxidation of water in photo-electrochemical devices reminiscent of photosynthesis. This project aims at the realization of hetero-structures based on oxides with intercalation properties (alkaline or alkaline earth) for applications in the field of electrochemical storage of energy (batteries). We intend to address a current issue in materials science, which is to understand how structural stresses induced by local variations in composition can influence the properties of the materials. In our case, we want to determine their influence on charge/discharge processes and their reversibility by developing core-shell hetero-structures to achieve a real strain engineering.

The first part of this internship will focus on the growth of multi-element oxides by colloidal routes. We want to characterize and determine which parameters control the distribution of a dopant within nanoparticles, that may lead to compositional gradients, surface segregation, or even differences of chemical composition between particles.

Spinel structure and various configurations for the distribution of the dopants





We propose to study three model systems of mixed spinel oxides for which the distribution of the cations between the tetrahedral and octahedral sites is well known in the bulk material: $CoAl_2O_4$ (assumed to be direct), $NiFe_2O_4$ (inverse), and $CuAl_2O_4$ (with random distribution). The distribution of cations within different particles will be studied by chemical mapping by STEM-EDX and powder x-ray diffraction.

The control of this stoichiometry will allow us to design core-shell hetero-structures combining two spinels or a spinel and a lamellar compound based on the same oxygen sublattice. Again, TEM and XRD will be the main tools used to characterize the obtained samples, specify the growth mode (heteroepitaxy) and highlight structural distortions in the shell reflecting a mechanical coupling with the core. The final objective is to test the electrochemical performances of these powders by inserting them into half-cells. These properties will be compared to those of single-phase materials of the same size (ie, of the same specific area) in order to highlight the influence of the coupling with the core on the charge/discharge rates, cycling and to outline future optimization strategies.