Titre de la thèse: *Simulation of functional mixed-oxides*

Oxides are the most abundant natural materials in our environment. Man has long utilized them but it is only recently that he realized that many technologies of the XXIst century will be based on oxides and more specifically on artificial nano-oxides. In particular doped and especially mixed (ternary) oxides represent an emerging research field with potential applications in materials for energy and environment, etc. However, there are presently large gaps in our understanding of the formation, structures and properties of such oxide nano-objects.

The goal of the thesis will be to bring fundamental understanding on important technological or natural oxide nano-objects, a large part of which have not been looked at before. Until now, most if not all studied nano-oxides have been binary oxides, while modern technology requires varying at will the cationic composition to obtain targeted specific properties (optical properties, surface reactivity, etc.). In the natural environment, the formation of solid-solutions is the law rather than the exception, foreign cation incorporation occurring easily in the first steps of mineral nucleation.

Using a multiscale strategy of numerical simulations, the study will focus on the changes in thermodynamic phase diagrams and in structure, composition and chemical ordering which occur at oxide solid-solution surfaces, interfaces, thin films, or nano-particles, due to low dimensionality and finite size effects --- presence of facets, edges and kinks. In particular, it will be interesting to demonstrate how the differences of cationic size, valence, structure and iono-covalent character of the constituents combine to determine the stability diagram of mixed nano-oxides, and derive the general laws they obey.

Techniques involved: numerical simulations