



Ph.D. defense

Institut de Chimie Séparative de Marcoule / CEA Marcoule
(UMR 5257, CEA, CNRS, Université Montpellier, ENSCM)

KÉVIN RUFFRAY

will present his Ph.D. dissertation

Synthesis and physicochemical study of molecular and self-assembled d-f heterometallic systems

The defense will take place on **Thursday, December 10, 2015 at 10.00 am**
in Visiatome Auditorium

The interactions between an f metal and its environment are studied in several fields (nuclear industry, electronics ...). However, those phenomena are often misunderstood in a fundamental point of view. The interactions which are able to settle between d and f metals are partly studied, mainly in the field of magnetism. The charge transfer phenomena were however less studied, despite an increasing interest in numerous systems. This study intends to develop molecular systems which allow studying numerous physicochemical properties of d-4f and d-5f systems, along with their transposability towards coordination polymers systems exhibiting d and f mixed metallic nodes. On the molecular systems, studies focused on photo-induced charge transfer from a d metal to an f metal and on their electrochemical properties. In order to do this, it was necessary to develop several molecular reference systems based on Ru allowing the addition of a 4f or 5f metal. The molecular systems, Ru and mixed Ru-f element, were characterized. Comparative photo-physical and electrochemical studies, experimental and theoretical (DFT and TD-DFT), between the monometallic Ru and the Ru-4f and Ru-5f systems have been achieved. Coordination polymers systems have been broached to enlarge the comparative study of the d-f mixed systems to 3D compounds. To that end, the synthesis of systems containing a d metal, an f metal and a ditopic ligand (2,5-dihydroxy-1,4-benzoquinone, DHBQ) has been studied, the aim being the controlled integration of the d metal in a well-known 4f-DHBQ polymeric structure. These studies showed that the introduction of a d metal in this type of coordination polymers is not possible in the study conditions for kinetic reasons. However, for the same kinetic reasons, the presence of the d metal during the synthesis influences in a significant way the morphology of the 4f-DHBQ compounds, opening other perspectives to these 4f systems. Thus, it is possible to use them as hard materials precursors (oxides, carbides) whose structural and microstructural aspects are controlled via structural and morphological properties of the coordination polymer.

Keywords: transition metals; lanthanides; natural actinides; coordination chemistry; reactivity

