

# Séminaire Labex ARCANE

Mardi 18/10/2016 - 14h à 16h30

*Salle de conférences de Nanobio – 570 rue de la chimie –  
Campus Saint Martin d'hères*

14h – 15h ***“Computational studies of oxygen activating enzymes and biomimetic model complexes”***

Sam P. De Visser

University of Manchester

Metalloenzymes perform vital functions for human health including the biosynthesis and biodegradation of compounds. In particular, the cytochrome P450s are heme based monooxygenases involved in drug metabolism reactions in the liver. Their catalytic cycle uses molecular oxygen, two reduction equivalents and two protons in order to transfer one oxygen atom to a substrate. Recently, a new class of P450 isozymes was discovered that utilizes  $H_2O_2$  instead and would not need a reduction partner. In this presentation, I will cover the catalytic mechanism of these P450 peroxygenases in a reaction with palmitic acid and discuss the bifurcation processes leading to terminal olefins and  $\alpha$ - and  $\beta$ -hydroxy palmitic acid. These product distributions are relevant to biotechnology where olefins find use as biofuels. The study implicates a spin-selective product distribution, which is explained with valence bond models and thermochemical cycles.



Sam de Visser received his B.Sc. degree from the College of Zeeland and M.Sc. and Ph.D. degrees from the University of Amsterdam (The Netherlands) in Organic Mass Spectrometry. Thereafter, he moved to the field of Theoretical Chemistry and performed postdoctoral research at King's College London (1997–1999) and at the Hebrew University of Jerusalem (1999–2004). He then moved to the United Kingdom, where he obtained a Lectureship position at the University of Manchester. His research interests are in the field of biomimetic and metalloenzyme reaction mechanisms using QM-cluster as well as QM/MM methodologies.

15h – 15h30 ***“Light-driven oxidation of organic substrates by activating small molecules ( $H_2O$  and  $O_2$ )”***

Olivier HAMELIN

Laboratoire de Chimie et Biologie des Métaux

15h30 – 16h ***“Formation of  $H_2O_2$  in Superoxide Reductase: Protonation or Dissociation First? Conformational and Mechanistic Study using MM Dynamics and QM/MM Metadynamics”***

Rolf DAVID

Equipe de Chimie Théorique, Département de Chimie Moléculaire

16h-16h30 ***Autour d'un café***