LABORATOIRE
DE CHIMIE
ENS DE LYON

Post-Doc

Modelling Catalyst Deactivation of Homogeneous Cross-Metathesis Catalysts

Olefin metathesis reactions promise to be powerful tools to switch from petro-chemistry to biomass-based commodities and fine chemicals such as essential oils. This last application has been exemplified by our experimental collaborator, Prof. Deryn Fogg (J. Am. Chem. Soc. 2012, 134, 18889). One major issue of olefin metathesis reactions of biomass is the presence of water: even traces of water tend to deactivate the ruthenium based homogeneous catalyst.

The aim of the project is to understand which species in the catalytic cycle is responsible for the deactivation and investigate possibilities to circumvent the deactivation by ligand design. Experimental studies at the University of Ottawa are underway. The computational study will be performed at the ENS Lyon, at the laboratory of chemistry. We will apply density functional theory in combination with implicit solvents and micro-solvation where required.

The exchange with Ottawa, Canada is part of an 8-years project (LIA FUN-CAT), which provides means for travelling.

The theoretical chemistry group of the Laboratoire de Chimie of the ENS de Lyon is a group of 20 to 30 people is expert in modeling chemical reactivity in a wide range of context, from excited state to ground state reactivity, from biochemistry to catalysis.

Lyon is internationally renown for Chemistry (especially in Catalysis and metathesis with the Nobel Prize of Yves Chauvin) but also for being a historical and architectural landmarks (UNESCO World Heritage Site) and being recognized as the French capital of gastronomy.

Supervisors	Dr. Carine Michel (carine.michel@ens-lyon.fr) Dr. Stephan Steinmann (stephan.steinmann@ens-lyon.fr)
Duration and start date	Duration: 18 months. Starting: as soon as possible.
Net Salary	Roughly 2'000 Euros per month
Academic requirements	PhD in computational chemistry
Language requirements	Fluency in French and/or English
Other requirements	Experience with modelling transition metal complexes is an advantage Knowledge of Linux Willing to travel to Ottawa roughly every 6 months, for 1-2 weeks each

UNIVERSITÉ DE LYON

ENS DE LYON