



## Postdoctoral position (2 year)

# Detailed chemical kinetic modeling of the impact of biofuels addition on the aging of conventional fuels

# Project description:

The increase of the share of biofuels in the transport sector, imposed by European regulations, requires studying their impacts on the aging of conventional fuels. This phenomenon finds its origin in the oxidation of liquid fuels and induces structural changes in the fuels, leading to safety problems and engine malfunction. Understanding and simulating these phenomena is therefore an important challenge. The microscopic mechanisms that govern these processes are identical to those involved in their combustion. Although the kinetic combustion models (gas) are well established in the literature, their adaptation to the liquid phase remains a major challenge. This project aims to study the impact of the addition of biofuels on the aging of conventional fuels using simulations tools. The hired candidate will be responsible for the development of a detailed kinetic model for the oxidation of the fuel / biofuel mixtures (surrogate molecules) by adapting the existing combustion models to the liquid phase, using an equilibrium thermodynamic code based on theoretical chemistry methods.

#### **Qualifications:**

The candidate must have a PhD in chemical engineering, physical chemistry, theoretical chemistry or other close fields. Knowledge in chemical kinetics and physical chemistry is required. Knowledge in detailed chemical combustion model development, ideal reactor simulation (e.g., Chemkin), and theoretical chemistry would be appreciable. Good oral and written communication skills are also required.

## Appointment:

The appointment period is for one year, starting December 1<sup>st</sup> 2018. Gross salary is about 2550 € and depends on the candidate experience.

## Application:

Prospective candidates should contact Dr Baptiste Sirjean (<u>baptiste.sirjean@univ-lorraine.fr</u>) and Pr Romain Privat (<u>romain.privat@univ-lorraine.fr</u>) and need to provide a detailed academic CV, including a list of publications.

## Laboratory and context:

The research will be perform in the Kinetic, Thermodynamic, Energy group of the Laboratory of Reactions and Process Engineering (http://lrgp-nancy.cnrs.fr/) in Nancy. This work will be perform within the ANR project BioACE that aims to study the impact of biofuels on the aging of conventional fuels.





