THESE MESRI

Experimental and Theoretical Study of Biofuel Oxidation Using Photoelectron Spectroscopy Coupled with Synchrotron Radiation and Chemical Quantum Calculations

Context

Although lignocellulosic biomass is recognized as a sustainable and renewable energy source, the impact of biofuels on pollutant emissions remains unclear, whether they are used as additives or as direct substitutes for conventional hydrocarbons. Biofuels have a complex molecular diversity, including alcohols, ethers, and carboxylic esters, making them more complex than conventional hydrocarbons. This complexity significantly influences their reactivity and combustion properties. Therefore, optimizing pollutant emissions in industrial processes involving wood or biofuel combustion requires a detailed understanding of the chemical reactions at the molecular level during the oxidation of alternative fuel compounds.

Thesis Objectives

The first stage of this doctoral project will involve conducting laboratory experiments to replicate oxidation reactions in a well-stirred reactor operating at atmospheric pressure and capable of reaching temperatures up to 1,000 K. This reactor will be linked to several analytical instruments to identify and quantify a wide range of reaction products. The thesis will primarily focus on using an innovative analytical method, photoelectron spectroscopy with synchrotron radiation, which will provide detailed information on the molecular structure of intermediate species formed by recording their vibrational signature. These experiments will be combined with quantum chemistry calculations to simulate the vibronic envelope of these intermediates to enhance their identification. Based on these data, the second stage will involve determining the main chemical transformation pathways of the oxidized compounds to develop kinetic models that will be validated by comparing their predictions with quantitative data obtained experimentally in the laboratory.

Candidate Profile:

We are looking for a candidate with an engineering degree or a master's in at least one of the following fields: molecular dynamics/chemical kinetics/combustion chemistry. Experience in mass spectrometry, gas chromatography, or spectroscopy is an advantage. Programming skills and familiarity with quantum chemistry software are also considered. While fluency in French is not required, good proficiency in English, both spoken and written, is necessary.

Scientific Supervisors:

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Jérémy Bourgalais, CR CNRS, jeremy.bourgalais@cnrs.fr

Salary: €2,074 gross monthly

Duration and Start Date of the Thesis: 3 years, starting on October 1, 2024

Practical Information: The thesis will be conducted at LRGP in Nancy and offers opportunities for international travel to meet collaborators. The candidate is expected to disseminate their results through scientific publications and conferences.