ResEX program

PhD defense notice

Anthony ABOU DIB

will publicly defend his PhD thesis entitled

Methodological development in FT-ICR MS for the analysis of bio-oils produced by pyrolysis of lignocellulosic biomass

on **Wednesday 3 May 2023 at 9:00 am**

at the Amphitheater of the Institut Supérieur d'Électronique et d'Automatique (ISEA), 7 Rue Marconi, 57070 Metz Technopôle

Jury members

Pr. Laurence CHARLES	Professor, ICR, University of Aix-Marseille	Rapporteur
Dr. Nadège CHARON	Research Engineer, IPF Energies Nouvelles	Rapporteur
Dr. Marie HUBERT-ROUX	Research Engineer, COBRA, University of Rouen Normandy	Examiner
Dr. Yann LE BRECH	Assistant professor, LRGP, University of Lorraine	Examiner
Pr. Guillaume VAN DER REST	Professor, ICP, University of Paris Saclay	Examiner
Pr. Stephanie HESSE	Professor, LCP-A2MC, University of Lorraine	Jury President
Dr. Vincent CARRÉ	Assistant professor, LCP-A2MC, University of Lorraine	Supervisor
Pr. Frédéric AUBRIET	Professor, LCP-A2MC, University of Lorraine	Supervisor

Keywords: *Bio-oils, pyrolysis, Fourier transform ion cyclotron resonance mass spectrometry, SPE, fractionation, derivatization, two-dimensional mass spectrometry, UVPD, petroleomic approach.*

Abstract:

Bio-oils from lignocellulosic biomass are promising sources for producing biofuels and high-added-value chemicals. Different processes, such as pyrolysis, allow the conversion of lignocellulosic biomass into bio-oils. The composition of these bio-oils is complex and contains highly oxygenated compounds, which limits their use. Therefore, these bio-oils must be upgraded by catalytic deoxygenation and/or cracking treatments. To determine the effectiveness of the catalytic treatments, a thorough knowledge of the chemical composition of bio-oils is required. A high-resolution mass spectrometer, such as Fourier Transform Ion Cyclotron Resonance (FT-ICR MS) coupled with ESI, APPI, and APCI, allows for in-depth study of the composition of the generated bio-oil at the molecular level. To evaluate the chemical characteristics of these compounds, the research conducted in this PhD thesis focuses on two aspects. The first is based on developing an analytical fractionation/derivatization method to label oxygen-containing compounds according to their functional groups. Combining solid-phase extraction (SPE) with an anion exchange sorbent and derivatization with stable isotope-labeled agents demonstrated, the identification of several oxygenated classes of bio-oil constituents by FT-ICR MS analyses. The second aspect is applied for the first time to bio-oil analysis. It uses two-dimensional ultra-violet photodissociation mass spectrometry (UVPD-MS) for structural analysis of the bio-oil components. Without using the conventional precursor ion isolation and fragmentation for MS/MS experiment, 2D-UVPD-MS has proven to be a powerful tool for performing tandem mass spectrometry experiments on such a complex system. 2D-UVPD-MS has showed to efficiently fragment small, single-charged molecules and to produce fragment ions from various chemical species, such as bio-oil components, thus providing useful structural information.