

ASMS 2024 Workshop Report

Interest Group “Energy, Petroleum and Biofuels“

Title “Aiding Energy Transition through Mass Spectrometry: Progress and Pathways Ahead”

Presiding: Christopher P. Ruger (University of Rostock) & David Stranz (Sierra Analytics)

Date: 4th of June, 5:45-7:00 PM

Participants: ~35 people

Christopher Ruger gave a short introduction of the speakers and program. He actively motivated everyone to check their interest group memberships. Three speakers had been invited to give a brief 5-10 min overview on current challenges in research on energy materials, petroleum and biofuels utilizing mass spectrometry.

Prof. Wolfgang Schrader from the Max-Planck-Institut fur Kohlenforschung (Muhlheim, Germany) started with a lively presentation on “Structural Elucidation in Complex Mixtures: What is really in a crude oil?”. He nicely motivated the combination of morphological and structural information retrieved by electron microscopy with data from high-resolution mass spectrometry and theoretical consideration via computational calculations. It can be concluded, that this sophisticated approach will definitely not only be useful for fossil matrices but also for modern challenges in bio- and recycling-fuel.

Prof. Boniek Gontijo Vaz from the Universidade Federal de Goias Goiania Goias (Brazil) presented on unraveling the complex chemical fingerprint of different crude oil products or fossil reservoirs with mass spectrometry (Opportunities for Mass Spectrometry in Oil & Gas through Energy Transition). This classical *Petroleomics* attempt was made possible by deploying different data analysis approaches with strong focus on chemometrics. Aside other findings, this workflow allowed for precise prediction of total acid number (TAN).

Dr. Pierre Giusti from TotalEnergies and CNRS (France) concluded the presentations with an exciting speech on lithium battery chemistry explored with ultra-high resolution mass spectrometry. This innovative research shows the broadening of mass spectrometry research for all variations of energy materials. In the specific case, only the superior mass resolving power and mass accuracy of Fourier-transform ion cyclotron resonance mass spectrometry enabled confident annotation of Lithium-organic degradation products in the electrolytes and membranes. Hereby, the strong sensitivity of the matrix to any oxygen and moisture required the usage of a vacuum MALDI approach.

The workshop ended with an active discussion. A key question was, if “Is energy transition and sustainability underrepresented in the ASMS?”. This aspect is of great importance as global climate change and various environmental problems, e.g., emerging pollutant, are interconnected to energy transition being one of the greatest challenges to humankind in the 21st century. Additionally, there has been an active discussion about renaming the interest group. This action should transform the interest group from its “fossil past” to a broader audience. However, this renaming has to be discussed with ASMS and should not interfere with other existing interest groups (even though there is none for “material science” specifically). Finally, to increase attendance at ASMS in this field, advertising this conference to colleagues from the field as an immense chance for networking in analytical science has been mentioned.