

ASMS 2023 Energy, Petroleum, and Biofuels Interest Group Workshop: “The Role of Mass Spectrometry in Emerging Energy Technologies Development”

Presiding: Yuri Corilo¹ and Leonard Nyadong²

1 - Environmental Molecular Sciences Laboratory, Pacific Northwest National *Laboratory*,
Richland WA, USA

2 - Phillips 66 Energy Research and Innovation, Bartlesville OK, USA

Date & Time: Monday, June 5, 2023. 5:45 – 7:00 pm

Place: George R. Brown Convention Center, Room 310 A

Workshop Outline

1. Yuri Corilo
 - o Welcome, Introduction and Workshop Overview
2. Two speakers (20 minutes each followed by a 5-minute question) on the topic of “The Role of Mass Spectrometry in Emerging Energy Technologies Development.”
 - o Ryan P. Rodgers (National High Magnetic Field Laboratory)
 - o Christopher Rüger (University of Rostock)
3. Leonard Nyadong
 - o Panel Discussion
4. Question from the audience
 - o General discussion points

Workshop Summary

The ASMS Energy, Petroleum, and Biofuels Interest Group held its workshop on Monday evening (June 5th, 2023) as part of the 71st ASMS Conference on Mass Spectrometry and Allied Topics in Houston, TX. Interest Group coordinators Yuri Corilo and Leonard Nyadong presided. Approximately 40 – 50 people were in attendance.

The workshop proceeded with an introduction of the topic, which was centered around three charged questions regarding the role of mass spectrometry in emerging energy technologies as follows: What innovations are needed in mass spectrometry in all emerging energy areas? What areas could benefit from existing mass spectrometry technologies? How could our community help?

Ryan P. Rodgers presented insights on the characterization of water and oil soluble polyfunctional oxygenates species using direct infusion ultra-high-resolution mass spectrometry data. The discussion focused on the ability to obtain quantitative data and the effects of ionization suppression in matrices different from petroleum. Another

essential discussion was the increased heteroatomic complexity of natural products compared to petroleum samples, which increased the complexity of the data and decreased the confidence of molecular formula assignments due to the increased heteroatomic content.

Christopher Ruger shared thoughts on biofuel upgrading and how mass spectrometry and other technologies can help characterize pyrolysis products and solids residue fractions.

This workshop concluded with a panel and questions and answers session led by Leonard Nyadong. At the end of the session, a call was put out for volunteers to organize subsequent interest group workshops. Two volunteers, namely, Christopher Ruger and David D. Stranz agreed to take on the role.

Respectfully,

Yuri Corilo and Leonard Nyadong.

June 2023