

# ***2024 Winter Conference on Plasma Spectrochemistry***

***Short Courses***

***Professional Development Courses***

***Friday – Saturday,  
January 12 – 20, 2024***

***Course Descriptions***

***Course Hours:***

***8 am - 12 noon***

***1 pm - 5 pm***

***7 pm - 11 pm***



# 2024 Winter Conference Short Courses

## Friday, January 12 – Saturday, January 20, 2024

### Schedule

#### Analysis by Plasma Spectrochemistry

- SA-01 LA-ICP-MS Elemental Analysis of Incremental Tissues as an Indicator of Past Pollution Events**, Friday, January 12, 7 pm, Dula Amarasiriwardena, daNS@hampshire.edu, Hampshire College, School of Natural Science, Amherst, MA 01002-3359
- SA-02 Environmental Isotope Geochemistry: Plasma Spectrochemistry as an Essential Tool**, Saturday, January 13, 8 am, Michael E. Ketterer, michael.ketterer@nau.edu, Department of Chemistry and Biochemistry, Northern Arizona University, Box 5698, Flagstaff, AZ 86011-5698
- SA-03 Speciation Analysis: Elemental, Isotopic and Molecular Mass Spectrometry in Life Sciences Studies**, Saturday, January 13, 7 pm, Olivier Donard, olivier.donard@univ-pau.fr, MARSS-IPREM, University of Pau, Pau, France
- SA-04 Fluorine Detection with and ESIMS and Applications**, Sunday, January 14, 7 pm, Jörg Feldmann, joerg.feldmann@uni-graz.at, j.feldmann@abdn.ac.uk, and Viktora Müller, TESLA - Analytical Chemistry Institute of Chemistry, University of Graz, Universitätsplatz 1, 8010 Graz, Austria
- SA-05 Implementing Clinical ICP-MS for Clinical Diagnosis, Biomonitoring and Emergency Response**, Sunday, January 14, 8 am, Cynthia D. Ward, CWard@cdc.gov, and Deanna Jones, DMJones1@cdc.gov, Centers for Disease Control and Prevention (CDC), 4770 Buford Hwy, Mailstop S110-5, Atlanta, GA 30341-3717
- SA-06 Tagging Approaches for Development of Immunoassays for ICP-MS Detection**, Saturday, January 13, 8 am, Norbert Jakubowski, norbi.jakubowski@gmail.com, Spetec GmbH, Am Kletthamer Feld 15, 85435 Erding, Germany;
- SA-07 Characterization of Nanomaterials: Focusing on Engineered Nanoproducs and Plastics in the Approach One Health?** Saturday, January 13, 7 pm, Petra Krystek, petra.krystek@uni-siegen.de, and Carsten Engelhard, engelhard@chemie.uni-siegen.de, University of Siegen, Department of Chemistry and Biology, Siegen, Germany
- SA-08 Analysis of Nano/microplastics and Their Role as Trojan Horses**, Sunday, January 14, 7 pm, Javier Jiménez-Lamana, j.Jimenez-lamana@univ-pau.fr, IPREM CNRS UMR 5254, Technopole Hélioparc, 2 avenue du president Angot, 64053 Pau, France
- SA-09 Analysis of Petroleum and Petroleum Products**, Monday, January 15, 7 pm, José Luis Todolí, jose.todoli@ua.es, Department of Analytical Chemistry, Nutrition and Food Sciences, University of Alicante, PO Box 99, 03080 Alicante, Spain
- SA-10 Single Particle and Single Cell ICP-MS Theory and Applications**, Saturday, January 13, 1 pm, Chady Stephan, chady.stephan@perkinelmer.com, and Ruth Merrifield, ruth.merrifield@perkinelmer.com, PerkinElmer, 501 Rowntree Dairy Rd, Woodbridge, ON L4L 8H1, Canada
- SA-11 New Inorganic and Isotopic Strategies for High Geographical Resolution Traceability. Application to Environmental and Food Related Issues**, Monday, January 15, 7 pm, Olivier Donard, olivier.donard@univ-pau.fr, MARSS-IPREM, University of Pau, Pau, France
- SA-12 Elemental Imaging at Micro- and Nanometer Scale for Applications in Biology, Nutrition, Toxicology, and Geology**, Saturday, January 13, 1 pm, Dirk Schaumlöffel, dirk.schaumloeffel@univ-pau.fr, IPREM CNRS UMR 5254, Heloparc, 2 avenue du president Angot, 64053 Pau, France
- SA-13 Edible Insects (& Other Novel Proteins). The Role of ICP-MS in a Safe and Sustainable Global Food System**, Sunday, January 14, 1 pm, Kelly LeBlanc, Kelly.Leblanc@nrc-cnrc.gc.ca, National Research Council Canada, Metrology Research Centre, 1200 Montreal Rd, Ottawa, ON, Canada K1A 0R6

#### Spectrochemical Instrumentation

- SI-01 New Calibration Strategies in Spectrochemical Analysis**, Tuesday, January 16, 7 pm, George L. Donati, donatigl@wfu.edu, Wake Forest University, Department of Chemistry, Winston-Salem, NC 27109
- SI-02 Opportunities, Challenges, and Application of Glow Discharge Techniques**, Sunday, January 14, 8 am, Volker Hoffmann, Leibniz Institute for Solid State and Materials, Research Dresden, PO Box 27 00 16, D-01171 Dresden, Germany, v.hoffmann@ifw-dresden.de; Peter K. Robinson, pete@masscare.co.uk, MassCare Ltd., 11 Waterside Way, Middlewich, Cheshire, CW 10 9HP, United Kingdom
- SI-03 ICP-TOFMS: Fundamental and Application for Single-Particle Analysis**, Friday, January 12, 1 pm, Alex Gundlach-Graham, alexgg@iastate.edu, Iowa State University, 1605 Gilman Hall, 2415 Osborne Dr, Ames, IA 50011
- SI-04 ICP-MS I: Introduction**, Saturday, January 13, 1 pm, John Olesik, olesik.2@osu.edu, Ohio State University, School of Earth Sciences, 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002
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- SI-06 Theory and Practical Use of Reaction Cells and Collision Cells for ICP-MS**, Sunday, January 14, 7 pm, Patrick Gray, patrick.gray@fda.hhs.gov, Center for Food Safety and Applied Nutrition, Office of Regulatory Science, U.S. Food and Drug Administration, College Park, MD
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- SI-09 Identification and Correction of Interferences in Practical ICP-MS**, Tuesday, January 16, 7 pm, Deborah Bradshaw, bradshawdk@cs.com, Atomic Spectroscopy Consulting, PO Box 536307, Orlando, FL 32853-6307
- SI-10 The Chemical Analysis of Things As They Are? Direct Atomic and Molecular Analyses with Ambient Mass Spectrometry**, Saturday, January 13, 7 pm, Carsten Engelhard, engelhard@chemie.uni-siegen.de, Department of Chemistry and Biology, University of Siegen, Siegen, 57076 Germany; Jacob T. Shelley, shellj@rpi.edu, Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Troy, NY 12180
- SI-11 Ultra-High Resolution in Plasma-Assisted Atomic/Isotopic/Molecular Analysis by Orbitrap Mass Spectrometry**, Sunday, January 14, 8 am, Kenneth Marcus, marcusr@clemson.edu, Clemson University, Department of Chemistry, Clemson, SC 29672, and Davide Bleiner, davide.bleiner@empa.ch, EMPA, Überlandstrasse 139, CH-8600 Dübendorf, Switzerland

### Sample Introduction Approaches

- SS-01 A Practical Guide to Nebulizers and the Part They Play in Modern Sample Introduction**, Saturday, January 13, 7 pm, Steve Mangum, steve.mangum@icpms.com, Elemental Scientific Inc., 7277 World Communications Dr, Omaha, NE 68132
- SS-02 Laser Ablation Mass Spectrometry**, Saturday, January 13, 1 pm, Detlef Günther, guenther@inorg.chem.ethz.ch, Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 1, 8093 Zurich, Switzerland
- SS-03 Latest Advances in Laser Ablation-Based Chemical Analysis and Emerging Applications: LIBS, LA-ICP-(OES/MS), and Tandem LA – LIBS**, Monday, January 15, 7 pm, Jhanis Gonzalez, jhanis@appliedspectra.com, jjgonzalez@lbl.gov, Applied Spectra, Inc., 950 Riverside Pkwy, Suite 90, West Sacramento, CA 95605-15071
- SS-04 Variations of Single Particle Inductively Coupled Plasma Mass Spectrometry**, Diane Beauchemin, diane.beauchemin@queensu.ca, Saturday, January 20, 1 pm, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada
- SS-05 Electrothermal Vaporization - ICP for the Direct Analysis of Solids**, Diane Beauchemin, diane.beauchemin@queensu.ca, Saturday, January 20, 8 am, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada
- SS-06 Artificial Intelligence (e.g., via Artificial Neural Networks, Machine Learning, Deep Learning) and Some Applications to ICP and to Microplasma Spectrochemistry**, Sunday, January 14, 1 pm, Vassili Karanassios, vkaranassios@uwaterloo.ca, University of Waterloo, Department of Chemistry and Waterloo Institute for Nanotechnology, Waterloo, ON N2L 3G1, Canada
- SS-07 Laser-Induced Breakdown Spectroscopy (LIBS)**, Tuesday, January 16, 7 pm, Vassilia Zorba, vzorba@lbl.gov, Laser Technologies Group, Lawrence Berkeley National Laboratory, Berkeley, CA 94720

### Plasma Spectrochemical Techniques

- ST-01 Critical Factors for Successful R&D Development Projects**, Saturday, January 13, 8 am, Andrew T. Zander, atzander1027@gmail.com, Technical Consultant, SCLS, Inc., 1112 Via Coronel, Palos Verdes Estates, CA 90274
- ST-03 High Precision and Accuracy Isotopic Analysis by MC-ICP-MS**, Saturday, January 13, 8 am, Lu Yang, lu.yang@nrc-cnrc.gc.ca, National Research Council Canada, 1200 Montreal Rd, Ottawa, ON, K1A 0R6, Canada
- ST-04 Starting a New Laboratory or Modifying Your Existing Laboratory for Trace Analyses**, Sunday, January 14, 8 am, Ela Bakowska, ela@bakowska.com, bakowskae@corning.com, Elba Elemental Consulting, PO Box 1053, Corning, NY 14830
- ST-05 Fundamentals, Plasma Diagnostics, Measurements, and Applications of Analytical Plasmas**, Sunday, January 14, 8 am, Igor B. Gornushkin, igor.gornushkin@bam.de, BAM, Federal Institute for Materials Research and Testing, Berlin, Germany
- ST-06 Triple Quad (QXQ) ICP-MS**, Sunday, January 14, 1 pm, R. Steven Pappas, rpappas@cdc.gov, Naudia Gray, NGray@cdc.gov, Centers for Disease Control & Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341-3717
- ST-07 sp-QQQ-ICP-MS, ETV-QQQ-ICP-MS, GC-QQQ-ICP-MS, HPLC-QQQ-ICP-MS, QQQ-ICP-MS: Method Development, Problem Solving, Troubleshooting and Optimization**, Saturday, January 13, 1 pm, Mark Fresquez, mwf6@cdc.gov, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341-3717

**ST-08 Sample Preparation Problem Solving for Atomic Mass Spectrometry**, Sunday, January 14, 7 pm, R. Steven Pappas, rpappas@cdc.gov, Naudia Gray, ngray@cdc.gov, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341-3717

**ST-09 Validation Assessment and ISO/IEC 17025: An Interactive Session**, Sunday, January 14, 1 pm, Rob Ritsema, robritsema@gmail.com, RR Quality Consultancy, Amersfoort, The Netherlands; Petra Krystek, petra.krystek@uni-siegen.de, University of Siegen, Department of Chemistry and Biology, Siegen, Germany

**ST-10 Metrology Concepts in Plasma Spectrochemistry**, Saturday, January 13, 8 am, Zoltan Mester, zoltan.mester@nrc-cnrc.gc.ca, National Research Council of Canada (NRC), 1200 Montreal Rd, Building M-58, Ottawa, ON K1A0R6, Canada

**ST-11 Sample Classification Using Elemental Fingerprint Analysis**, Saturday, January 13, 7 pm, Andreas Limbeck, andreas.limbeck@tuwien.ac.at, and Lukas Brunnbauer, TU Wien, Institute of Chemical Technologies and Analytics, Getreidemarkt 9/164, A-1060 Vienna, Austria

**ST-12 Nanomaterials: Advances in Standardization, Measurement Methods, Reference Materials and Remaining Challenges Imposed by Regulation**, Monday, January 15, 7 pm, Heidi Goenaga-Infante, LGC Limited, Queens Road, Teddington, Middlesex TW1 1 OLY, U K, heidi.goenaga-infante@lgcgroup.com

**ST-13 Agilent ICP-Expert/ Masshunter Workshop**, Tuesday, January 16, 7 pm, Chuck Schneider et al., chuck.schneider@agilent.com, Agilent Technologies, 2850 Centerville Rd, Wilmington, DE 19808

### Schedule by Date and Time

#### Friday, January 12, 1 pm

**SI-03 ICP-TOFMS: Fundamental and Application for Single-Particle Analysis**, Alex Gundlach-Graham, alexgg@iastate.edu, Iowa State University, 1605 Gilman Hall, 2415 Osborne Dr, Ames, IA 50011

#### Friday, January 12, 7 pm

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#### Saturday, January 13, 8 am

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**SA-06 Tagging Approaches for Development of Immunoassays for ICP-MS Detection**, Norbert Jakubowski, Spetec GmbH, Am Kletthamer Feld 15, 85435 Erding, Germany; norbi.jakubowski@gmail.com

**ST-01 Critical Factors for Successful R&D Development Projects**, Andrew T. Zander, atzander1027@gmail.com, Technical Consultant, SCLS, Inc., 1112 Via Coronel, Palos Verdes Estates, CA 90274

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**SS-02 Laser Ablation Mass Spectrometry**, Detlef Günther, guenther@inorg.chem.ethz.ch, Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 1, 8093 Zurich, Switzerland

**ST-07 sp-QQQ-ICP-MS, ETV-QQQ-ICP-MS, GC-QQQ-ICP-MS, HPLC-QQQ-ICP-MS, QQQ-ICP-MS: Method Development, Problem Solving, Troubleshooting and Optimization**, Mark Fresquez, mwf6@cdc.gov, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341-3717

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**SA-07 Characterization of Nanomaterials: Focusing on Engineered Nanoproducs and Plastics in the Approach 'One Health'**, Petra Krystek, petra.krystek@uni-siegen.de, and Carsten Engelhard, engelhard@chemie.uni-siegen.de, University of Siegen, Department of Chemistry and Biology, Siegen, Germany

**SI-10 The Chemical Analysis of Things As They Are? Direct Atomic and Molecular Analyses with Ambient Mass Spectrometry**, Carsten Engelhard, engelhard@chemie.uni-siegen.de, Department of Chemistry and Biology, University of Siegen, Siegen, 57076 Germany; Jacob T. Shelley, shellj@rpi.edu, Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Troy, NY 12180

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**SA-05 Implementing Clinical ICP-MS for Clinical Diagnosis, Biomonitoring and Emergency Response**, Cynthia D. Ward, CWard@cdc.gov, and Deanna Jones, DMJones1@cdc.gov, Centers for Disease Control and Prevention (CDC), 4770 Buford Hwy, Mailstop S110-5, Atlanta, GA 30341-3717

**SI-02 Opportunities, Challenges, and Application of Glow Discharge Techniques**, Volker Hoffmann, v.hoffmann@ifw-dresden.de, Leibniz Institute for Solid State and Materials, Research Dresden, PO Box 27 00 16, D-01171 Dresden, Germany; Peter K. Robinson, pete@masscare.co.uk, MassCare Ltd., 11 Waterside Way, Middlewich, Cheshire, CW10 9HP, United Kingdom

**SI-11 Ultra-High Resolution in Plasma-Assisted Atomic/Isotopic/Molecular Analysis by Orbitrap Mass Spectrometry**, Kenneth Marcus, marcusr@clemson.edu, Clemson University, Department of Chemistry, Clemson, SC 29672, and Davide Bleiner, davide.bleiner@empa.ch, EMPA, Überlandstrasse 139, CH-8600 Dübendorf, Switzerland

**ST-04 Starting a New Laboratory or Modifying Your Existing Laboratory for Trace Analyses**, Ela Bakowska, ela@bakowska.com, bakowskae@corning.com, Elba Elemental Consulting, PO Box 1053, Corning, NY 14830

**ST-05 Fundamentals, Plasma Diagnostics, Measurements, and Applications of Analytical Plasmas**, Igor B. Gornushkin, igor.gornushkin@bam.de, BAM, Federal Institute for Materials Research and Testing, Berlin, Germany

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**ST-09 Validation Assessment and ISO/IEC 17025: An Interactive Session**, Rob Ritsema, robritsema@gmail.com, RR Quality Consultancy, Amersfoort, The Netherlands; Petra Krystek, petra.krystek@uni-siegen.de, University of Siegen, Department of Chemistry and Biology, Siegen, Germany

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**SA-08 Analysis of Nano/microplastics and Their Role as Trojan Horses**, Javier Jiménez-Lamana, j.Jimenez-lamana@univ-pau.fr, IPREM CNRS UMR 5254, Technopole Hélioparc, 2 avenue du president Angot, 64053 Pau, France

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**ST-12 Nanomaterials: Advances in Standardization, Measurement Methods, Reference Materials and Remaining Challenges Imposed by Regulation**, Heidi Goenaga-Infante, heidi.goenaga-infante@lgcgroup.com, LGC Limited, Queens Road, Teddington, Middlesex TW1 1 OLY, UK

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### Saturday, January 20, 8 am

**SS-05 Electrothermal Vaporization - ICP for the Direct Analysis of Solids**, Diane Beauchemin, diane.beauchemin@queensu.ca, Saturday, January 20, 8 am, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada

### Saturday, January 20, 1 pm

**SS-04 Variations of Single Particle Inductively Coupled Plasma Mass Spectrometry**, Diane Beauchemin, diane.beauchemin@queensu.ca, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada

## **2022 Winter Conference Short Courses** **Friday, January 12 – Saturday, January 20, 2024**

### **Descriptive Abstracts**

#### **Analysis by Plasma Spectrochemistry**

**SA-01 LA-ICP-MS Elemental Analysis of Incremental Tissues as an Indicator of Past Pollution Events**, Friday, January 12, 7 pm, Dula Amarasiriwardena, duNS@hampshire.edu, Hampshire College, School of Natural Science, Amherst, MA 01002-3359

Human teeth, hair, shells, tree rings and fish otolith are examples of incrementally deposited tissues with a defined time axis. These tissues are repositories of trace metals and excellent materials for detection of past pollution episodes. We will introduce how microprobe techniques like LA-ICP-MS methods can be used for analysis of these incremental tissues. We will present LA-ICP-MS instrumentation, theory practice, troubleshooting hints, as well as sample preparation, and instrument calibration strategies for LA-ICP-MS. Unique applications in biology, environmental sciences, archeology, anthropology, and forensic science will be presented. Analytical advantages and limitations of each method will be discussed.

#### **Key Learning Objectives:**

- We will learn about theory, fundamentals of LA-ICP-MS,
- Analytical advantages and limitations, and trouble shooting skills.
- We will introduce how microprobe techniques like LA-ICP-MS methods can be used for analysis of these incremental tissues to gain valuable archived elemental information for interdisciplinary applications.

#### **Course outline:**

- LA-ICP-MS principles and instrumentation.
- Analytical advantages, limitations and trouble shooting skills.

- What are incremental biological tissues?
- What is the archived elemental information in hard tissues (teeth, bones, tree rings, hair etc.,)?
- Sample preparation and calibration strategies
- Data analysis
- Elemental bioimaging
- Applications in biology, environmental sciences, anthropology, and archaeology.

**Dula Amarasiriwardena**, Emeritus Professor of Chemistry at Hampshire College, Amherst, Massachusetts received his Ph.D. in Analytical Chemistry from North Carolina State University, Raleigh, NC. Dula teaches analytical chemistry, environmental chemistry, and general chemistry. His research is focused on the transport properties and the fate of trace metals and metal nanoparticles in soil and aquatic environments. Dula is also interested in the application of laser ablation (LA)-ICP-MS for investigation of trace metal nutrition and the exposure to toxic metal pollutants using hard tissues such as human teeth and hair. Professor Amarasiriwardena served as a *Fulbright Specialist in Chile*. He serves on the editorial boards of *Environmental Pollution* and *Applied Spectroscopy Practica*. Instructor's Web site: <http://helios.hampshire.edu/~daNS/index.html>

**SA-02 Environmental Isotope Geochemistry: Plasma Spectrochemistry as an Essential Tool**, Saturday, January 13, 8 am, Michael E. Ketterer, [michael.ketterer@nau.edu](mailto:michael.ketterer@nau.edu), Department of Chemistry and Biochemistry, Northern Arizona University, Box 5698, Flagstaff, AZ 86011-5698

The majority of the chemical elements possess multiple isotopes. Natural or synthetic variation of isotope compositions are widely used in geochemistry and the environmental sciences for gaining insight into the sources, transport, and fate of these elements in the natural and human-affected environment. This course provides a broad overview of the isotope geosciences, with emphasis on sources of these variations, and the use of plasma spectrochemistry to generate the requisite data. Applications to environmental/geochemical studies of important elements such as Pb, Sr, Nd, U, and Pu will be discussed, using examples from the literature.

Keywords: Isotopes, environmental sciences, geochemistry, ICPMS, source/transport/fate processes

**Michael E. Ketterer** obtained his primary and secondary education in Buffalo, NY, and received a B.S. in Chemistry from University of Notre Dame in 1980. He pursued graduate studies in electron transfer and interfacial chemistry at the University of Colorado under the direction of Prof. Carl A. Koval, receiving a Ph.D. in 1985. After brief employment as an industrial electrochemist, he worked from 1987-1993 at the US Environmental Protection Agency's forensic laboratory, and was Assistant Professor at John Carroll University from 1993-1998. Mike has since taught at Northern Arizona University (1998-2013) and Metropolitan State University of Denver (2013-2018), and is presently Professor Emeritus at Northern Arizona University. His research interests include plasma spectrochemistry, an interest that began when he first used an Elan 250 in 1988, and applications of isotope measurements in the environmental geosciences. Mike has published ~90 peer-reviewed papers in his career, is a prolific collaborator, and has traveled and lectured worldwide in pursuit of his scientific interests. As an Emeritus, Mike is pursuing consulting and *pro bono* work, focusing on assistance to communities affected by legacy Cold War-era nuclear contamination.

**SA-03 Speciation Analysis: Elemental, Isotopic and Molecular Mass Spectrometry in Life Sciences Studies**, Saturday, January 13, 7 pm, Olivier Donard, [olivier.donard@univ-pau.fr](mailto:olivier.donard@univ-pau.fr), MARSS-IPREM, University of Pau, Pau, France

The development of speciation analysis was a response to the increasing concerns about the role of chemical elements, even when present at trace concentrations, in living organisms. The short course addresses elemental, isotopic and molecular information to study the status, pathways, and transformations of trace elements in biota. The first part presents the concept of elemental speciation, the occurrence and classification of metal species, the techniques used and the criteria of their choice. The second part discusses selected case studies of trace metal speciation in environmental processes, plant and animal physiology, food safety and metallodrug metabolism.

Keywords: speciation analysis, environmental analysis, food analysis, food supplements, metallodrugs, trace metals, ESI MS, chromatography

**SA-04 Fluorine Detection with and ESIMS and Applications**, Sunday, January 14, 7 pm, Jörg Feldmann, [joerg.feldmann@uni-graz.at](mailto:joerg.feldmann@uni-graz.at), [j.feldmann@abdn.ac.uk](mailto:j.feldmann@abdn.ac.uk), and Viktora Müller, TESLA - Analytical Chemistry Institute of Chemistry, University of Graz, Universitätsplatz 1, 8010 Graz, Austria

Fluorine is one of the elements that cannot directly be detected by conventional ICPMS. This course will give some background, how environmental analysis for organofluorines such as F-containing pesticides and F-containing pharmaceuticals and PFAS (Per and polyfluorinated alkylated substances) is routinely analyzed by target LC-MS/MS. Furthermore, will be demonstrated how ICPMS can be used for non-target HR-ESIMS. Applications about PFAS in food contact materials, ski wax, accumulation in wildlife as well as fluorinated compounds in sewage water. Additionally, we will feature how LA-ICPMS can be conducted for fluorine.

**Jörg Feldmann** received his PhD at University of Essen (Germany) in 1995; he studied volatile metal and metalloids in the environment by using GC-ICP-MS. He was Feodor Lynen Postdoc (Alexander von Humboldt) at University of British Columbia, Canada in 1995-1997 when he investigated complimentary use of GC-MS and GC-ICP-MS for volatile tin, antimony, and bismuth compounds. Since 1997 he was a Lecturer at University of Aberdeen, Scotland and became full Professor in 2003. Recently he moved to the University of Graz in Graz, Austria. He has published more than 100 papers in peer-reviewed journals mainly about arsenic speciation. His focus is on the determination of the arsenosugar metabolism by seaweed-eating sheep and the transport and biotransformation of arsenic in plants and the pro and cons of ES-MS and ICP-MS and the on line combination of both MS techniques.

**SA-05 Implementing Clinical ICP-MS for Clinical Diagnosis, Biomonitoring and Emergency Response.** Sunday, January 14, 8 am, Cynthia D. Ward, CWard@cdc.gov, and Deanna Jones, DMJones1@cdc.gov, hii4@cdc.gov, Centers for Disease Control and Prevention (CDC), 4770 Buford Hwy, Mailstop S110-5, Atlanta, GA 30341-3717 Successful application of inductively coupled plasma mass spectrometry (ICP-MS) in a clinical laboratory is dependent upon addressing several key issues such as method validation, contamination control, CLIA regulations, quality control, and method troubleshooting. We will discuss these issues in detail as well as the key requirements for a clean-room type of laboratory environment. Laboratory infrastructure and methodological considerations to provide analytical support for biomonitoring studies, epidemiological assists, and emergency response will be covered. This course is of interest to scientists involved with or responsible for the testing of clinical samples in research, public health, or diagnostic labs.  
Keywords: Clinical ICP-MS, method validation, biomonitoring, clinical diagnosis, quality control, emergency response

**Cynthia Ward** is the Deputy Branch Chief of the Inorganic and Radiation Analytical Toxicology (IRAT) Branch. Her responsibilities include assisting with the planning, implementation, oversight, and execution of laboratory programs focused on research and development of analytical methods, the analysis of trace, toxic, and essential metals such as mercury (total and organic), arsenic (total and speciated), cadmium, lead, cobalt, tungsten, uranium, molybdenum, and antimony. The Branch produces population-based exposure levels segmented by age, sex, and race or ethnicity as part of the National Health and Nutrition Examination Survey (NHANES). The Branch also collaborates with academic institutions and other partners, including state public health departments, on exposure studies and studies that examine the connection between exposure levels and health effects.

**Deanna Jones** is the Chief of the Speciation and Lot Screening Laboratories in the IRAT Branch. She has over 15 years of experience at the CDC developing methods for measuring trace elements in biological samples using chromatography and ICP-MS. Her laboratory performs arsenic and mercury speciation methods and provides technical support to state and local public health labs. She is proficient in qualitative and quantitative statistical data analysis, method validation and evaluating analytical figures of merit, Clinical Laboratory Improvement Amendments (CLIA) regulations including Proficiency Testing (PT) requirements, and Quality Assurance/Quality Control (QA/QC) review.

**SA-06 Tagging Approaches for Development of Immunoassays for ICP-MS Detection**, Saturday, January 13, 8 am, Norbert Jakubowski, norbi.jakubowski@gmail.com, Spetec GmbH, Am Kletthamer Feld 15, 85435 Erding, Germany

In this short course the chemistry of metal tagging and staining of biomolecules for ICP-MS detection will be introduced and selected examples how these techniques can be used analytically in different applications will be discussed.

In the first part of this short course the tagging and staining chemistry for ICP-MS applications will be discussed in detail. In summary, mainly bifunctional ligands have been investigated in literature as tagging reagents. They consist of two parts, a metal chelating compound, and a reactive group, which connects the chelate covalently to the biomolecule of interest, such as the antibody. Concerning the reactive group, reagents will be discussed which are commercially available and which can either tag free amino-groups or alternatively free thiol groups of proteins or antibodies. The advantages and disadvantages of different tagging reagents will be discussed in detail.

In the second part selected applications will be discussed. A special focus will be set on mass and Imaging Cytometry for which the instrumentation and workflows will be presented. Applications will focus on Alzheimer and cancer research, the regulation of cytochromes, micro-tissue arrays, measurement of the cell status and cell differentiation. An outline is available on request.

Keywords: Metal tags and stains, antibody tagging, ICP-MS, mass cytometry, imaging mass cytometry, LA-ICP-MS

**Norbert Jakubowski** graduated as from the University in Essen/Duisburg and obtained his doctorate (Dr. rer. nat.) in 1991 from the University of Stuttgart/Hohenheim. In 1981 he joined the Institute for Analytical Sciences (ISAS) in Dortmund to work as a research scientist in the laboratory for inorganic analysis. He became the head of the division 1.1 (Inorganic Trace Analysis) of the Federal Institute of Materials Research and Testing in Berlin in 1999, and he retired in 2018. His present activities are mainly focused on analytical chemistry with special interest in development of instruments, methods and problem-orientated procedures based on the use of plasma sources (inductively coupled plasma, glow discharge) for elemental mass spectrometry of solid and liquid samples. Key Topics of his research



include speciation of P, Pt, Gd; metallomics; bioconjugation of antibodies for clinical assays; bio-imaging; analytical characterization of nanoparticles and their interaction with cells.

**SA-07 Characterization of Nanomaterials: Focusing on Engineered Nanoproducs and Plastics in the Approach “One Health”**, Saturday, January 13, 7 pm, Petra Krystek, [petra.krystek@uni-siegen.de](mailto:petra.krystek@uni-siegen.de), and Carsten Engelhard, [engelhard@chemie.uni-siegen.de](mailto:engelhard@chemie.uni-siegen.de), University of Siegen, Department of Chemistry and Biology, Siegen, Germany

Smallest particles (such as engineered inorganic nanoparticles (NPs) and nanomaterials (NMs) in e.g. consumer products as well as micro-, and nanoplastics (MNPs)) are subject of analysis in current multidisciplinary research because the knowledge on exposure and possible toxicity of nanotechnological as well as plastic degradation products is still limited. “One Health” is an approach wherein human health and environmental health are linked and various analytical challenges arise. A selection of case studies will be discussed including:

- a) Human exposure scenarios (inhalation, ingestion, dermal contact, injection) and biodistribution of engineered nanomaterials
- b) Solution routes for micro-, nanoplastics (MNPs) formation with respect to the approach “One Health”

During this interactive session, we will discuss aspects from sampling and sample storage, to sampling pre-treatment and analysis with inductively coupled plasma mass spectrometry (ICPMS) as the characterization technique of choice. Next to integrated approaches based on different uses of ICPMS and hyphenated fractionation techniques (e.g. asymmetric flow field flow fractionation (AF4)), other complementary techniques and quality control aspects will be discussed as well.

During this short course, an intermezzo on instrumental and fundamental aspects of single particle (sp)ICPMS for engineered nanoparticles as well as microplastics will be given by Carsten Engelhard, University of Siegen, Germany.

**Petra Krystek** received her PhD in 1999 at the University of Mainz, Germany. She has more than 20 years' experience in the field of ICPMS. Her research is application focused, especially regarding to ultra-trace, speciation, and nano-analysis mainly in the field of health and environmental aspects, and she has been involved in many interdisciplinary projects. She has worked at research institutes like the National Institute for Public Health and the Environment (RIVM) and Deltares in the Netherlands as well as in industries as Thermo and Philips. From 2009 to 2022, she also had a fellowship at the department Environment & Health at the Vrije Universiteit (VU) Amsterdam, the Netherlands. Since 2018, she is visiting lecturer and scientist at the University of Siegen in Germany.

Petra Krystek has published over 65 peer-reviewed articles and book chapters; she is a regularly invited lecturer and speaker at international symposia and organized many workshops. Within her international network, she has been associate member of the analytical chemistry division of International Union of Pure and Applied Chemistry (IUPAC) and expert in the working group for ICP spectrometry of the European Pharmacopoeia Commission (EDQM). Petra Krystek is also member of the editorial board of the journal *Chemosphere* and since 2022 she is a work package leader of the project MOMENTUM (microplastics and human health consortium).

**Carsten Engelhard** is an Associate Professor of Analytical Chemistry and the Department Chair of the Department of Chemistry and Biology at the University of Siegen. He received his Dr. rer. nat. degree in 2007 from the University of Muenster, Germany, and was a post-doctoral fellow at Indiana University from 2008 to 2010 under the guidance of Prof. G.M. Hieftje. Carsten has 10 years of experience in ultratrace elemental analysis, mass spectrometry, instrumentation, surface analysis, and nanoparticle detection. He has published more than 75 peer-reviewed articles and two book chapters in this field. Since 2023 he is chairman of the board of the German Working Group for Analytical Spectroscopy (DAAS) in the Analytical Division of the German Chemical Society (GDCh).

**SA-08 Analysis of Nano/microplastics and Their Role as Trojan Horses**, Sunday, January 14, 7 pm, Javier Jiménez-Lamana, [j.Jimenez-lamana@univ-pau.fr](mailto:j.Jimenez-lamana@univ-pau.fr), IPREM CNRS UMR 5254, Technopole Hélioparc, 2 avenue du président Angot, 64053 Pau, France

The ubiquitous presence of plastics debris, including micro and nanoplastics, as well as their role as carriers of metals and other pollutants is causing a growing concern among society and the scientific community. In this context, the assessment of nano and microplastics pollution requires the development and validation of new protocols, going from the sample preparation and separation schemes to the detection of the micron and submicron plastic particles as well as the metallic pollutants they can carry on. In this short course we will address all the steps necessary for the analysis of these emerging pollutants. It will not only focus on the use of inductively coupled plasma mass spectrometry (ICPMS) for this purpose, but it will also show how surface analytical techniques, like Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS), X-ray Photoelectron Spectroscopy (XPS) or Laser Ablation (LA) can provide critical information about the interactions of micro and nanoplastics with metal pollutants.

Keywords: nanoplastics, microplastics, plastic pollution, metal pollution, Trojan horse, mass spectrometry, single particle, trace metals, sample preparation

**Javier Jiménez-Lamana** is assistant professor at the University of Pau and Pays de l'Adour (UPPA). Since he started his PhD his research interest has been focused on the analysis of pollutants at the nanoscale in the environment. He has developed analytical methodologies based on Single Particle ICP-MS to study engineered nanoparticles in

different environmental and biological matrices. Currently, he is adapting the SP-ICP-MS methodology to the detection and quantification of nanoplastics and their potential role as carriers of heavy metals.

**SA-09 Analysis of Petroleum and Petroleum Products**, Monday, January 15, 7 pm, José Luis Todolí, jose.todoli@ua.es, Department of Analytical Chemistry, Nutrition and Food Sciences, University of Alicante, PO Box 99, 03080 Alicante, Spain

This course will provide an overview of the analysis of petroleum and petrochemicals by ICP OES and ICP-MS techniques and, in depth, information on specific applications and challenges. Sample types will include crude oil, distillate fractions, volatile hydrocarbons and solvents, used oils and other materials found in petrochemical processing. Sample preparation and sample introduction will be highlighted. Existing methods, calibration standards, and certified samples will be evaluated, as well as result validation and quality. The advantages of ICP-MS hyphenation with separation techniques will be discussed. Time for class discussion on topics of individual interest will be provided, and advice will be available on carrying out the ICP-OES and ICP-MS analysis of different petroleum products.

Keywords: ICP OES, ICPMS, plasma spectrometry, petroleum, crude oil, metals, organic solvents, sample preparation, sample introduction, HPLC

**SA-10 Single Particle and Single Cell ICP-MS Theory and Applications**, Saturday, January 13, 1 pm, Chady Stephan, chady.stephan@perkinelmer.com, and Ruth Merrifield, ruth.merrifield@perkinelmer.com, PerkinElmer, 501 Rowntree Dairy Rd, Woodbridge, ON L4L 8H1, Canada

This course will briefly review the theory of SP-ICP-MS focusing on the state-of-the-art innovations in hardware and software with relation to the latest applications in environmental, forensic and semiconductor sciences. We will introduce the concept of single cell-ICP-MS and discuss the challenges faced when analyzing cells suspensions with an in-depth focus on the necessary hardware and software requirements to quantify accurately the number of particles and/or metal content in individual unicellular organisms. Various applications to human and environmental health applications of this technique will be discussed.

Keywords: Single cell ICP-MS, single particle ICP-MS, bioaccumulation, nanoparticles, environment, cancer, semiconductor, forensic

**ChadyStephan** holds a Ph.D. in Analytical Chemistry from the University of Montreal. He worked as a project manager for QSAR risk assessment services before joining PerkinElmer as an Inorganic Product Specialist supporting the various elemental analysis platforms. He then managed the development of various nanotechnology applications that focus on measurement techniques for nano-object characterization using various analytical platforms. He currently leads a multifunctional team composed of marketing, technical marketing, application scientist and strategists focusing on delivering complete market solutions. He is a thought leader in elemental analysis with over 20 peer-reviewed published papers and book chapters. Over the past few years, his main research activities at PerkinElmer have been in developing single-particle ICP-MS and more recently Single Cell ICP-MS.

**SA-11 New Inorganic and Isotopic Strategies for High Geographical Resolution Traceability. Application to Environmental and Food Related Issues.** Monday, January 15, 7 pm, Olivier Donard, olivier.donard@univ-pau.fr, MARSS-IPREM, University of Pau, Pau, France

Metal speciation is gaining increasing importance in a wide variety of fields, for example, clinical, environmental, nutritional, industrial, and geochemical applications. It is well understood now that the determination of the chemical form of metals is essential for the correct evaluation of their fate, impact, and "risk assessment" in all traditional compartments where inorganic analysis is involved. In the past 20 years considerable effort has been made by academic, regulation and industrial communities to identify, rationalize, and promote simple and effective analytical procedures that will improve our understanding of metal related issues in the environment, nutrition, hygiene, and industry. Now, non-traditional isotopic analyses are of paramount importance in a variety of field such as the environment, food, cosmetics,... The aim of this course is to detail the status of metal speciation analysis and the later extension for isotopic analysis and will consist of the following topics: a. Overview of traditional and classical aspects of sampling, extraction and detection of analyte species; b. Current status of metal species and non traditional isotopic determination strategies (elemental speciation, isotopic signatures); c. Identification of the areas of growing demand; d. Review, examination and critically assess major developments in sample collection, preservation, preparation, analyte detection and validation for both speciation and isotopic analysis, and e. Description of analytical speciation and isotopic procedures using examples from environment, nutrition and industrial applications.

Keywords: Sampling, metal speciation, non-traditional isotopic signatures detection, applications, environment, nutrition, and industry

**Olivier F.X. Donard** is a Research Director at the French CNRS, He is the head of the Mass Spectrometry Center for Reactivity and Speciation Sciences and is the codirector of a commercial enterprise (Ultra Traces Analyses Aquitaine - UT2A) dedicated to speciation analysis. He has recently been the co-funded of a new company on isotopic signatures for traceability (AIA Advanced Isotopic Analysis). He has developed analytical strategies and promoted speciation

related issues for a large variety of international environmental organizations (USA EPA, Dutch Ministry of Water and Environment, and French Fisheries IFREMER). He has pioneered several approaches for sample preparation, derivatization, and detection using atomic absorption, atomic fluorescence, ICP-AES, and mass spectrometries that facilitate routine elemental speciation and is now developing similar approach in isotopic analysis both applied for fundamental research of commercial analytical applications. He is the author of more than 300 international publications in analytical and environmental chemistry. He has delivered over 150 plenary and invited lectures at international meetings and more than 500 poster and oral presentations on the topic of atomic spectrometry, speciation and now isotopic signatures applied to a large array of applications. He has an h factor of 50 (ISI Web Sciences). He is the cofounder and an executive member of the European Virtual Institute of Speciation Analysis-EVISA. He collaborates with instrument and sample preparation manufacturers in order to improve instrument performance and preserve the integrity of the species of interest and is now involved in sample preparation for isotopic analysis by MC ICP/MS.

**SA-12 Elemental Imaging at Micro- and Nanometer Scale for Applications in Biology, Nutrition, Toxicology, and Geology.** Saturday, January 13, 1 pm, Dirk Schaumlöffel, dirk.schaumloeffel@univ-pau.fr, IPREM CNRS UMR 5254, Heloparc, 2 avenue du president Angot, 64053 Pau, France

This course provides in the first part an overview of different element specific imaging techniques such as Laser Ablation ICP-MS, TEM-X/EDS, synchrotron radiation XRF, and secondary ion mass spectrometry. Specifications and limitations regarding spatial resolution and sensitivity will be discussed. The second part will focus on the technique and challenges of nanoscale secondary ion mass spectrometry (NanoSIMS) for elemental and isotopic imaging at the submicrometer level. The third part of this course will highlight different applications including sample preparation techniques for NanoSIMS. Applications from our work on plant and animal tissue, cell cultures as well as geological samples will be presented and discussed. Finally, in the last part, solutions for the treatment of imaging data and their limitations will be presented.

Keywords: Elemental imaging, SIMS, nm resolution, sample preparation, plant and animal tissue, subcellular

**Dirk Schaumlöffel** obtained his doctorate in analytical chemistry in 1995 at the Philipps University in Marburg, Germany, and then carried out research at the GKSS research center in Geesthacht. After a stay in the USA, he went to the University of Pau, France where he obtained his habilitation in analytical chemistry in 2008. Since 2011 he has been a research professor at the French National Center for Scientific Research (CNRS) and he teaches at the University of Pau. His research includes analytical-chemical developments for the determination of essential and toxic trace elements in biological organisms. Main research activities are imaging methods for the localization of trace elements in tissue and cells in the nanometer level using secondary ion mass spectrometry (NanoSIMS) with applications in the environment, biomedicine, and toxicology. Dirk Schaumlöffel is also editor of the *Journal of Trace Elements in Medicine and Biology*, and president of the German Society for Minerals and Trace Elements (GMS).

**SA-13 Edible Insects (& Other Novel Proteins). The Role of ICP-MS in a Safe and Sustainable Global Food System,** Sunday, January 14, 1 pm, Kelly LeBlanc, Kelly.LebLANC@nrc-cnrc.gc.ca, National Research Council Canada, Metrology Research Centre, 1200 Montreal Rd, Ottawa, ON, Canada K1A 0R6

This course will address the challenges associated with the analysis of trace elements and trace element species in new and emerging high-protein foods. We will discuss the sample preparation requirements to achieve the complete digestion needed for total elemental analysis and ways to address the differences between total and biologically-relevant analyte contents. Specific focus will be given to speciation analysis of trace elements in these foods and the challenges related to quantitative extraction while maintaining chemical speciation. As an element often associated with proteins, selenium is of particular interest, and we will discuss the tools that can be used to examine its distribution and biological relevance in novel high-protein foods. Additionally, we will look at the calibration approaches used to achieve the most accurate and precise results while also considering observed interferences during ICP-MS detection, and will examine the role of Certified Reference Materials in ensuring high quality data. Keywords: novel foods, alternative protein, food analysis, speciation analysis, sample preparation, microwave digestion, bioaccessability, Certified Reference Materials, metrology

**Kelly LeBlanc** received her PhD in Analytical Environmental Chemistry from Trent University (Peterborough, Ontario, Canada) in 2016. Later that year she joined the Inorganic Chemical Metrology group at the National Research Council Canada, where she holds a position as a Research Officer. Her research focuses on metal speciation with particular interest in selenium. At NRC, she is part of the Certified Reference Material team where she has been involved in a number of certification campaigns for materials including uranium ore concentrates, selenized yeast, fish protein, and a series of novel high-protein foods (*i.e.*, crickets, mealworms, canola meal). Since 2023, Kelly has been serving as the President of the Canadian Society for Analytical Sciences and Spectroscopy.

## **Spectrochemical Instrumentation**

**SI-01 New Calibration Strategies in Spectrochemical Analysis,** Tuesday, January 16, 7 pm, George L. Donati, donatigl@wfu.edu, Wake Forest University, Department of Chemistry, Winston-Salem, NC 27109

Calibration is a crucial component of quantitative spectrochemical analysis. In recent years, alternative calibration methods have been proposed to improve accuracy and sample throughput. Five of these new strategies will be discussed in this short course: standard dilution analysis (SDA), multi-energy calibration (MEC), interference standards (IFS), multi-isotope calibration (MICal), and multispecies calibration (MSC). The theoretical basis of each method and their application in atomic absorption, atomic emission and inorganic mass spectrometry will be discussed. There will also be opportunity for hands-on data processing using MS Excel and ICP-OES and ICP-MS experimental results. Bring your computer with MS Excel installed.

Keywords: Accuracy; Sample throughput; External standard calibration; Standard additions; Standard dilution analysis; Multi-energy calibration; Interference standard; Multi-isotope calibration; Multispecies calibration; Non-traditional calibration methods.

**George L. Donati** received his M.Sc. in Analytical Chemistry from the Federal University of Sao Carlos (UFSCar, Brazil, 2006), and his Ph.D. in Analytical Chemistry from Wake Forest University (WFU, USA, 2010). During his postdoctoral fellowship at UFSCar, George collaborated with Prof. Joaquim Nobrega and Dr. Renata Amais to develop the first concepts of the interference standard method (IFS). George is a Research Professor at the Department of Chemistry of Wake Forest University, in Winston-Salem, NC, where he developed the methods of multi-energy calibration (MEC), multi-isotope calibration (MICal) and multispecies calibration (MSC), and contributed to the development of Prof. Bradley Jones's standard dilution analysis method (SDA). His research interests include portable instrumentation and novel calibration methods for spectrochemical analysis, as well as the use of machine learning tools to diagnose diseases and improve the performance of different analytical methods. George is a member of the advisory board of the *Journal of Analytical Atomic Spectrometry*, and the editorial board of the *Brazilian Journal of Analytical Chemistry*. He has published more than 110 peer-review papers and four book chapters, and he was awarded with the 2020 JAAS Emerging Investigator Lectureship.

**SI-02 Opportunities, Challenges, and Application of Glow Discharge Techniques**, Sunday, January 14, 8 am, Volker Hoffmann, Leibniz Institute for Solid State and Materials, Research Dresden, PO Box 27 00 16, D-01171 Dresden, Germany, v.hoffmann@ifw-dresden.de; Peter K. Robinson, pete@masscare.co.uk, MassCare Ltd., 11 Waterside Way, Middlewich, Cheshire, CW 10 9HP, United Kingdom

This course is designed to review the application of GD-OES and -MS in modern material science. Advantages and disadvantages of the technique and different instruments will be discussed from practical point of view. Hard- and software (quantification) will be explained, and applications will be compared with other methods of direct solids elemental analysis. Analytical figures of merit for the two spectrometric methods will be presented. We offer all participants a discussion about their actual analytical problems. Finally, the session will be concluded with a discussion of future trends in instrumentation and applications, as e.g. imaging spectroscopy and new detectors. Keywords: GD-OES, GD-MS, application, solid-state analysis

**Volker Hoffmann** graduated from the Technical University in Dresden and obtained his doctorate (Dr. rer. nat.) in 1986. The same year he joined the Central Institute of Solid State Physics and Materials Research in Dresden (now Leibniz Institute of Solid State and Materials Research) to work as a research scientist in the laboratory for spectral analysis, where he became the head in 1996. His present activities are mainly focused on the research and development of glow discharge optical (GD-OES) and mass spectrometry (GD-MS), which are performed in cooperation with different companies and research groups in Europe and USA. In cooperation with LECO Germany and USA, a new radio frequency (rf) technology for the analysis of non-conductors by glow discharge spectroscopy was developed. In the field of GD-MS he worked in cooperation together with PTB Braunschweig and developed a new fast flow source principle, which after further development is now used in commercial GD-MS equipment. His present research includes pulsed discharges to improve thin layer analysis and plasma imaging. From 2006 to 2012 he was chairman of the European Working Group for Glow Discharge Spectroscopy, and he was secretary of the corresponding German workgroup until 2022.

**Peter K. Robinson** started working with MS in 1980 when he joined the VG group. Initially he was employed as a software engineer and started by working on static gas instruments. In 1982 Peter led the development of software for the first generation of ICP-MS instruments, the Plasma Quad. Later in 1984 he moved over to join the team that developed the first commercially available GD-MS instrument, the VG9000. Peter worked with the VG9000 until 2003 (as part of VG, Fisons, and Thermo) when the instrument production was stopped. Having moved away from software in the 1980's, Peter had roles in manufacturing and development before focusing on after sales leading the team that was responsible for instrument test, installation, and support. In 2004 after leaving Thermo, Peter established the small firm MassCare Ltd. and to this day supports the VG9000 in the field. He also works closely with manufacturers of modern instruments, the Astrum, the Element, and the Auto Concept. Away from direct support of instruments, Peter is current Chair of the EW-GDS, a body that organizes GDS-focused symposia and has the basic aim to develop young scientists in the field. He is also chairing the GD Subcommittee of ISO/ TC20 Surface Chemical Analysis and contributes toward the development of international standards.



**SI-03 ICP-TOFMS: Fundamental and Application for Single-Particle Analysis.** Friday, January 12, 1 pm, Alex Gundlach-Graham, alexgg@iastate.edu, Iowa State University, 1605 Gilman Hall, 2415 Osborne Dr, Ames, IA 50011

We will explore the fundamentals of contemporary ICP-TOFMS instruments, including operating principles, performance characteristics, noise distributions unique to TOFMS, and advanced data treatment strategies. Participants will leave the course with an understanding of the limitations and benefits of ICP-TOFMS, and an arsenal of new strategies for treating their own TOFMS datasets. We will discuss in detail strategies for single-particle analysis with ICP-TOFMS; specific topics include calibration *via* microdroplets, defining accurate critical values to find nanoparticle signals, predicting homoparticle and heteroparticle coincidences, and automating multi-element single-particle data analysis. Practitioners of sp-ICP-MS and those interested in ICP-TOFMS and Individuals interested in advanced signal-to-noise characterization and automated single-particle data analysis should take this course.

Keywords: Time-of-Flight Mass Spectrometry, Detection Science, Nanoparticles, Microdroplets, Matrix Effects, Automation in Data Analysis, Compound Poisson Distribution, Elemental Fingerprinting

**Alex Gundlach-Graham** is an assistant professor of chemistry at Iowa State University. He received his PhD in 2013 in the Hieftje group at Indiana University, where his research focused on the development and characterization of distance-of-flight mass spectrometry. Alex moved to the group of Detlef Günther at ETH Zurich for, initially, his postdoctoral studies as a Marie-Curie Fellow, and then as a research scientist through a Swiss NSF fellowship. At ETH, Alex's research centered on the combination of laser ablation ICP-TOFMS for high-resolution elemental imaging and on the measurement of engineered nanoparticles by single-particle ICP-TOFMS. At ISU, the Gundlach-Graham group pursues research in atomic mass spectrometry with a focus on automated and high-throughput sp-ICP-TOFMS analysis.

**SI-04 ICP-MS I: Introduction**, Saturday, January 13, 1 pm, John Olesik, olesik.2@osu.edu, Ohio State University, School of Earth Sciences, 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002

This course is intended mainly for the newcomer to ICP-MS. ICP characteristics as an ion source, ion extraction, operating principles of ion optics, ion focusing, quadrupole and sector mass analysis, and detectors will be described. The general analytical capabilities, applications survey, and an introduction to matrix effects will be presented.

Keywords: ICP-MS characteristics, instrumentation, interferences, applications

**SI-05 ICP-MS II: Advanced Topics**, Sunday, January 14, 1 pm, John Olesik, olesik.2@osu.edu, Ohio State University, School of Earth Sciences, 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002

This course is intended for those who complete Part I and for the experienced ICP-MS user. Detailed consideration will be given to basic cases of matrix effects, removal of polyatomic ion interferences (solvent removal, collisional dissociation, high resolution, and cool plasma), alternate mass analyzers, solid sampling, analysis of limited solution volumes, and combining ICP-MS with chromatography for speciation and removal of interferences.

Keywords: ICP-MS operation and measurement effects, interference corrections, sampling, chromatography

**SI-06 Theory and Practical Use of Reaction Cells and Collision Cells for ICP-MS**, Sunday, January 14, 7 pm, Patrick Gray, patrick.gray@fda.hhs.gov, Center for Food Safety and Applied Nutrition, Office of Regulatory Science, U.S. Food and Drug Administration, College Park, MD

The design and operation of reaction cells and collision cells used for isobaric interference removal in ICP-MS will be discussed. The course begins with an introduction to the principals and kinetics of ion-molecule reactions and the operation of the rf devices (quadrupoles, hexapoles, octapoles, *etc.*). The various efficiencies of the ion chemistry (primarily ion reactivity, reactivity, production of the ions within the cell) will be evaluated, concluding that where high efficiency of the primary chemistry is obtained, reaction of the analyte ion with impurities and the formation of new interferences within the cell becomes important. Various means of suppressing these effects, including kinetic energy discrimination and band pass operation of the cell will be contrasted and compared, and effects related to the order of the multipole device will be considered. Examples of the application of reaction cell and collisions cell methods in the semiconductor, environmental, clinical, geochemical, and isotopic analysis will be presented.

Keywords: Collision cell, reaction cell, spectral interference, chemical resolution, pressurized multipole, chemistry, ion dynamics, ion-molecule chemistry, in-cell produced interferences, multipole operating point, energy discrimination

**Patrick Gray** is a Chemist at U.S. Food & Drug Administration based in Silver Spring, Maryland. Previously, Patrick was a Research Chemist at U.S. Department of Defense.

**SI-07 Interferences in ICP Spectroscopy**, Sunday, January 14, 7 pm, José Luis Todolí, jose.todoli@ua.es, Department of Analytical Chemistry, Nutrition and Food Sciences, University of Alicante, PO Box 99, 03080 Alicante, Spain

Matrix effects make difficult the use of ICP techniques for some particular applications. The first step to overcome them is to understand the mechanisms and the main sources of interferences. The present course deals with the detection of the origin of the ICP-OES and ICP-MS interferences. The discussions will be based on selected applications (clinical, organic, food analysis...). Advice to improve the accuracy of the determinations will be given.

Keywords: Matrix effects, liquid sample introduction system, inorganic acids, organic solvents, easily ionized elements, ICP-AES, ICP-MS, clinical analysis, fuel analysis, food analysis

**SI-08 Identification and Correction of Interferences in Practical ICP-OES**, Monday, January 15, 7 pm, Deborah Bradshaw, bradshawdk@cs.com, Atomic Spectroscopy Consulting, PO Box 536307, Orlando, FL 32853-6307

The identification and correction of interferences for ICP-OES can be critical to obtain accurate data in the analytical laboratory. The interferences and their corrective techniques that will be addressed include sample transport, sample matrix, and spectral. Procedures used to correct for transport and matrix interferences include the use of appropriate internal standards, matrix matching, optimizing plasma conditions, using buffer solutions, and the correct choice of sample introduction systems. Spectral interference correction approaches include optimizing the method parameters as well as choosing the appropriate correction technique such as interelement corrections and multiple linear regression techniques. Some of these may be limited to the specific instrumental hardware and software available to the analyst. The merits and disadvantages of the various correction approaches that are used will be examined, with practical examples of the use of these corrections to obtain accurate data. This course is recommended for new to intermediate users.

Keywords: Transport interferences, matrix interferences, spectral interferences, interelement correction, multiple linear regressions, inductively coupled plasma atomic emission

**Deborah Bradshaw** is an analytical chemist who has been working the field of atomic spectroscopy for over 35 years. She started working as a chemist using flame atomic absorption and then migrated into graphite furnace in the 1980s, developing methods using Zeeman background corrected techniques for the analysis of seawater samples. It was then a natural progression to migrate into the plasma techniques. For the past 20 years, she has been working as a consultant in the field of atomic spectroscopy, conducting training classes and giving technical support for AA, ICP-OES and ICP-MS. Debbie is a Fellow of the Society for Applied Spectroscopy (SAS) and is a recipient of their Distinguished Service Award. For 14 years, she was the News Column Editor for the journal *Applied Spectroscopy*, SAS's monthly publication. She continues to be a reviewer for publications and journals in her field. She has organized symposia in atomic spectroscopy at FACSS (now SciX) and PittCon and has been a short course instructor at the Winter Conference on Plasma Spectrochemistry since 2000.

**SI-09 Identification and Correction of Interferences in Practical ICP-MS**, Tuesday, January 16, 7 pm, Deborah Bradshaw, bradshawdk@cs.com, Atomic Spectroscopy Consulting, PO Box 536307, Orlando, FL 32853-6307

The identification and correction of interferences for ICP-MS can be critical to obtain accurate data in the analytical laboratory. The interferences and their corrective techniques that will be addressed include sample transport, sample matrix, and spectral. Procedures used to correct for transport and matrix interferences include the use of appropriate internal standards, matrix matching, optimizing plasma conditions, and the correct choice of sample introduction systems. Spectral interference correction approaches include optimizing the method parameters as well as choosing the appropriate correction equations. The merits and disadvantages of the various correction approaches that are used will be examined, with practical examples of the use of these corrections to obtain accurate data. This course is suitable for new to intermediate users.

Keywords: Transport interferences, matrix interferences, spectral interferences, correction equations, inductively coupled plasma mass spectrometry

**SI-10 The Chemical Analysis of Things As They Are? Direct Atomic and Molecular Analyses with Ambient Mass Spectrometry**, Saturday, January 13, 7 pm, Carsten Engelhard, engelhard@chemie.uni-siegen.de, Department of Chemistry and Biology, University of Siegen, Siegen, 57076 Germany; Jacob T. Shelley, shellj@rpi.edu, Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Troy, NY 12180

The ultimate goal of analytical chemistry is to provide, what G.E.F. Lundell described as, "The chemical analysis of things as they are" such that a comprehensive assessment of sample constituents is directly obtained in a way that is nondestructive, while the sample is interrogated in its native environment. Recent efforts in mass spectrometry ionization source development have demonstrated these attributes to be possible. In such ambient mass spectrometry experiments, the source desorbs molecules from a surface, softly ionizes them, and transfers these ions into a mass spectrometer. This course will cover fundamental principles of desorption/ionization processes, as well as applications of these ionization sources. A particular emphasis will be placed on plasma-based systems.

People who wish to learn about methods to perform direct, mass-spectrometric analyses with a particular focus on portable/ field able methods, plasma-based sources, and emerging elemental approaches should be interested in this course.

Keywords: Direct Analysis, Molecular Mass Spectrometry, Glow Discharge, Ambient Ionization, DART, DESI, FAPA

**SI-11 Ultra Ultra-High Resolution in Plasma-Assisted Atomic/Isotopic/Molecular Analysis by Orbitrap Mass Spectrometry**, Sunday, January 14, 8 am, Kenneth Marcus, marcusr@clemson.edu, Clemson University, Department of Chemistry, Clemson, SC 29672, and Davide Bleiner, davide.bleiner@empa.ch, EMPA, Überlandstrasse 139, CH-8600 Dübendorf, Switzerland

While atomic mass spectrometry has made major progress with a large selection of commercially available architectures, one gap has never been filled: Fourier transform mass spectrometry (FT-MS). The capabilities for ultra-high mass resolution was never a need for ICP-MS, until more and more cases of complex mixtures have challenged the field. We describe here the coupling of plasma sources, predominately micro plasmas having combined atomic and molecular (CAM) capabilities, with commercial Orbit rap MS platforms. Focus on the operation principles of the Orbit rap FTMS and it application to plasma source mass spectrometry will be the heart of the short course.

Keywords: Orbit rap, Atmospheric Pressure Glow Discharge; Combined Atomic and Molecular (CAM) Ionization; Fourier Transform; Plasma source mass spectrometry; Ion Trap; Ultra-high mass resolution; Isotope ratios; Metal speciation

**R. Kenneth Marcus** earned B.S. degrees (1982) in chemistry and physics from Longwood College and a Ph.D. (1986) in analytical chemistry from the University of Virginia. He serves on the editorial advisory board for three international journals and was the recipient of the 2001 S.C. Governor's Award for Excellence in Science Research. In 2010, Professor Marcus was named a Fellow of the Royal Society of Chemistry (FRSC), in 2012 a Fellow of the American Association for the Advancement of Science (FAAAS), in 2016 a Fellow of the Society for Applied Spectroscopy, and in 2018 a Fellow of the National Academy of Inventors. In 2019, Marcus was awarded the inaugural Clemson University Researcher of the Year designation. Marcus has been on the Clemson faculty for 35 years, graduating 43 Ph.D. and 15 MS students.

**Davide Bleiner** studied in Rome (Italy) and got his Summa cum laude Mac in Earth Sciences in 1998. In 2002 he got his PhD under the guidance of Detlef Günther at the ETH Zürich. After a postdoc at the Swiss Federal Laboratories for Materials Science & Technology (Empa) he moved to the group of Annemie Bogaerts in 2005. In 2007 he was appointed Senior Assistant at the ETH Zurich working on plasma sources for Extreme Ultraviolet lithography. In 2010 he moved to the University of Bern where in 2011 was appointed Assistant Professor for X-ray Laser Physics. He has finally moved back to Empa in 2014 as a Head of Advanced Analytical Technologies. In 2026 he got the Venia Legendi and PhD Awarding Right at the University of Zurich. He has published more than 100 papers on laser microanalysis, advanced laser sources based on plasmas, and advanced methods.

### Sample Introduction Approaches

**SS-01 A Practical Guide to Nebulizers and the Part They Play in Modern Sample Introduction**, Saturday, January 13, 7 pm, Steve Mangum, [steve.mangum@icpms.com](mailto:steve.mangum@icpms.com), Elemental Scientific Inc., 7277 World Communications Dr, Omaha, NE 68132

This course will give participants an overview of the popular methods for introducing liquid samples used by today's instruments. A wide variety of nebulizers will be presented along with a discussion of how they work, which ones to use for particular matrices, and how to properly care for them. Along the way we will also feature ideas for best connecting pump tubing of a wide variety of sizes to these various devices. Once a firm understanding of nebulizers and their operation is established, the course will continue with a detailed discussion of sample matrices, properties of aerosols and segregation chambers that are important for good spectrochemical analysis, how matrices affect nebulizer performance and what can be learned about these matrices from the spectroscopic results. Since nebulization implies working with aerosols, participants will be provided a window into novel sample collection techniques that use nebulizers as part of the whole sample introduction scheme. Engaging discussions among the participants will be encouraged, so that everyone can share their experiences and come away with new and practical information with which to return to the lab.

Keywords: Nebulizers, spray chambers, desolvation, aerosol diagnostics, process monitoring, transport efficiency

**Steve Mangum** has over 30 years of experience in atomic spectroscopy, spending his first 10 years working in a certified environmental laboratory running flame/furnace, ICP and ICP-MS. Steve then spent the next 20 years as a spectroscopy Product Specialist for one of the large instrument manufacturers, helping laboratories implement new instrumentation and developing analytical methods. This experience has given Steve a strong background in methods and instrumentation, especially in environmental, nutritional supplement and semiconductor applications. Steve holds a Masters degree from the University of Utah and is currently working as a Field Application Scientist for Elemental Scientific, helping customers improve their analytical capabilities.

**SS-02 Laser Ablation Mass Spectrometry**, Saturday, January 13, 1 pm, Detlef Günther, [guenther@inorg.chem.ethz.ch](mailto:guenther@inorg.chem.ethz.ch), Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 1, 8093 Zurich, Switzerland

The course is designed to give participants an introduction to the analytical capabilities of laser ablation - inductively coupled plasma spectrometry and should be of particular benefit to spectroscopists interested in developing a laser ablation facility. LA-ICP-MS has become one of the most common solid sampling technique for major, minor and trace element analysis. The course will explain how LA-ICP-MS works. Details about basics in lasers and ICP-MS instrumentation and their combination will be explained. Examples for transient data acquisition, method development, and a large number of applications will be discussed to give a feel for the quantification capabilities of this analytical technique. Topics also will include terms and terminology, laser selection, ablation cell design and

interfacing, ablation processes, transport phenomena, and measurement systems. Participants do not need previous knowledge about this technique.

Keywords: Lasers, ablation, aerosol transport systems, carrier gas, calibration, atomization and ionization, ICP-MS, interface, applications

**Detlef Günther** is full professor for Trace Element and Micro Analysis at the Department for Chemistry and Applied Biosciences (D-CHAB) at ETH Zurich. His research in the field of Analytical Chemistry is focused on instrument and method development for trace and ultra-trace element analysis and isotope ratio determinations using high spatial resolution laser ablation and inductively coupled plasma mass spectrometry. His group contributed publications to fundamental and applied research in Analytical Chemistry. He received the Lester Strock Award, the European Award for Plasma Mass Spectrometry, the Widmer Award. In 2014 he became member of the German National Academy of Science Leopoldina. From 2015 until 2022 he served as Vice President for Research and Corporate Relations at ETH Zurich.

**SS-03 Latest Advances in Laser Ablation-Based Chemical Analysis and Emerging Applications: LIBS, LA-ICP-(OES/MS), and Tandem LA – LIBS**, Monday, January 15, 7 pm, Jhanis Gonzalez, jhanis@appliedspectra.com, jjgonzalez@lbl.gov, Applied Spectra, Inc., 950 Riverside Pkwy, Suite 90, West Sacramento, CA 95605-15071

Laser ablation has advanced over the last 50 years to become a successful technology for numerous chemical analysis applications. Breakthroughs in understanding the science of the ablation process and development of improved laser and detector components have led to reliable analytical measurement performance. The course will summarize key underlying mechanisms of the ablation process that are critical for accurate and precise measurements using LIBS and ICP-MS. This course will cover state of art system and performance, example applications and directions for future capabilities.

Keywords: Laser ablation, ICP-MS, LIBS, chemical analysis, elemental isotopic and molecular analysis, nano-analysis, imaging

**Jhanis José Gonzalez Chacon** is director of Applications Lab Operations, Applied Spectra, Inc, and project scientist at Lawrence Berkeley National Lab, Berkeley, CA. He received a BS and PhD in chemistry from Central University of Venezuela, and he joined the Laser Spectroscopy and Applied Materials Group at Lawrence Berkeley National Laboratory, under the supervision of Dr. Richard E. Russo. He was a postdoctoral fellow from 2004 to 2007. His research is focused on fundamental mechanisms of laser-material interaction, including laser energy coupling to solid samples, laser induced plasma properties, particle formation and transport, and developing new applications for laser technologies, in particular laser induced breakdown spectroscopy (LIBS) and laser ablation inductively coupled plasma mass spectroscopy (LA-ICP-MS).

**SS-04 Variations of Single Particle Inductively Coupled Plasma Mass Spectrometry**, Diane Beauchemin, diane.beauchemin@queensu.ca, Saturday, January 20, 1 pm, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada

Coupling flow injection (FI), where a known volume of NPs suspension is injected into a continuous carrier flow, or monosegmented flow analysis (MSFA), where injection is done within an air bubble in a continuous carrier flow, to single particle inductively coupled plasma mass spectrometry (spICPMS) simplifies the analysis. Indeed, FI-spICPMS or MSFA-spICPMS eliminates the need to measure the sample uptake rate, which is required with conventional spICPMS. Also, the transport efficiency is not required for measurement of NP size, unlike with conventional spICPMS, and is only needed for measurement of NPs concentration if total sample introduction is not achieved.

Keywords: single particle inductively coupled plasma mass spectrometry, flow injection, monosegmented flow analysis; nanoparticle measurement

**Diane Beauchemin** obtained a B.Sc. in 1980 and a Ph.D. in 1984 (supervisor: Joseph Hubert) at l'Université de Montreal. She then worked as a Research Associate at the National Research Council of Canada where she did seminal work on the first commercial inductively coupled plasma (ICP) mass spectrometry (MS) instrument (an ELAN 250). She joined the Department of Chemistry at Queen's University in 1988. She progressed through the ranks and became Full Professor in 2001. Her research efforts focus on ICPMS and ICP optical emission spectrometry from both fundamental and application perspectives. Her work has been recognized by the Alan Date Memorial Award (in ICPMS) in 1988, the 1991 Maccoll Prize, a Senior Industrial Fellowship from the Natural Sciences and Engineering Research Council of Canada to work in the R&D Division of SCIEX (sole Canadian ICPMS manufacturer) in 1995, the 2017 Maxxam Award from the Canadian Society for Chemistry (she was the first woman to receive it), the 2018 Gerhard Herzberg Award from the Canadian Society for Analytical Sciences and Spectroscopy (she was the first woman to receive it), and the 2019 Clara Benson Award from the Canadian Society for Chemistry. Amongst research-active Canadians, she has the most experience with ICPMS and on ways to expand its capabilities.

**SS-05 Electrothermal Vaporization - ICP for the Direct Analysis of Solids**, Diane Beauchemin, diane.beauchemin@queensu.ca, Saturday, January 20, 8 am, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada



A commercially available electrothermal vaporization (ETV) system is readily coupled to an inductively coupled plasma (ICP) optical emission spectrometry (OES) or mass spectrometry (MS) instrument for the direct analysis of solids as well as liquids and slurries. The pyrolysis step preceding analyte vaporization enables external calibration with solutions. Depending on the boiling points of analytes and interferents, isobaric interferences can be eliminated in ETV-ICPMS. Because ICPOES is inherently more robust than ICPMS, ETV-ICPOES has been applied to the analysis of various solid samples, including food, metals and alloys, slag, solder, bones, hair, *etc.*, and is well suited for forensic analysis.

Keywords: electrothermal vaporization, inductively coupled plasma optical emission spectrometry, inductively coupled plasma mass spectrometry, direct solid analysis, forensic analysis, analysis of refractory materials

**SS-06 Artificial Intelligence (e.g., via Artificial Neural Networks, Machine Learning, Deep Learning) and Some Applications to ICP and to Microplasma Spectrochemistry**, Sunday, January 14, 1 pm, Vassili Karanassios, vkaranassios@uwaterloo.ca, University of Waterloo, Department of Chemistry and Waterloo Institute for Nanotechnology, Waterloo, ON N2L 3G1, Canada

Artificial Intelligence (and its variants) are receiving significant attention in the scientific journals and the popular press [1, 2] (with expected significant future increases in market size). This short course is divided into two unequal parts. Part 1 deals with an introduction and fundamentals of AI and Part 2 with applications of AI in plasma spectrometry.

[1] V. Karanassios *et al.*, "Artificial Neural Networks (ANNs) for spectral interference correction using a large-size spectrometer and ANN-based deep learning for a miniature one", invited **open access** book chapter, In Tech Publishing, Chapter 12, Pages 227-249, In Tech Publishing, Dec. 20, 2017, DOI: 10.5772/intechopen.71039

[2] C. Tat and V. Karanassios, "Artificial intelligence, machine learning and deep learning in plasma and microplasma spectrochemistry", SPIE Proc., in press

Keywords: Artificial Intelligence (AI); Deep Learning (DL); Artificial Neural Networks (ANNs); Spectral Interference correction using ANNs; Deep learning Approaches using optical emission data obtained by a microplasma.

**Vassili Karanassios** is a Professor of Chemistry at the University of Waterloo (Ontario, Canada) and a co-founder of a degree-program in nano-technology engineering at the same University. Professor Karanassios received his Ph.D. from the University of Alberta (Edmonton, Canada) and was a Post Doctoral Fellow at McGill University (Montreal, Canada). In 2009, he held a Leverhulme award in the UK where he was a visiting Professor in Chemistry (Sheffield University), an Overseas Fellow of Churchill College (Cambridge University, UK), and a visiting Professor of Engineering (Cambridge University, UK) in the Center for Advanced Photonics and Electronics (CAPE). Karanassios and his group published (among others) on 3D printing, on microfluidics and nanofluidics, on and on rapid prototyping, on spectral interference correction using Artificial Neural Networks (ANNs) and Deep Learning, and on smartphone-enabled data acquisition and signal-processing from a variety of sensors for *on-site* chemical analysis and (potentially) for IoT applications and on microplasmas for elemental analysis.

**SS-07 Laser-Induced Breakdown Spectroscopy (LIBS)**, Tuesday, January 16, 7 pm, Vassilia Zorba, vzorba@lbl.gov, Laser Technologies Group, Lawrence Berkeley National Laboratory, Berkeley, CA 94720

This course will cover the basic principles, mechanisms, and instrumentation of laser-induced breakdown spectroscopy (LIBS). Laser-induced breakdown spectroscopy (LIBS) has emerged as a unique analytical technique for the qualitative and quantitative analysis of a variety of solid materials. The minimal sample preparation requirements, high spatial resolution capabilities, rapid analysis time, simple instrumentation, and applicability to all media make LIBS especially appealing to industry. This course will introduce the fundamentals and instrumentation of LIBS and provide a brief review of current applications. The utility of LIBS for the analysis of solid materials will be covered, including its application to coating analysis, homogeneity determination, contaminant identification, and elemental quantitative analysis.

Keywords: LIBS, atomic spectroscopy, mechanisms, instrumentation, solid analysis

### **Plasma Spectrochemical Techniques**

**ST-01 Critical Factors for Successful R&D Development Projects**, Saturday, January 13, 8 am, Andrew T. Zander, atzander1027@gmail.com, Technical Consultant, SCLS, Inc., 1112 Via Coronel, Palos Verdes Estates, CA 90274  
Once a basic research project shows advantageous outcomes, that is, that it actually works, it may be selected for development into a new product. At that stage a variety of factors, some of them competing, can directly affect the successful development of the target product.

In this short course, some specific aspects leading to the success of an R&D product development project will be covered. They are aspects of high tech development that are rarely covered in conventional curricula. Among the topics to be covered will be budgeting and finances; innovation; and leadership.

Keywords: Product development. Innovation. Leadership. Budgeting.

**Andrew Zander** is a successful technology developer and manager of engineering and scientific professionals. The majority of his product development experience is in the analytical instrument industry. He also has managerial and technical development experience in Defense Dept. RDT&E from a 30-year career in the U. S. Naval Reserve as a Senior Scientific Liaison Officer with the Office of Naval Research.

**ST-03 High Precision and Accuracy Isotopic Analysis by MC-ICP-MS**, Saturday, January 13, 8 am, Lu Yang, lu.yang@nrc-cnrc.gc.ca, National Research Council Canada, 1200 Montreal Rd, Ottawa, ON, K1A 0R6, Canada  
This short course focuses on the latest developments related to isotopic fractionation/mass bias and its correction models for the accurate and precise determination of both absolute isotope ratios and delta isotope ratios by MC-ICP-MS. In addition to commonly believed mass-dependent fractionation (MDF) phenomenon, recognition and reporting of mass-independent fractionation (MIF) within MC-ICP-MS itself has proliferated in the last couple decades. MIF has a significant impact on the choice of these isotopic fractionation correction models, as the use of mass-dependent models to correct for instrumental bias for isotopes which display mass-independent fractionation would result in biased isotope amount ratios. Implication of MIF on several popular mass bias correction models, the core concepts and assumptions for each model, its pros and cons, and individual practical aspects for isotope amount ratio measurements will be discussed in details.  
Keywords: Delta isotope ratio, absolute isotope ratio, MC-ICP-MS, isotopic fractionation, mass bias, correction models, mass-dependent fractionation, mass-independent fractionation

**Lu Yang** is a Senior Research Officer at National Research Council of Canada (NRC, Ottawa, Canada) and a Fellow of Royal Society of Chemistry, leading research in applications of ICP-MS and MC-ICP-MS. She has published over 140 research papers. The isotopic measurements for mercury, germanium, indium, iridium, osmium, hafnium, and lead from her lab have been adopted by IUPAC as the best available isotopic composition measurements; and the standard atomic weights of Hg, Ge, Ir and Hf are based on her lab's results. She is a NRC's representative at the Isotope Ratio Working Group of CCQM (Consultative Committee for Amount of Substance) of the BIPM (International Bureau of Weights and Measures), and services as an Associate Editor of *Frontiers in Chemistry* (Analytical Chemistry) and Editorial Board member of *Spectroscopy* and the Advisory board member of JAAS.

**ST-04 Starting a New Laboratory or Modifying Your Existing Laboratory for Trace Analyses**, Sunday, January 14, 8 am, Ela Bakowska, ela@bakowska.com, bakowskae@corning.com, Elba Elemental Consulting, PO Box 1053, Corning, NY 14830

The course would benefit scientists and managers adapting their current laboratory (renovating or remodeling) or designing a new laboratory to optimize the performance of ICP-MS instrumentation. Reducing and eliminating sources of elemental contamination and by optimizing the laboratory layout improve trace or ultra-trace capabilities. Based on my own experience of building seven new labs and modifying few existing labs, I will share the best practices of minimizing the contamination, optimizing the workflow and guidelines for procurement of new instrumentation. Cost saving alternatives for lab design and operation will be presented. Sample preparations considerations for different applications will be discussed.  
Keywords: Laboratory design/upgrade, contamination prevention, supplies, instrumentation, sample preparation, safety, automation.

**Ela Bakowska** is a Senior Research Associate at Corning RDC and Technical Director at Elba Elemental Consulting and has more than 30 years of experience in ICP-MS. Ela holds M.S. in Physical Chemistry from the Warsaw University (Poland) and Ph.D. in Analytical Chemistry from the University of Massachusetts, Amherst. During her career Ela established the first application ICP-MS lab at HP (now Agilent Technologies) and expanded and modernized several other labs. For eight years she was ICP-MS application chemist for HP/Agilent, and in this role, she assisted multiple customers in modernizing and upgrading their labs. Since 2001 (again a user), she purchased multiple ICP-MS systems from various vendors. Ela's experience includes development of methods for preparation and analysis of various types of glass, ceramics, raw materials, plastics, semiconductor, clinical, forensic, environmental, nuclear, and pharmaceutical samples. Since 2010 Ela is continuously upgrading and automating her seven labs at Corning RDC, including sample preparation areas dedicated to ultra-trace levels testing. During 13 years at Corning RDC Ela purchased two HR-ICP-MS systems, six Q-ICP-MS, one ICP-MS-QQQ and two LA.

**ST-05 Fundamentals, Plasma Diagnostics, Measurements, and Applications of Analytical Plasmas**, Sunday, January 14, 8 am, Igor B. Gornushkin, igor.gornushkin@bam.de, BAM, Federal Institute for Materials Research and Testing, Berlin, Germany

This course will introduce you to plasma diagnostic techniques. The focus of the course will be on a discussion of practical procedures as well as the basic physical principles for measuring fundamental plasma characteristics. Topics to be covered include thermal equilibrium, line profiles, temperatures, electron densities, excitation processes, micro reactions, pump and probe diagnostics, tomography, temporal and spatial resolution. Particular attention will be paid to laser induced plasma, but other types of analytical plasmas will be used as examples if necessary. A brief introduction to plasma modeling will also be offered.  
Keywords: Thermal equilibrium, plasma processes, plasma diagnostics, emission line profiles, temperature and density measurements, spatial information

**Igor B. Gornushkin** is a physicist and analytical chemist with major expertise in fundamental and applied spectroscopy including LIBS, emission, absorption, fluorescence, and Raman. He received his PhD from the University of Florida in 1998 and at present works at BAM Federal Institute of Material Research, Berlin (Germany).

He develops spectroscopic methods for environmental, industrial, and laboratory applications, and he has strong background in physics, optics, and computer modeling.

**ST-06 Triple Quad (QXQ) ICP-MS**, Sunday, January 14, 1 pm, R. Steven Pappas, rpappas@cdc.gov, Naudia Gray, NGray@cdc.gov, Centers for Disease Control & Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341-3717

Development of the Agilent 8900 QQQ, the ThermoFisher iCAPTQ, and the PerkinElmer 5000 were major steps in next generation quadrupole instrumentation development, adding new capabilities, increased sensitivity, and new approaches for addressing analytical interferences. Basic instrument designs and how they address analytical problems will be discussed. This course will describe choice of reactive gas to accomplish "mass shift" to avoid interferences, how to use internal standards in different modes, how to use instrument settings to overcome problems with high intensity analytes in the same method with low intensity analytes.

Analysts who are investigating the potential of triple quad ICP-MS instrumentation, how to take advantage of its capabilities, how to apply it to multielement, multimode methods, internal standard choices, practical applications will find this course useful.

Keywords: TripleQuad, QQQ-ICP-MS, interference, reactive gas, quadrupole, reaction cell

**Steve Pappas** earned his B.S. in Chemistry at Middle Tennessee State University and his Ph.D. in Biochemistry at Vanderbilt University. After faculty positions at Middle Tennessee State University and Georgia State University, he was employed at the Centers for Disease Control and Prevention (CDC) to develop methods for analysis of toxic metals in urine and blood within the Clinical Laboratory Improvement Act (CLIA) framework and later became the Tobacco Inorganics Group Project Lead responsible for development of methods for analysis of toxic metals in tobacco, cannabis, tobacco smoke, electronic cigarette liquids and aerosols within the ISO 17025 framework, and electronic cannabinoid delivery device aerosols during the 2019-2020 CDC E-Cigarette and Vaping Associated Lung Injury emergency response.

In addition to authoring analytical manuscripts and presenting on good analytical practices in ASTM, AOAC and Spectroscopy symposiums, Steve has written Annex 1 (Toxic Metals in Tobacco and in Cigarette Smoke) in World Health Organization Technical Report Series 967, the pre-edited metals section in "A Report of the Surgeon General (2010): How Tobacco Smoke Causes Disease", toxicological reviews in Metallomics (Toxic elements in tobacco and in cigarette smoke: inflammation and sensitization) and International Journal of Environmental Research and Public Health (Cadmium and cadmium/zinc ratios and tobacco-related morbidities), and book chapters in "Measuring Heavy Metal Contaminants in Cannabis and Hemp" and "Applied Mass Spectroscopy Handbook, Homeland Security".

**Naudia Gray** received her Bachelors and Masters in Environmental Science at Duquesne University under Dr. Skip Kingston in 2012. After completing her masters, she began to work in the Tobacco and Volatiles Branch of CDC in the Tobacco Inorganics group under Dr. Steve Pappas. Her assignments have included determination of cigarette and little cigar physical properties, development and utilization of methods for analysis of toxic metals in tobacco and tobacco smoke using microwave digestion, development of a low metals trap for e-cigarette aerosol, quadrupole ICP-MS, "Triple Quadrupole" ICP-MS, and combustion mercury analyzer.

**ST-07 sp-QQQ-ICP-MS, ETV-QQQ-ICP-MS, GC-QQQ-ICP-MS, HPLC-QQQ-ICP-MS, QQQ-ICP-MS: Method**

**Development, Problem Solving, Troubleshooting and Optimization**, Saturday, January 13, 1 pm, Mark Fresquez, mwf6@cdc.gov, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341-3717

This short course will cover hyphenated techniques related to ICP-MS enabling ultra-trace elemental analysis with minimal interferences. Course will discuss selectivity, optimization, troubleshooting, problem solving, and method development of these specific techniques and the issues involved in the analyses of difficult matrices with an emphasis on especially troublesome blank contaminations. Discussion on isotope dilution, sp-QQQ-ICP-MS, desolvating sample introduction systems, sample preparation, and troubleshooting of ICP-MS hyphenated systems and ICP-MS instrumentation in general.

Anyone interested in achieving selectivity and sensitivity increases related to hyphenated techniques involving ICP-MS, and analysts interested in interference removal, analysis of difficult matrices, maintenance strategies and troubleshooting of instrumentation should attend.

Keywords: ICP-MS, sp-QQQ-ICP-MS, Desolvating, Sample, Introduction, interferences, hyphenated, troubleshooting, method, ultra- trace

**Mark Fresquez** earned his B.S. in Chemistry in 1988, and subsequently his M.S. in Analytical Chemistry at New Mexico State University. Mark began his career in commercial environmental trace metal analysis laboratories working with a wide variety of matrices and instrumentation including ETV-AAS, CV-AAS, ICP-OES and ICP-MS for 13 years. Afterwards he was employed at the Centers for Disease Control and Prevention (CDC) working with arsenic speciation in urine utilizing HPLC-ICP-MS and mercury speciation in blood using GC-ICP-MS. Subsequently at CDC he was responsible for development of methods for analysis of tobacco and smoke for toxic metals. He has over 30 years of inorganic trace metals analysis experience with a wide range of instrumentation including ETV-AAS, ICP-OES/AES, ICP-MS, HPLC-ICP-MS, GC-ICP-MS, and ETV-ICP-MS.

**ST-08 Sample Preparation Problem Solving for Atomic Mass Spectrometry**, Sunday, January 14, 7 pm, R.

Steven Pappas, rpappas@cdc.gov, Naudia Gray, NGray@cdc.gov, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341-3717

Topics include preparation of liquid samples such as water, urine, and blood, biological solid sample digestion, very brief coverage of difficult inorganic oxide and metal sample dissolution, chemistry related to analytes of interest including chelation and avoiding memory effects. Approaches to optimization and the use of desolvating introduction systems for increased sensitivity and decreased interferences will be discussed. Limited discussion will touch on special needs such as considerations necessary for organic solvents and use of electrothermal vaporization.

Analysts new to inorganic analysis or who are struggling with common or challenging samples, internal standard choices, or who have problems with memory effects will find this course useful.

Keywords: Sample preparation, memory effects, chelation, digestion, desolvation, environmental and biological samples, electrothermal vaporization

**ST-09 Validation Assessment and ISO/IEC 17025: An Interactive Session**, Sunday, January 14, 1 pm, Rob

Ritsema, robritsema@gmail.com, RR Quality Consultancy, Amersfoort, The Netherlands; Petra Krystek, petra.krystek@uni-siegen.de, University of Siegen, Department of Chemistry and Biology, Siegen, Germany

This course will give an overview about the validation of analytical methods and procedures, which is an integral part of any good analytical practice. Method validation is the process used to confirm that the analytical procedure employed for a specific test is suitable for its intended use. Results from method validation can be used to judge the quality, reliability, and consistency of analytical results.

For making this information as practice relevant as possible, several examples like a procedure for the determination of selected elements in water by ICPMS will be discussed in detail. Special attention will be given to sampling and storage. Other examples from the inorganic analytical field of environmental, food and biological matrices will be covered too.

Besides the methodological aspects and the obtained analytical results, the ten most relevant performance characteristics (limit of detection, recovery, repeatability, reproducibility, measuring range, trueness, lack of fit, expanded uncertainty of measurement, robustness, and selectivity) are defined, calculated, and discussed; also in relation if the analytical method should fulfill of the accreditation standard ISO/IEC 17025.

More aspects of ISO/IEC 17025 will be discussed too.

This course will be held as an interactive session.

**Rob Ritsema** is an analytical chemist and obtained his PhD in 1997 at the Université de Pau et des Pays de l'Adour, Pau, France. He was working at the accredited laboratory of the National Institute of Public Health and the Environment (RIVM) in the field of ICPMS during 15 years, focussing on environmental, food and body fluid analysis. Since 2019, he has his own company RR Quality Consultancy.

Since 1998, he is a freelance assessor at the Dutch Accreditation Council (RvA) performing approx. twenty ISO/IEC 17025 technical assessments on a yearly base at accredited laboratories in the Netherlands and Belgium. In 2015, he started at RvA as a freelance lead assessor.

He is board member of the working group Atomic Spectrometry of the Royal Netherlands Chemical Society (KNCV).

**Petra Krystek** received her PhD in 1999 at the University of Mainz, Germany. She has more than 20 years' experience in the field of ICPMS. Her research is application focused, especially regarding to ultra-trace, speciation and nano-analysis mainly in the field of health and environmental aspects, and she has been involved in many interdisciplinary projects. She has worked at research institutes like the National Institute for Public Health and the Environment (RIVM) and Deltares in the Netherlands as well as in industries as Thermo and Philips. From 2009 to 2022, she also had a fellowship at the department Environment & Health at the Vrije Universiteit (VU) Amsterdam, the Netherlands.

Since 2003, she is a lead assessor and technical assessor in inorganic analytical chemistry at the Dutch Accreditation Council (RvA) for auditing laboratories mainly in the Netherlands, which are accredited according to ISO/IEC 17025.

Since 2018, she is visiting lecturer at the University of Siegen in Germany.

Petra Krystek has published over 65 peer reviewed articles and book chapters; she is a regularly invited lecturer and speaker at international symposia and organized many workshops. She is also member of the editorial board of the journal Chemosphere.

**ST-10 Metrology Concepts in Plasma Spectrochemistry**, Saturday, January 13, 8 am, Zoltan Mester,

zoltan.mester@nrc-cnrc.gc.ca, National Research Council of Canada (NRC), 1200 Montreal Rd, Building M-58, Ottawa, ON K1A0R6, Canada

An overview of the basics concepts of chemical measurement science will be given. The international infrastructure supporting measurement comparability consists of a constellation of documentary standards, laboratory accreditation infrastructure and an organizational framework maintaining physical measurement standards, etalons.

The role of these three pillars will be discussed with a particular focus on the National Metrology Institutes.

Measurement scales, concepts related to measurement traceability, comparability, and uncertainty will also be explored. Special attention will be given to the selection and proper use of certified reference materials (CRMs).



Keywords: Chemical metrology, traceability, uncertainty, CRM

**Zoltan Mester** completed his PhD in chemistry splitting his time between his alma mater in Budapest and Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA), Rome, Italy. After his graduation he joined University of Waterloo, Canada and developing novel microextraction methodologies. In 1999 accepted a position at the National Research Council Canada (NRC) in Ottawa, Canada where since 2010 he is heading the inorganic chemical measurement science research program. His research interest is focused on the analytical use of mass spectrometry. Since 2005, he has been active at the International Union of Pure and Applied Chemistry (IUPAC), in increasingly senior roles, where he is currently completing his second term as the President of the Analytical Chemistry Division. Since 2010 he has been representing Canada at the Consultative Committee for Amount of Substance (CCQM) of the Metre Convention (international treaty, curating the system of units, the SI). Apart from research and international outreach activities he is also involved training the next generation of analytical chemists by hosting students in his laboratories at NRC. He delivered/contributed to courses at universities in more than 20 countries and maintained adjunct professorships at two Canadian universities. He has published over 230 peer-reviewed papers, 3 book chapters and one book. His papers receive around 500 citations annually. Over the years he gave numerous invited/keynote presentations at conferences around world.

**ST-11 Sample Classification Using Elemental Fingerprint Analysis**, Saturday, January 13, 7 pm, Andreas Limbeck, andreas.limbeck@tuwien.ac.at, and Lukas Brunnbauer, TU Wien, Institute of Chemical Technologies and Analytics, Getreidemarkt 9/164, A-1060 Vienna, Austria

In recent years, much progress has been made in sample discrimination based on elemental fingerprinting techniques. To achieve this, elemental analysis is combined with multivariate statistical analysis of the obtained data to gain information about differences or variations within the investigated samples. In this short course, we will briefly present the concepts and approaches used for assessing elemental contents and provide an overview of common chemometric methods and their potential for sample classification. Finally, we will discuss some descriptive application examples from the fields of food analysis, geology, life sciences and material science.

Keywords (limit 10): multi-element analysis, elemental fingerprint, chemometrics, statistical analysis, machine learning, sample authentication, product adulteration, and forensic analysis

**Andreas Limbeck** is an expert in the field of atomic spectroscopy with more than 20 years research experience. In the last years, he developed advanced expertise in the application of LA-ICP-MS and LIBS for the chemical analysis of solid materials, in particular for the quantitative determination of element distributions in various sample types. Since 2021 he is full professor for “Analytical Chemistry of Materials” at the Faculty of Technical Chemistry at TU Wien.

**Lukas Brunnbauer**, received his PhD in Technical Chemistry from the TU Wien. Currently he is working as PostDoc at TU Wien in the research group “Surface Analytics, Trace Analytics and Chemometry”. His research is mainly focused on spatially resolved polymer characterization using LIBS and LA-ICP-MS.

**ST-12 Nanomaterials: Advances in Standardization, Measurement Methods, Reference Materials and Remaining Challenges Imposed by Regulation**, Monday, January 15, 7 pm, Heidi Goenaga-Infante, LGC Limited, Queens Road, Teddington, Middlesex TW1 1 OLY, U K, heidi.goenaga-infante@lgcgroup.com

This short course will discuss advances in regulatory aspects of the use of engineered nanomaterials by industry, linked to the existing nanomaterial definitions, and in measurement methods and reference nano-materials. It will also discuss progress made so far in standardization, the learning experience from collaborative international comparison studies for assessment of methods and materials and, will generate a discussion on remaining analytical challenges driven by regulation.

It will be divided into three parts as follows: The first part of the course will cover recent guidance and scientific opinions on the safe use of nanomaterials and key regulations, which have emerged from the increasing use of nanomaterials in several industrial applications (e.g., novel food, food contact materials, cosmetics, medical devices, etc.). It will also discuss the measurement capability needed to comply with those regulations and for future risk assessment. The second part of the course will discuss existing analytical technology and advances in measurement capabilities for the characterization of nanomaterials and their input on key relevant ISO standards. Focus will be on inorganic nanomaterials and on multi-modal platforms combining hyphenated ICP-MS with spectroscopy and microscopy techniques. Examples of key analytical challenges and recommendations for overcoming such challenges will be given through (i) the quantification and characterization of metal oxide nanoparticles in food and cosmetics by asymmetrical field-flow-fractionation hyphenated to multiple detectors and (ii) the characterization of complex nanomaterial mixtures released from medical devices by single particle ICP-MS and AF4-ICPMS/light scattering for toxicology testing. Finally, the short course will touch on measurement lessons learnt from international intercomparisons as well as highlight future measurement and technology requirements and associated challenges. It will also provide the attendees with information on the existing reference materials for method development and validation and discuss remaining gaps for matrix/measurand combinations. The course presentation will be informal allowing for questions or remarks from the participants to be raised and discussed at any time.

Keywords: Regulations, standardization, engineered nanomaterials, reference nano-materials, measurement, characterization, AF4, international comparisons, ICP-MS, light scattering, microscopy.

**ST-13 Agilent ICP-Expert/Masshunter Workshop**, Tuesday, January 16, 7 pm, Chuck Schneider, et al., chuck.schneider@agilent.com, Agilent Technologies, 2850 Centerville Rd, Wilmington, DE 19808

Come hone your skills with our software bootcamps. Learn about the latest in software solutions for spectroscopy, discuss the entire analytical process from method development to data analysis with our experts. PCs provided with the latest software loaded. Half the course will cover the ICP Expert software followed by a session on MassHunter software for ICP-MS. ICP Expert is for ICP-OES systems and MassHunter is for ICP-MS and ICP-QQQ systems. Current and prospective users of Agilent atomic spectroscopy equipment should take this course.

Keywords: software, Agilent