2022 Winter Conference on Plasma Spectrochemistry

Short Courses

Professional Development Courses

Saturday – Tuesday,
January 14 – 18, 2022

Course Descriptions

Course Hours:

8 am - 12 noon

1 pm - 5 pm

7 pm - 11 pm

2022 Winter Conference Short Courses

Friday, January 14 – Tuesday, January 18, 2022

Schedule

Analysis by Plasma Spectrochemistry

SA-01 Practical Guide to ICP-MS for Toxicology, Sunday, January16,8am,RileyMurphy, riley.murphy@nmslabs.com, NMS Labs, 200 Welsh Road, Horsham PA 19044

SA-02 Environmental Isotope Geochemistry: Plasma Spectrochemistry as an Essential Tool, Michael E. Ketterer, Saturday, January 15, 8 am, Department of Chemistry and Biochemistry, Northern Arizona University, Box 5698, Flagstaff, AZ 86011-5698, michael.ketterer@nau.edu

SA-03 Speciation Analysis: Complementarity of Elemental, Isotopic and Molecular Mass Spectrometry in Life Sciences Studies, Monday, January 17, 7 pm, Joanna Szpunar, joanna.szpunar@univ-pau.fr, and Ryszard Lobinski, Institute for Analytical Sciences and Physicochemistry of the Environment and Materials, CNRS UMR 5254-IPREM, Hélioparc, 2, Av. Président Angot, 64053 Pau, France

SA-04 Arsenic and Mercury Speciation in Biological Samples, Sunday, January 16, 7 pm, Jörg Feldmann, ESLA - Analytical Chemistry Institute of Chemistry, University of Graz, Universitätsplatz 1, 8010 Graz, Austria, joerg.feldmann@uni-graz.at, j.feldmann@abdn.ac.uk

SA-05 Clinical ICP-MS: **Inorganic Chemical Exposure Evaluations for Clinical Diagnosis, Biomonitoring and Emergency Response.** Sunday, January 16, 1 pm, Robert Jones, rljones@cdc.gov, Cynthia Ward, dmo9@cdc.gov, CDC, Inorganic and Radiation Analytical Toxicology Branch, 4770 Buford Hwy, Mailstop S103-1, Atlanta, GA 30341-3724

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

SA-07 ICPMS for the Characterization of Nanomaterials: Focusing on the Human Exposure to Nanoproducts, Saturday, January 15, 7 pm, Petra Krystek, Vrije University (VU) Amsterdam, Amsterdam, The Netherlands, petra.krystek@vu.nl

SA-08 Environmental Sampling Techniques for Laboratory Analysts in Fair and Foul Weather, Saturday, January 15, 7 pm, Brian Buckley, Rutgers University, EOHSI 681 Frelinghuysen Rd, Piscataway NJ 08854, bbuckley@eohsi.rutgers.edu

SA-09 Analysis of Petroleum and Petroleum Products, Monday, January 17, 7 pm, José Luis Todolí, Department of Analytical Chemistry, Nutrition and Food Sciences, University of Alicante, PO Box 99, 03080 Alicante, Spain, jose.todoli@ua.es

SA-10 Single Particle and Single Cell ICP-MS Theory and Applications, Sunday, January 16, 7 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 Speciation and Non Traditional Isotopic Analyses for Environmental, Forensic, Biomedical, and Industrial Applications. Sunday, January 15, 7 pm, Olivier Donard, MARSS-IPREM, University of Pau, Pau, France, olivier.donard@univ-pau.fr

SA-12 Elemental Bioimaging of Tissues and Cells. Saturday, January 15, 1 pm, Dirk Schaumlöffel, dirk.schaumloeffel@univ-pau.fr, IPREM CNRS UMR 5254, Hélioparc, 2 avenue du president Angot, 64053 Pau, France

SA-13 Tracing Element Metabolism in Animals and Humans Using Stable Isotope Techniques, Monday, January 17, 7 pm, Thomas Walczyk, Department of Chemistry, National University of Singapore, Science Drive 4, Singapore 117543, walczyk@nus.edu.sg

SA-14 Fundamentals in Metals Toxicology; How Metals Got Their Biological Species, Tuesday, January 18, 7 pm, Brian Buckley, Rutgers University, Environmental and Occupational Health Sciences Institute, 681 Frelinghuysen Road, Piscataway NJ 08854, bbuckley@eohsi.rutgers.edu

Spectrochemical Instrumentation

SI-01 New Calibration Strategies in Spectrochemical Analysis, Tuesday, January 18, 7 pm, George L. Donati, Wake Forest University, Department of Chemistry, Winston-Salem, NC 27109, donatigl@wfu.edu

SI-02 Opportunities, Challenges, and Application of Glow Discharge Techniques, Sunday, January 16, 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, MassCare Ltd., 11 Waterside Way, Middlewich, Chesire, CW10 9HP, United Kingdom; pete@masscare.co.uk

SI-03 ICP-TOFMS: Principles and Application for Single-Particle Analysis. Friday, January 14, 7 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 15, 1 pm, John Olesik, Ohio State University, School of Earth Sciences, 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002, olesik.2@osu.edu

SI-05 ICP-MS II: Advanced Topics, Sunday, January 16, 1 pm, John Olesik, Ohio State University, School of Earth Sciences, 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002, olesik.2@osu.edu

SI-06 Theory and Practical Use of Reaction Cells and Collision Cells for ICP-MS, Monday, January 17, 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, Maryland

SI-07 Interferences in ICP Spectroscopy, Sunday, January 16, 1 pm, José Luis Todolí, Department of Analytical Chemistry, Nutrition and Food Sciences, University of Alicante, PO Box 99, 03080 Alicante, Spain, jose.todoli@ua.es

SI-08 Identification and Correction of Interferences in Practical ICP-OES, Sunday, January 16, 8 am, Deborah Bradshaw, Atomic Spectroscopy Consulting, PO Box 536307, Orlando, FL 32853-6307, bradshawdk@cs.com

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

SI-10 "The Chemical Analysis of Things As They Are": Direct Atomic and Molecular Analyses with Ambient Mass Spectrometry, Saturday, January 15, 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

Sample Introduction Approaches

SS-01 A Practical Guide to Nebulizers and the Part They Play in Modern Sample Introduction, Saturday, January 15, 7 pm, Steve Mangum, Elemental Scientific Inc., 7277 World Communications Dr, Omaha, NE 65132; steve.magnum@icpms.com

SS-02 Laser Ablation Mass Spectrometry I, Friday, January 14, 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 17, 7 pm, Jhanis Gonzalez, Applied Spectra, Inc., 46661 Fremont Blvd, Fremont, CA 94538, jhanis@appliedspectra.com, jjgonzalez@lbl.gov; Rick Russo, Lawrence Berkeley National Laboratory, 1 Cyclotron Rd, Berkeley, CA 94720, rerusso@lbl.gov

SS-04 Variations of Single Particle Inductively Coupled Plasma Mass Spectrometry, Diane Beauchemin, Sunday, January 16, 8 am, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada, diane.beauchemin@queensu.ca

SS-05 Microplasma for Chemical Analysis, Saturday, January 15, 7 pm, Vassili Karanassios, University of Waterloo, Department of Chemistry and Waterloo Institute for Nanotechnology, Waterloo, ON N2L 3G1, Canada, vkaranassios@uwaterloo.ca

SS-06 Laser-Induced Breakdown Spectroscopy (LIBS), Tuesday, January 18, 7 pm, Vassilia Zorba, Laser Technologies Group, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, vzorba@lbl.gov

Plasma Spectrochemical Techniques

ST-01 Soft Skills Supporting Scientific Success, Saturday, January 15, 8 am & 1 pm, Andrew T. Zander, Consultant, 1632 Hickory Ave, Torrance, CA 90503, atzander1027@gmail.com

ST-02 Isotopic Measurements Using ICP-MS, Sunday, January 16, 1 pm, Frank Vanhaecke, Ghent University, Department of Analytical Chemistry, Campus Sterre, Krijgslaan 281 - S12, 9000 Ghent, Belgium, frank.vanhaecke@ugent.be, and Nancho Garcia Alonso, University of Oviedo, Ovideo, Spain, jiga@uniovi.es

ST-03 Accurate, Precise and SI Traceable Measurements by ICP-MS, Lu Yang, National Research Council Canada, 1200 Montreal Rd., Ottawa, ON, K1A 0R6, Canada, lu.yang@nrc-cnrc.gc.ca

ST-04 Isotopic Fingerprinting for Source Identification and Apportionment of Lead in a Child's Environment, Tuesday, January 18, 7 pm, Cathleen Doherty, cld133@eohsi.rutgers.edu, Rutgers University, EOHSI 170 Frelinghuysen Rd, Piscataway NJ 08854

ST-05 Contamination Control for Elemental Analysis, Sunday, January 16, 1 pm, Brad McKelvey, Seastar Chemicals Inc., 10005 McDonald Park Rd., Sidney, BC V8L 5Y2, Canada, bmckelvey@seastarchemicals.com

ST-06 Launching or Modifying Your Laboratory for Trace Analyses, Sunday, January 16, 8 am, Ela Bakowska, Elba Elemental Consulting, PO Box 1050, Corning, NY 14830, ela@bakowska.com, bakowskae@corning.com

ST-07 Why IUPAC Tables of Isotopic Abundances and Atomic Weights Should Matter to Plasma Spectrochemists, Sunday, January 16, 8 am, Johanna Irrgeher, Montanuniversität Leoben, Department of General, Analytical and Physical Chemistry, Chair of General and Analytical Chemistry, Isotope Research Group; Franz Josef-Strasse 18, 8700 Leoben, Austria, johanna.irrgeher@unileoben.ac.at

ST-08 Plasma Diagnostics: Fundamentals, Measurements, and Applications, Sunday, January 16, 7 pm, Igor B. Gornushkin, BAM, Federal Institute for Materials Research and Testing, Berlin, Germany, igor.gornushkin@bam.de

ST-09 Triple Quad (QXQ) ICP-MS, Sunday, January 16, 1 pm, R. Steven Pappas, and Nathalie Gonzalez-Jimenez, Centers for Disease Control & Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341, rpappas@cdc.gov

ST-10 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 15, 1 pm, Mark Fresquez, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341, mwf6@cdc.gov

ST-11 Sample Preparation Problem Solving for Atomic Mass Spectrometry, Sunday, January 16, 7 pm, R. Steven Pappas and Naudia Gray, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341, rpappas@cdc.gov

ST-12 Validation Assessment and ISO/IEC 17025: An Interactive Session, Sunday, January 16, 1 pm, Rob Ritsema, RR Quality Consultancy, Amersfoort, The Netherlands; robritsema@gmail.com; Petra Krystek, VU Amsterdam, The Netherlands, petra.krystek@vu.nl

ST-13 Uncertainty of Measurements: Practical Approaches to Determine Measurement Uncertainty Budgets, Sunday, January 16, 7 pm, Thomas Prohaska, Chair General and Analytical Chemistry, Montan-universitaet Leoben, Franz Josef-Strasse 18, 8700 Leoben, Austria, thomas.prohaska@unileoben.ac.at

ST-14 Nanomaterials: Advances in Standardization, Measurement Methods, Reference Materials and Remaining Challenges Imposed by Regulation, Monday, January 17, 7 pm, Heidi Goenaga-Infante, LGC Limited, Queens Road, Teddington, Middlesex TW11 OLY, UK, heidi.goenaga-infante@lgcgroup.com

ST-15 Metrology Concepts in Plasma Spectrochemistry, Saturday, January 15, 7 pm, Zoltán Mester, National Research Council of Canada (NRC), 1200 Montreal Rd, Building M-58, Ottawa, ON K1A 0R6, Canada, zoltan.mester@nrc-cnrc.gc.ca

Schedule by Date and Time

Friday, January 14, 1 pm

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

Friday, January 14, 7 pm

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

Saturday, January 15, 8 am

SA-02 Environmental Isotope Geochemistry: Plasma Spectrochemistry as an Essential Tool, Michael E. Ketterer, Department of Chemistry and Biochemistry, Northern Arizona University, Box 5698, Flagstaff, AZ 86011-5698, michael.ketterer@nau.edu

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ST-01A Soft Skills Supporting Scientific Success, Andrew T. Zander, Consultant, 1632 Hickory Ave, Torrance, CA 90503, atzander1027@gmail.com

ST-15 Metrology Concepts in Plasma Spectrochemistry, Zoltán Mester, National Research Council of Canada (NRC), 1200 Montreal Rd, Building M-58, Ottawa, ON K1A 0R6, Canada, zoltan.mester@nrc-cnrc.gc.ca

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SA-12 Elemental Bioimaging of Tissues and Cells. Saturday, Dirk Schaumlöffel, dirk.schaumloeffel@univ-pau.fr, IPREM CNRS UMR 5254, Hélioparc, 2 avenue du president Angot, 64053 Pau, France

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ST-01B Soft Skills Supporting Scientific Success, Andrew T. Zander, Consultant, 1632 Hickory Ave, Torrance, CA 90503, atzander1027@gmail.com

ST-10 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 15, 1 pm, Mark Fresquez, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341, mwf6@cdc.gov

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SI-02 Opportunities, Challenges, and Application of Glow Discharge Techniques, 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, MassCare Ltd., 11 Waterside Way, Middlewich, Chesire, CW10 9HP, United Kingdom; pete@masscare.co.uk

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ST-03 Accurate, Precise and SI Traceable Measurements by ICP-MS, Lu Yang, National Research Council Canada, 1200 Montreal Rd., Ottawa, ON, K1A 0R6, Canada, lu.yang@nrc-cnrc.gc.ca

ST-06 Launching or Modifying Your Laboratory for Trace Analyses, Ela Bakowska, Elba Elemental Consulting, PO Box 1050, Corning, NY 14830, ela@bakowska.com

ST-07 Why IUPAC Tables of Isotopic Abundances and Atomic Weights Should Matter to Plasma Spectrochemists. Johanna Irrgeher, Montanuniversität Leoben, Department of General, Analytical and Physical Chemistry, Chair of General and Analytical Chemistry, Isotope Research Group; Franz Josef-Strasse 18, 8700 Leoben, Austria, johanna.irrgeher@unileoben.ac.at

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SA-05 Clinical ICP-MS: **Inorganic Chemical Exposure Evaluations for Clinical Diagnosis, Biomonitoring and Emergency Response.** Robert Jones, Cynthia Ward, Jeff Jarrett, CDC, Inorganic and Radiation Analytical Toxicology Branch, 4770 Buford Hwy, Mailstop S103-1, Atlanta, GA 30341, rljones@cdc.gov, dmo9@cdc.gov

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ST-12 Validation Assessment and ISO/IEC 17025: An Interactive Session, Rob Ritsema, RR Quality Consultancy, Amersfoort, The Netherlands, robritsema@gmail.com; Petra Krystek, VU Amsterdam, The Netherlands, petra.krystek@vu.nl

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

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Monday, January 17, 7 pm

SA-03 Speciation Analysis: Complementarity of Elemental, Isotopic and Molecular Mass Spectrometry in Life Sciences Studies, Joanna Szpunar, joanna.szpunar@univ-pau.fr, and Ryszard Lobinski, Institute for Analytical Sciences and Physicochemistry of the Environment and Materials, CNRS UMR 5254-IPREM, Hélioparc, 2, Av. Président Angot, 64053 Pau, France

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SS-03 Latest Advances in Laser Ablation-Based Chemical Analysis and Emerging Applications: LIBS, LA-ICP-(OES/MS), and Tandem LA – LIBS, Jhanis Gonzalez, Applied Spectra, Inc., 46661 Fremont Blvd, Fremont, CA 94538, jhanis@appliedspectra.com, jjgonzalez@lbl.gov; Rick Russo, Lawrence Berkeley National Laboratory, 1 Cyclotron Rd, Berkeley, CA 94720, rerusso@lbl.gov

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Descriptive Abstracts

Analysis by Plasma Spectrochemistry

SA-01 Practical Guide to ICP-MS for Toxicology, Sunday, January 16, 2022, 8 am, Riley Murphy, riley.murphy@nmslabs.com, Frederick Strathmann, Justine Titko, NMS Labs, 200 Welsh Road, Horsham PA 19044

Topics to be covered will be part of a practical focus on the utility of using ICP-MS in clinical and forensic testing laboratories. Tales from the front line will be given by a scientist developing and troubleshooting elemental analyses, a board certified clinical and toxicological laboratory director, and a lab supervisor keeping everything in order. Topics around method requirements and design, quality control, utility and case studies, and lab management will be discussed. Lastly, novel and future applications of ICP-MS in clinical aFnd forensic testing will be highlighted. The course is designed for laboratory supervisors, laboratory technologists, researchers, and medical directors.

Keywords: ICP-MS, toxicology, workflow, quality control, test menu design, clinical presentation

Riley Murphy is the Technical Director of the Metals Department at NMS Labs and more recently began technical oversight of the Special Chemistry, and QC Departments as well. He received his BS in chemistry at the University of Vermont in Burlington and his PhD in physical chemistry at Temple University in Philadelphia.

Frederick Strathmann is currently the Senior Vice President of Operations and an Assistant Laboratory Director at NMS Labs in Horsham, Pennsylvania. Dr. Strathmann received his MS and PhD in Pathology & Laboratory Medicine from the University of Rochester in NY, completed an academic postdoctoral fellowship in Biomedical Genetics at the University of Rochester in NY, completed a ComACC accredited clinical chemistry fellowship at the University of Washington in Seattle, and received an MBA from the University of Utah. Dr. Strathmann is board certified in Clinical Chemistry and Toxicological Chemistry from the American Board of Clinical Chemistry and has over 50 peer-reviewed publications in areas ranging from basic research in the neurosciences to laboratory test design and utilization.

Justine Titko is the current supervisor for the Metals and Alcohols departments at NMS Labs. She received her BS in Biology with a minor in Criminal Justice from Lycoming College, and she received her MS in Forensic Science from Arcadia University. Immediately following her graduation from Arcadia, she began working at NMS Labs as a lab support specialist. Through her time at NMS, she worked her way up through the management track to land in her current position, and she will be celebrating her 10-year anniversary with the company in 2022.

SA-02 Environmental Isotope Geochemistry: Plasma Spectrochemistry as an Essential Tool, Michael E. Ketterer, michael.ketterer@nau.edu, Saturday, January 15, 8 am, 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, teaches part-time at University of Denver, and focuses on assistance to communities affected by legacy Cold War-era nuclear contamination.

SA-03 Speciation Analysis: Complementarity of Elemental, Isotopic and Molecular Mass Spectrometry in Life Sciences Studies, Monday, January 17, 7 pm, Joanna

Szpunar, joanna.szpunar@univ-pau.fr, and Ryszard Lobinski, Institute for Analytical Sciences and Physicochemistry of the Environment and Materials, CNRS UMR 5254-IPREM, Hélioparc, 2, Av. Président Angot, 64053 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 the complementarity of 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

Joanna Szpunar is research engineer at the French National Research Council (CNRS) in Pau, France. She has a broad experience in the field of bio-inorganic speciation analysis with a focus on the identification and quantification of trace elements in biological systems and in the chemistry of metal-biomolecule interactions. She is the author or co-author of a book and more than 130 scientific publications in peer-reviewed international journals. Her works have received more than 5500 citations (h-factor 51). Dr. Szpunar (fellow of RSC) has given 30 invited lectures and is a member Advisory Boards of *JAAS*, *Metallomics* and *Brazilian Journal of Analytical Chemistry.* The investigations carried out under her supervision and/or with her active participation resulted in the identification of molecular targets of metals in biological systems including, among others, Bi-binding proteins in *Helicobacter pylori*, Cd-metallothionein complexes in kidney cell lines upon exposure to CdS nanoparticles, I-contaning protein in algae as well as selenoproteins in bacteria and plants. Her research involves severall collaboration projects (University of Zaragoza (Spain), Italian National Institute of Health, University of Vigo (Spain), University of Santiago de Compostela (Spain), University of Naples (Italy), the Norwegian University of Life Sciences, Hongkong University and Mahidol University (Thailand) laboratories. She has supervised six PhD theses and several post-doctoral fellows.

SA-04 Arsenic and Mercury Speciation in Biological Samples, Sunday, January 18, 7 pm, Jörg Feldmann, ESLA - Analytical Chemistry Institute of Chemistry, University of Graz, Universitätsplatz 1, 8010 Graz, Austria, joerg.feldmann@uni-graz.at, j.feldmann@abdn.ac.uk; https://chemie.uni-graz.at/en/analytical-chemistry/research/tesla/

This course is divided into three parts. Part 1 shows how speciation analysis is done when only an element-selective detector is available. In particular identification strategies of known and unknown species using HPLC-ICP-MS will be elaborated. Part 2 introduces electrospray mass spectrometry and discusses the advantages and limitation of this technique for complex sample matrices. Part 3 focuses on quantitative aspects in element speciation analysis when chromatographic separations are used.

Keywords: Electrospray MS, ICP-MS, food analysis, arsenic, arsenosugars, mercury, phytochelatins, plant physiology

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 online combination of both MS techniques

SA-05 Clinical ICP-MS: Inorganic Chemical Exposure Evaluations for Clinical Diagnosis, Biomonitoring and Emergency Response, Sunday, January 16, 1 pm, Robert L. Jones, rljones@cdc.gov, Cynthia Ward, dmo9@cdc.gov, Inorganic and Radiation Analytical Toxicology Branch, Centers for Disease Control and Prevention (CDC), 4770 Buford Hwy, Mailstop S103-1, Atlanta, GA 30341

Successful application of inductively coupled plasma mass spectrometry (ICP-MS) is dependent upon correctly addressing numerous pre-analytical, analytical, and post-analytical issues. This workshop will address key issues including matrix selection, contamination control, sample collection/processing/transport, short and long-term quality control, method validation, quality assurance, CLIA regulations, and human subject issues (IRB). Topics will also include discussion of laboratory environment/infrastructure, considerations for automation of sample processing and analysis, and considerations for Biomonitoring versus clinical diagnosis and emergency response preparedness. This course is of interest to scientists involved with or responsible for the testing of clinical samples for biomonitoring, clinical diagnosis, or emergency response.

Keywords: Clinical ICP-MS, matrix, method validation, biomonitoring, clinical diagnosis, quality control, emergency response

Robert L. Jones is Chief of the Inorganic and Radiation Analytical Toxicology Branch. His responsibilities include the planning, implementation, oversight, and completion of laboratory programs related to public health that involves possible exposures to non-radioactive and radioactive elements or their isotopes. These programs involve research and development of a wide variety of analytical

methods to enable the Centers for Disease Control and Prevention to assay and monitor the exposure of populations to toxic or essential elemental or radioactive exposures. In addition, the laboratory group responds to Epidemiological (EPI) Aids, "emergency responses", and is involved with inorganic and radiological laboratory terrorism preparedness.

Cynthia Ward is Chief of the Speciation and Lot Screening Laboratories. Her responsibilities include the planning, implementation, oversight, and completion of programs implementation, oversight, and completion of laboratory speciation programs related to public health that involves possible exposures to non-radioactive elements or elemental species. These programs involve research and development of a wide variety of analytical methods to enable the Centers for Disease Control and Prevention to assay and monitor the exposure of populations to toxic or essential elemental exposures. Her other responsibilities include the implementation and laboratory aspects of multiple local, state, regional, national and international studies or investigations.

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

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 "Diplom-Physiker" 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 ICPMS for he Characterization of Nanomaterials: Focusing on Human Exposure to Nanoproducts. Saturday, January 15, 7 pm, Petra Krystek, Vrije Universiteit (VU), Amsterdam, The Netherlands; petra.krystek@vu.nl

This course will provide an overview about the role of ICPMS in the characterization of (engineered) nanomaterials, the analysis of (contact) matrices from human exposure scenarios to nanoproducts as well as in assessments regarding occupational exposure.

The stepwise procedures from sampling, sample pretreatment and measurements by ICPMS will be discussed while aspects of validation and quality control will be involved too. In these cases, ICPMS is used for elemental identification and quantification. The possibilities by single particle (sp) ICPMS will be shown as well.

The knowledge on exposure and possible toxicity of nanotechnological products is still limited; resulting in a great relevance of human risk assessments while exposure can occur by inhalation, ingestion, injection and/or skin contact. For answering these questions, integrated approaches based on the use of ICPMS including hyphenation to *e.g.* asymmetric flow field flow fractionation (AF4) and other complementary techniques are needed. An overview about the selection criteria of matrices, sampling strategies and analytical procedures by ICPMS will be given. Examples with *e.g.* body fluids, saliva, tissues (organs) and skin will be discussed more closely.

Passive and active nanomaterials will be discussed and this course will be held as an interactive session.

Petra Krystek received her PhD in 1999 at the University of Mainz, Germany. She has more than 25 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 TNO in the Netherlands as well as in industries as Thermo and Philips. She is a visiting scientist at the Department of Environment & Health at the Vrije Universiteit (VU) Amsterdam, the Netherlands, and since 2018, she is a part-time lecturer at the University of Siegen, Germany. Since 2003, she is a lead assessor and freelance assessor in inorganic analytical chemistry at the Dutch Accreditation Council (RvA) for auditing laboratories in the Netherlands, which are accredited according to ISO/IEC 17025. 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* and associate member of the analytical chemistry division of IUPAC.

SA-08 Environmental Sampling Techniques for Laboratory Analysts In Fair and Foul Weather. Saturday, January 15, 7 pm, Brian Buckley, Rutgers University, EOHSI 170 Frelinghuysen Road, Piscataway NJ 08854, bbuckley@eohsi.rutgers.edu

You never know what you will encounter when you leave the pristine laboratory to go to the field to collect less than pristine samples, especially true after a disaster. This course will cover the fundamentals of environmental sampling for metals and organics with a focus on how to obtain a "clean" sample. Post disaster sampling scenarios and working with the incident command to obtain time sensitive samples will also be described. Targeted for the analyst with field sampling responsibilities this course provides a basic understanding of sample collection, preservation and transport, so that useful analytical information is obtainable. Maintaining a clean sampling environment during sample collection, preparation for going into the field, cleaning apparatus, equipping a sampling kit, preparing an itinerary, and sample transport will be discussed. Sample matrices will include soil, sediment, dust, air, and biologicals. Finally, we discuss working within emergency management offices to safely obtain your samples following a disaster.

Keywords: Sampling, environmental media, post-disaster sampling

Brian Buckley is Executive Director at the Environmental and Occupational Health Sciences Institute and a member of the graduate faculty at Rutgers University. His research involves trace metal quantification and speciation by chromatography coupled ICP-MS as well as development of novel field sampling techniques.

SA-09 Analysis of Petroleum and Petroleum Products, Monday, January 17, 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, Sunday, January 16, 7 pm, Chady Stephan and Ruth Merrifield, PerkinElmer, 501 Rowntree Dairy Rd, Woodbridge, ON L4L 8H1, Canada, chady.stephan@perkinelmer.com, ruth.merrifield@-perkinelmer.com

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

Chady Stephan holds a Ph.D. in Analytical Chemistry from the Université de Montréal. 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 Speciation and Non Traditional Isotopic Analyses For Environmental, Forensic, Biomedical, and Industrial Applications. Sunday, January 16, 7 pm, Olivier Donard, olivier.donard@univ-pau.fr, MARSS-IPREM, CNRS UMR 5034 (LCABIE), 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 is sample preparation for isotopic analysis by MC ICP/MS.

SA-12 Elemental Bioimaging of Tissues and Cells. Saturday, January 15, 1 pm, Dirk Schaumlöffel, dirk.schaumloeffel@univ-pau.fr, IPREM CNRS UMR 5254, Hélioparc, 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 biological applications including sample preparation techniques for NanoSIMS. Applications from our work on plant and animal tissue as well as cell cultures 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 Tracing Element Metabolism in Animals and Humans Using Stable Isotope Techniques, Monday, January 17, 7 pm, Thomas Walczyk, Department of Chemistry, National University of Singapore, Science Drive 4, Singapore 117543, walczyk@nus.edu.sg

Participants will be familiarized in this course with the basic principles and practicalities of tracing element uptake, utilization and excretion from the body in living organisms. This includes a basic introduction to human physiology, metabolism and bioavailability of the most relevant essential elements (iron, zinc, calcium, selenium), theoretical concepts of element tracing in living organisms based on isotope dilution principles, standard methods and protocols to study element metabolism in animals and humans, aspects to consider in the design of such studies, practicalities of sample collection and preparation as well as mass spectrometric analysis and, finally, principles and algorithms for translation of analytical data into physiological information. Participants with a background either in inorganic mass spectrometry or life sciences with an interest to conduct stable isotope studies in animals or humans are encouraged to attend. Expertise in isotope analysis and/or basic physiology is an advantage but not a prerequisite for attending the course

Keywords: Stable isotopes, element metabolism, biomedical research, human studies, animal studies, isotope dilution mass spectrometry

Thomas Walczyk is a chemist by training who earned his PhD degree in isotope sciences/isotope ratio mass spectrometry. For more than 20 years he has been exploring the potential of stable isotope techniques in biomedical research and contributed significantly to the shaping of the field and its recognition as a research domain in inorganic mass spectrometry. After more than a decade at the Laboratory of Human Nutrition at ETH Zurich, he joined the National University of Singapore as a faculty member in 2007, jointly appointed by the Department of Chemistry (Science) and the Department of Biochemistry (Medicine).

SA-14 Fundamentals in Metals Toxicology; How Metals Got Their Biological Species, Tuesday, January 18, 7 pm, Brian Buckley, Rutgers University, Environmental and Occupational Health Sciences Institute, 681 Frelinghuysen Road, Piscataway NJ 08854, bbuckley@eohsi.rutgers.edu

Did you ever wonder why some forms of metals are bioavailable and others are not? Speciation of metals, especially toxic metals, is important because the fate and transport through an environmental system is governed by the species of the metal. The chemical form of the metal also governs the fate of the metal within a biological system, and the differences in species can radically alter a metal's toxicity. The chemical form of the metal as well as their toxicological endpoints also determines the target organ. Biological systems often add organic moieties as conjugates to detoxify a metal once it has been incorporated into the living system, but sometimes this attempt to detoxify a metal (*e.g.*, arsenic) actually makes the metal more toxic. Understanding the mechanisms associated with metal metabolism is key in understanding which species of the metal to look for in a biological fluid when assessing exposure or calculating dose. This course will discuss in general terms the toxicology associated with many of the metals most often quantified in the environment (Pb, Cd, Hg, As, Cr, Ni, Cu Ag, *etc*.) and in human biological fluids, because of their toxicity. The mechanisms of detoxification and common conjugation processes will be described in detail and the proteins that play the most significant role in metal metabolism within the human will be presented in detail. Differences in detoxification efficacy based on metal adduction will be highlighted.

Keywords: Metal toxicology, metal species, detoxification, and mechanisms

Spectrochemical Instrumentation

SI-01 New Calibration Strategies in Spectrochemical Analysis, Tuesday, January 18, 7 pm, George L. Donati, Department of Chemistry, Wake Forest University, Salem Hall, Box 7486, Winston-Salem, NC 27109, donatigl@wfu.edu

Calibration is a crucial component of quantitative spectrochemical analysis. In recent years, several 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, as well as 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, ICP-MS, MIP OES and HR-CS FAAS 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 São 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 Nóbrega and Dr. Renata Amais to develop the first concepts of the interference standard method (IFS). George is an Associate 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 atomic spectrometry and advanced statistical tools to diagnose and understand diseases. George is a member of the advisory board of the *Journal of Analytical Atomic Spectrometry*, and the editorial board of the *Microchemical Journal*. He has published more than 100 peer-review papers and three book chapters on several topics associated with spectrochemical and trace element analysis, and he was awarded with the 2020 *JAAS* Emerging Investigator Lectureship.

SI-02 Opportunities, Challenges, and Application of Glow Discharge Techniques, Sunday, January 16, 8 am, Volker Hoffmann, Leibniz Institute for Solid State and Materials, Research Dresden, Helmholtzstrasse 20. 01069 Dresden, Germany, V.Hoffmann@IFW-Dresden.de; Peter K. Robinson, MassCare Ltd., 11 Waterside Way, Middlewich, Chesire, CW10 9HP, United Kingdom; pete@masscare.co.uk

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 as "Diplom-

Physiker" 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 joint 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 is secretary of the corresponding German workgroup.

Dr. Peter J. Robinson started working with MS in 1980 when he joined the VG group. Initially he was employed as a software engineer and stared by working on static gas instruments. In 1982 Peter led he 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 AutoConcept. 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 chair the he GD Subcommittee of ISO/TC20 Surface Chemical Analysis and contributes toward the development of international standards.

SI-03 ICP-TOFMS: Principles and Application for Single-Particle Analysis. Friday, January 14, 7 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 15, 1 pm, John Olesik, Ohio State University, School of Earth Sciences, 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002, olesik.2@osu.edu

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 16, 1 pm, John Olesik, Ohio State University, School of Earth Sciences, 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002, olesik.2@osu.edu

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, Monday, January 17, 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 20740

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 16, 1 pm, José Luis Todolí, jose.todoli@ua.es, jose.todoli@gcloud.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, Sunday, January 16, 8 am, Deborah Bradshaw, bradshawdk@cs.com, Atomic Spectroscopy Consulting, POB 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, Sunday, January 16, 7 pm, Deborah Bradshaw, bradshawdk@cs.com, Atomic Spectroscopy Consulting, POB 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 15, 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/fieldable 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

Sample Introduction Approaches

SS-01 A Practical Guide to Nebulizers and the Part They Play in Modern Sample Introduction, Saturday, January 15, 7 pm, Steve Mangum, Elemental Scientific Inc., 7277 World Communications Dr, Omaha, NE 65132; steve.magnum@icpms.com

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

SS-02 Laser Ablation Mass Spectrometry I, Friday, January 14, 1 pm, Detlef Günther, Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 1 8093 Zurich, Switzerland, guenther@inorg.chem.ethz.ch

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 was born in Köthen, Germany in 1963. He obtained his Diploma degree in Chemistry in 1987 and a Ph.D. degree in Analytical Chemistry from the Martin-Luther-University Halle-Wittenberg under supervision of L. Moenke - Blankenburg in 1990. After carrying out postdoctoral work in the Institute of Plant Biochemistry Halle where he worked on the development of analytical methods to characterize heavy metal-binding proteins using HPLC-ICP-MS, he joined the group of H.P. Longerich at the Memorial University of Newfoundland, Canada. From 1995 until 1998 he was in the group of C.A. Heinrich at the Institute of Isotope Geology and Mineral Resources at ETH Zürich. In 1998 he was appointed Assistant Professor in the Laboratory of Inorganic Chemistry at the ETH Zürich. He was promoted to Associate Professor for Trace Element and Micro Analysis in 2003 and became Full Professor in 2008. From 2010 until 2012 he was Chair of the Department of Chemistry and Applied Biosciences at ETH Zurich and since 2015 he is Vice President for Research and Corporate Relations at ETH Zurich. He is recipient of the Ruzicka Award (2002), the European Award for Plasma Spectrochemistry (2003), the Fresenius Award (2007), and the Lester Strock Award (2007), and he received in 2013 the "Einstein Visiting Fellowship" to Humboldt University Berlin (Germany) and the "Thousand Talent Fellowship" (Wuhan University, China). In 2014 he became a member of the German National Academy of Science Leopoldina. His research program focuses on fundamental and applied studies in inductively coupled plasma-mass spectrometry (ICP-MS) and laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS), including studies on laser-sample interaction, aerosol transport, and plasma-related excitation processes. As well particle plasma interaction and particle vaporization for single nanoparticle analysis have been studied. Fundamental processes of UV-ns and UV-fs laser ablation used with Q-ICP-MS, SF-ICP-MS, TOF-ICP-MS, and MC-ICP-MS as well as alternative excitation sources,

such as glow discharge are currently under investigation. The improvements in trace element and microanalysis and isotope ratio determinations have been demonstrated on a wide variety of applications (*e.g.*, quantification of fluid inclusions, gemstones, metals, minerals, ceramic, and various nano materials).

SS-03 Latest Advances in Laser Ablation-Based Chemical Analysis and Emerging Applications: LIBS, LA-ICP-(OES/MS), and Tandem LA – LIBS, Monday, January 17, 7 pm, Jhanis Gonzalez, Applied Spectra, Inc., 46661 Fremont Blvd, Fremont, CA 94538, jhanis@appliedspectra.com, jjgonzalez@lbl.gov; Rick Russo, Lawrence Berkeley National Laboratory, 1 Cyclotron Rd, Berkeley, CA 94720, rerusso@lbl.gov

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 González Chacon is director of Applications Lab Operations, Applied Spectra, Inc, Fremont, CA, 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).

Richard E. Russo is founder and scientific director of the laser material interactions group at the Lawrence Berkeley National Laboratory (LBNL). His group has pioneered the development of laser ablation for chemical analysis, with an almost 30 year contribution to fundamental and applied research topics. Programs in this group are closely integrated to DOE basic science, industrial technologies and nonproliferation activities. His research has led to breakthroughs in laser ablation understanding and development. Dr. Russo has an international scientific reputation in chemistry and physics related to nanosecond and femtosecond laser-material-interactions (laser ablation), is co-inventor of the nanowire laser, and developer of a real-time standoff laser ultrasonic sensor (R&D100 2006). He also is co-inventor of a process for ion nano-texturing (ITEX) thin-films, lead-inventor of the ion-assisted pulsed laser deposition (IBAD) process, and a pioneer in elucidating fundamental laser heating and laser ablation processes for chemical analysis. The group achieved 450 nm spatial resolution and a detection limit of 220 ag using a single laser pulse for LIBS (laser induced breakdown spectroscopy) measurements. By pioneering near-field scanning optical microscopy (NSOM) with laser ablation, the group achieved 30-nm diameter sampling and analysis. Finally, the group demonstrated and patented the use of laser plasmas (LIBS) for real-time measurement of isotopes. Russo has over 220 scientific publications; 45 refereed proceedings; 250 (115 Invited) presentations, nine book chapters, and nine patents. Fourteen students have received their PhD degree under his direction at the University of California, Berkeley.

Dr. Russo is president and founder of Applied Spectra, Inc. (ASI). The company is the world leader in laser ablation based chemical analysis using LIBS and laser ablation with ICP-OES and ICP-MS. The ASI staff members are experts in utilizing laser ablation for solving the most challenging chemical analysis problems. Applied Spectra's LIBS and laser ablation instruments offer superior performance in commercial, military, and security markets. These LIBS and LA-ICP-MS systems provide significant cost benefits to traditional chemical analysis, delivering real time elemental and isotopic analysis with excellent spatial and depth resolution, and without sample digestion. The ASI bench top RT100 LIBS system is successfully deployed in energy, environmental, health, industrial and security markets. The company continues to drive laser ablation capabilities and instrumentation based on strong in-house research, and instrumentation and applications (methods) development.

SS-04 Variations of Single Particle Inductively Coupled Plasma Mass Spectrometry, Sunday, January 16, 8 am, Diane Beauchemin, diane.beauchemin@queensu.ca, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7l 3N6, Canada

Variations of single particle inductively coupled plasma mass spectrometry (spICPMS) for the measurement of nanoparticles (NPs) in solution will be discussed. Coupling flow injection (FI), where a discreet 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, simplifies the analysis. 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.

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 Montréal.

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 MICROPLASMAS FOR CHEMICAL ANALYSIS, Sunday, January 16, 7 pm, Vassili Karanassios, vkaranassios@uwaterloo.ca, Department of Chemistry and Waterloo Institute for Nanotechnology, University of Waterloo, 200 University Ave West, Waterloo, ON Canada N2L 3G1

Microplasmas have been arbitrarily defined as those with one "critical" dimension (*e.g.*, depth, height, radius) in the µm or sub-mm regime [1]. In this short course, micoplasmas for optical emission and mass spectrometry described in the literature will be reviewed. Battery-operated microplasmas fabricated on-chips using a variety of technologies (ranging from clean room-based and micro-machining to 3D-printing) will be emphasized. Analytical performance characteristics will be discussed and selected applications will be highlighted.

[1] V. Karanassios, "Microfluidics and Nanofluidics: Science, fabrication technology (from cleanrooms to 3D printing) and their application to chemical analysis by battery operated microplasmas on-chips." Invited, open-access book-chapter (free down load), Chapter 1, Pages 1-34, InTech Publishing, Aug. 22, 2018, DOI: 10.5772/intechopen.74426.

[2] V. Karanassios, "Microplasmas for portable optical emission spectrometry", chapter 11 (invited), in *Portable Spectroscopy and Spectrometry 1: Technologies and Instrumentation (portable Spectroscopy and Spectrometry)*, R.A. Crocombe, P.E. Leary and B.W. Kammrath (Eds.), John Wiley & Sons, in press (2021); ISBN-13: ý978-1119636366.

[3] A. Cebula and V. Karanassios, "Chromium speciation using graphene oxide as a chemo-mechanical material and a battery operated microplasma on a polymeric substrate", *Proceedings, IEEE FLEPS* (Flexible and Printable Sensors and Systems (2021, accepted).

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 (https://uwaterloo.ca/future-students/programs/nanotechnology-engineering). 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). Professor Karanassios and his group published (among others) on microplasmas, on microfluidics and nanofluidics, on 3D printing 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. Since 2016, he has been presenting a short course on 3D printing (primarily) on IEEE sensors conferences.

SS-06 Laser-Induced Breakdown Spectroscopy (LIBS), Tuesday, January 18, 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-01A, 01B Soft Skills Supporting Scientific Success, Saturday, January 15, 8 am and 1 pm, Andrew Zander, Technical Consultant, 1632 Hickory Ave., Torrance, CA 90503, atzander@earthlink.net (One full day of two 4 hour sessions, back-to-back)

Technical professionals will stay in demand in industry, but tomorrow's most valuable professionals will not be geniuses in the cubicle; rather they will be those who can build relationships, brainstorm and lead. "The people who master the human abilities that are fading all around us will be the most valuable. Organizations are finding not only that they have no jobs for the disengaged and socially inept, but that such people are toxic to the enterprise and must be removed," G. Colvin, p 210, *Humans are Underrated*, 2015.

In this short course, skills "softer" than hard-core science and engineering skills will be covered. These are the human abilities and skills that technical professionals need to succeed in their jobs, but were rarely covered in conventional curricula. Among the topics to be covered will be (not inclusive) the culture of a work environment; enumeration of soft skills; teaming; being organized; confidential materials; credentialing; electronic communications; basic project management; basic personnel management; managing diverse employees; relationship building; budgeting and finances; innovation; disciplines for success; leadership.

The material in this course is geared toward finishing graduate students about to embark on corporate positions and new hires in industry. It is also beneficial for seasoned technology developers wishing to upgrade their soft skills or who have been recently promoted to leadership positions in technical departments.

Keywords: Professional development, Soft Skills, Personal development

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 Department 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. Andy has had published 29 peer-reviewed journal articles, 21 non-refereed publications (*e.g.*, book chapters) and authored multiple manuals and training documents for project management. He has four patents. Andy is a technical consultant with SCLS, Inc., a non-profit community service organization.

ST-02 Isotopic Analysis Using ICP-MS, Sunday, January 16, 1 pm, Frank Vanhaecke, Ghent University, Department of Chemistry, Atomic & Mass Spectrometry – A&MS research unit, Campus Sterre, Krijgslaan 281 – S12, 9000 Ghent, Belgium. frank.vanhaecke@ugent.be; José Ignacio García Alonso, Department of Physical and Analytical Chemistry. Faculty of Chemistry. University of Oviedo. Julian Clavería 8 , 33006 Oviedo, Spain, jiga@uniovi.es

In this short course, we will discuss the measurement of isotope ratios by ICP-MS from two points of view: i) natural variations and ii) Isotope Dilution Mass Spectrometry (IDMS) applications after the addition of enriched isotopes. In the first part, specific attention will be devoted to elements with radiogenic nuclides (*e.g.*, Sr, Pb) and to mass-dependent and mass-independent isotope fractionation. The importance of isotope ratio precision will be underlined and hints for optimization of the instrument settings and data acquisition parameters aiming at an optimum isotope ratio precision will be provided for single-collector and multi-collector ICP-MS. Correction for detector dead time (pulse counting detectors) and for instrumental mass discrimination, required to convert the raw measurement data into "true" isotope ratios, will be discussed. Examples of applications relying on the determination and quantification of natural isotope ratio variation will include provenance determination of raw materials used in the manufacturing of ancient artifacts, environmental applications, geo-/cosmochemical applications and the use of isotopic analysis for medical diagnosis.

In the second part of the course we will discuss the use of enriched stable isotopes and isotope abundance measurements for IDMS in elemental analysis, speciation, traceability and metabolism studies. The theory of IDMS applied to the different fields will be described in detail as it is recognized by the Bureau International des Poids et Mesures (BIPM) as a potential primary measurement method, directly traceable to the International System of units. Trace element speciation is another field where enriched stable isotopes have been applied successfully as they can correct for degradation and interconversion reactions, which can occur during sample preparation or measurement. Another application field for enriched isotopes is in the traceability of manufactured goods and living organisms. We will describe a double-isotopic labelling technique, which can be applied for traceability purposes.

Keywords: Isotope ratio, isotopic composition, isotope fractionation, radiogenic nuclide, MC-ICP-MS, Isotope Dilution Mass Spectrometry, speciation, metabolism, traceability.

J. Ignacio García Alonso obtained his PhD in analytical chemistry from the University of Oviedo, Spain in 1985 and subsequently became a postdoctoral fellow at the University of Plymouth, UK before returning to Oviedo in 1987. For five years he was a scientific officer of the European Commission, based in Karlsruhe, Germany, and in 1995 he returned to the University of Oviedo, where he is now Full Professor of Analytical Chemistry. He is head of the research group on Enriched Stable Isotopes. Prof. Garcia Alonso is founding member of the spin-off company ISC-Sciences (www.isc-science.com) devoted to the synthesis and commercialization of isotopically labelled compounds particularly for speciation and food analysis. He is co-author of the book *Isotope Dilution Mass Spectrometry* published by the Royal Society of Chemistry in the UK.

Frank Vanhaecke received a PhD from Ghent University (Belgium) in 1992. Currently, he is Senior Full Professor in Analytical Chemistry at Ghent University, where he leads the 'Atomic & Mass Spectrometry – A&MS' research group that is specialized in the determination, speciation and isotopic analysis of (trace) elements *via* ICP-mass spectrometry (ICP-MS). His group studies fundamentally oriented aspects of the technique and develops methods for solving challenging scientific problems in an interdisciplinary context. High-precision isotopic analysis using multi-collector ICP-MS is an important research line in his group. Methods for high-precision isotopic analysis are developed for applications in, among other, the fields of geo- and cosmochemistry, archaeometry, the environmental sciences, and medicine ("isotopic diagnosis"). Frank was co-editor of the book *Isotopic Analysis – Fundamentals and Applications using ICP-MS* published by Wiley-VCH.

ST-03 Accurate, Precise and SI Traceable Measurements by ICP-MS, Sunday, January 16, 8 am, Lu Yang, National Research Council Canada, 1200 Montreal Rd., Ottawa, ON, K1A 0R6, Canada, lu.yang@nrc-cnrc.gc.ca

This short course provides an overview of the fundamentals of isotope dilution technique and recent developments in this area. Single, double, triple and quadruple isotope dilution techniques will be discussed in details. Standard addition method will be discussed as well. In addition, this short course provides metrological principles and rules in order to achieve accurate, precise and SI traceable measurements. Examples of the determination of trace metals in a biological tissue using ICPMS will be provided. Excel file template for the calculation of combined uncertainty of final result obtained by double isotope dilution methods will be provided to the participants.

Keywords: Isotope dilution, standard addition, accurate, precise, SI traceable measurements, trace metals, ICPMS

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 *JAAS* and *Spectroscopy*.

ST-04 Isotopic Fingerprinting for Source Identification and Apportionment of Lead in a Child's Environment. Tuesday, January 18, 7 pm, Cathleen Doherty, cld133@eohsi.rutgers.edu, Rutgers University, EOHSI 170 Frelinghuysen Road, Piscataway NJ 08854

Identifying the sources of lead in a child's environment is required for an intervention strategy and remediation plan. Biological samples (teeth, blood, *etc.*) have the potential to identify the sources, if we can narrow the suspects. Lead concentrations are critical for decisions on chelation or household remediation. However, concentration alone cannot identify the source, which may include paint, dust, pipes, lead solder, and plumbing fixtures.. Lead isotopic ratios are highly effective in tracing sources of environmental contamination because of the processes that control isotopic ratios: (1) the abundance of the parent isotopes (*i.e.*, ^{238}U, ^{235}U, ^{232}Th), (2) the radioactive decay rate of these isotopes to daughter isotopes (^{206}Pb, ^{207}Pb, and ^{208}Pb), and (3) the age of the metal ore deposit. These factors cause variations in isotopic ratios from one source to the next, resulting in a highly specific isotopic fingerprint that is traceable to the contamination source. This course will focus on creation of a source apportionment model for lead using isotopic fingerprinting. We describe how to accurately measure lead isotopes in environmental samples, evaluate data in 3D space, and create a mixing curves that are critical in successful identification of multiple sources when other techniques fall short. Finally, we will describe the potential sources within the home and where to look for them in the child.

Key words: Isotopic fingerprinting, source apportionment, mixing curves

Cathleen Doherty is the Director of Inorganic Analysis Facility/Instrument Specialist at the Environmental and Occupational Health Sciences Institute, Rutgers University. A geologist by training from the Lamont-Doherty Earth Observatory, she is an expert on precision ICPMS measurement of isotopic ratios for source identification in environmental samples

ST-05 Contamination Control for Elemental Analysis, Sunday, January 16, 1 pm, Brad McKelvey and Lucas Choma, Seastar Chemicals Inc., 2061 Henry Ave West, Sidney, BC V8L 5Z6, Canada, bmckelvey@seastarchemicals.com

Current instrumentation has the ability to determine many elements down to the ppt and ppq level. However, many analytical techniques for trace element determinations are limited by the blank. The focus of this course will be contamination control and strategies to determine and eliminate contamination sources. This course will discuss contamination sources from the environment, labware, reagents, sample handling and sample introduction systems. Participants will be encouraged to discuss their contamination problems and experiences.

Keywords: Contamination control, trace element analysis, blanks

Brad McKelvey is Senior Research Scientist at Seastar Chemicals Inc. Seastar Chemicals is a global supplier of high purity reagents for trace element analysis. Dr. McKelvey has over 30 years experience in ICP-MS analysis, sample preparation, and contamination control for ultra-trace elemental analysis.

Lucas Choma earned his master's degree in chemistry from Queen's University under the supervision of Diane Beauchemin, focusing on sample introduction techniques for ICP. This included analysis of environmental samples, an electrolyte fuel, as well as single particle detection methodology. Presently he has been working at Seastar Chemicals for the past three years doing ultra-trace elemental analysis on ICP-MS.

ST-06 Building or Modifying Your Laboratory for Trace and Ultratrace Analyses, Sunday, January 16, 8 am, Ela Bakowska, 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 new or existing ICP-MS instrumentation.

Reducing and eliminating sources of elemental contamination and by optimizing the laboratory layout achieve the improvements of trace or ultra-trace capabilities. Based on my own experience of building two new labs and modifying another

two, 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 (semiconductor, environmental, clinical) will be discussed.

Keywords: Laboratory design/upgrade, contamination prevention, supplies, instrumentation, sample preparation, automation

Ela Bakowska is 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 an 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 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 new users in modernizing and upgrading their labs. Since 2001 (being 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, especially sample preparation areas dedicated to ultra-trace levels testing. Her research focus is testing of glass, raw materials, Extractables and Leachables (E&L), and surface contamination. During 11 years at Corning RDC Ela purchased two HR-ICP-MS systems, four Q-ICP-MS and one LA.

ST-07 Why IUPAC Tables of Isotopic Abundances and Atomic Weights Should Matter to Plasma Spectrochemists. Johanna Irrgeher, Sunday, January 16, 8 am, Montanuniversität Leoben, Department of General, Analytical and Physical Chemistry, Chair of General and Analytical Chemistry, Isotope Research Group; Franz Josef-Strasse 18, 8700 Leoben, Austria, johanna.irrgeher@unileoben.ac.at

This short course gives an introduction to the Commission, its key tasks and functions as well as current projects relevant to the mass spectrometric community. Practical considerations for the plasma spectrochemist are provided concerning (1) the appropriate/inappropriate use of the CIAAW publications and the tabulated atomic-weight and isotope-abundance values; (2) the importance of correct and transparent extraction and application of these values and recommendations and in analytical chemistry; (3) isotope-abundance measurements and certified reference materials, and (4) the importance of measurement uncertainty along with a guide on how to calculate and extract uncertainties from tabulated values. Recommendations will be discussed interactively on examples taken from daily lab routine. This short course is relevant to all users of standard atomic-weight and isotopic-abundance values, spanning from undergraduate students to experienced plasma spectrochemists. Insights into how tabulated values and their uncertainties are generated within the Commission are explained along with guidelines on how to extract values and associated uncertainties for different analytical questions and calculations. Colleagues from academia and industries as well as instrument manufacturers are welcome.

Keywords: CIAAW, IUPAC, isotopic abundances, atomic weight, uncertainty, isotope ratio measurements

Johanna Irrgeher has held a position as head of the Isotope Research Group at the Montanuniversität Leoben since January 2019. She graduated from the University of Natural Resources and Life Sciences (BOKU), Vienna with honors in 2013. Amongst others, she was visiting researcher at the NRC Canada, the National Cheng Kung University Tainan, the University of Calgary, and the University of Alaska, Fairbanks. From 2015 to 2018, she was post-doctoral fellow at the Helmholtz Centre in Geesthacht, Germany. Johanna is a lecturer at BOKU and in 2018 she was appointed adjunct professor at the University of Calgary. Currently, she is chair of the Subcommittee on Isotopic Abundance Measurement of the IUPAC Commission on Isotopic Abundances and Atomic Weights (CIAAW). Her current research interests are dedicated to analytical mass spectrometry and the application of isotope tools in medical, environmental and material sciences including the implementation of fundamental metrological methods. Among other awards, she received the Agilent Rising Star Award at the EWCPS 2017.

ST-08 Plasma Diagnostics: Fundamentals, Measurements, and Applications, Sunday, January 16, 7 pm, Igor Gornushkin, igor.gornushkin@bam.de, BAM, Federal Institute for Materials Research and Testing, Richard-Willstätter-Strasse 11, 12489 Berlin, Germany

This course will provide an introduction to plasma diagnostic techniques. The major focus of the course will be on the discussions of the practical procedures as well as the underlying physical principles for the measurements of plasma fundamental characteristics (*e.g.*, temperatures, thermodynamic properties, and electron number density). Particular emphasis will be placed on inductively coupled plasma–atomic emission spectrometry, but other analytical plasmas will also be used as examples when appropriate. Selected examples on how one can manipulate the operating conditions of the plasma source, based on the results of plasma diagnostic measurements, to improve its performance used for spectrochemical analysis will also be covered. Topics to be covered include thermal equilibrium, line profiles, temperatures, electron densities, excitation processes, microreactions, pump and probe diagnostics, tomography, temporal and spatial resolution. Basis of plasma computer modeling will be presented.

Keywords: Thermal equilibrium, plasma processes, electron number density, temperatures, emission line profiles, spatial information, plasma modeling

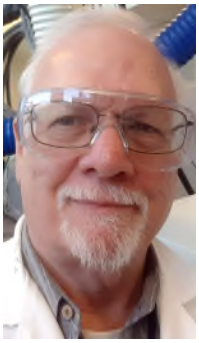
Igor B. Gornushkin is a physicist and analytical chemist with major expertise in fundamental and applied spectroscopy including LIBS, emission, absorption, fluorescence and Raman. He received his PhD from the University of Florida in 1998 and at present works at BAM Federal

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-09 Triple Quad (QXQ) ICP-MS, Sunday, January 16, 1 pm, R. Steven Pappas and Nathalie Gonzalez-Jimenez, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341, rpappas@cdc.gov

Development of the Agilent 8800/8900 QQQ, the ThermoFisher iCAP TQ, 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. Questions are welcomed. 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: Triple Quad, QQQ-ICP-MS, interference, reactive gas, quadrupole, reaction cell



Steve Pappas earned his B.S. in Chemistry at Middle Tennessee State University in 1986. He completed his doctoral training in Biochemistry at Vanderbilt University. After holding 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 for emergency response state health department laboratory training. In the second phase of his work at CDC, he became responsible for development of methods for analysis of tobacco and smoke for toxic metals. He subsequently became the Tobacco Inorganics Group Team Lead. He oversees method development, ISO 17025 accreditation, and analyses for toxic metals in tobacco and smoke. He is responsible for publishing and interpreting data in terms of public health risks. In addition to application manuscripts, he has written the Annex behind World Health Organization Technical Report Series 967 on toxic metals in tobacco and smoke with emphasis on inflammation and sensitiza-tion responses in animal and human studies, and a *Metallomics* review on the same topic, and a review on cadmium and cadmium/zinc ratios in tobacco-related disease.

Nathalie Gonzalez Jimenez earned her bachelor's degree in chemistry at the Interamerican University of Puerto Rico in San German and her master's in public health at the Mercer University in Atlanta, Georgia. Nathalie has been working at the Centers for Disease Control and Prevention (CDC) for eight years and has dedicated her work to research and development projects for analysis of toxic metals in tobacco, smoke, electronic cigarette liquids, and aerosol. Nathalie contributed to the 2019 E-cigarette and vaping associate lung injury (EVALI) response by assisting in developing procedures for the sample recovery and preparation and method development for analysis of aerosols from cannabinoid delivery devices. Nathalie has earned a National Center for Environmental Excellence in Response award for her contributions during EVALI. Nathalie has contributed as co-author to eight publications on analysis of toxic metals in different tobacco products and their emissions. Her two most recent publications are: Chapter 24 "Measurement of Elemental Constituents of Cannabis Vaping Liquids and Aerosols by ICP-MS" in the CRC book, *Measuring Heavy Metal Contaminants in Cannabis and Hemp*, and "Analysis of Toxic Metals in Liquid from Electronic Cigarettes" in the *International Journal of Environmental Research and Public Health*.

ST-10 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 15, 1 pm, Mark Fresquez, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341, mwf6@cdc.gov

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.

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-11 Sample Preparation Problem Solving for Atomic

Mass Spectrometry, Monday, January 17, 7 pm, R. Steven Pappas and Naudia Gray, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS S110-4, Atlanta, GA 30341, rpappas@cdc.gov

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.

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

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.

Steve Pappas earned his B.S. in Chemistry at Middle Tennessee State University and his Ph.D. in Biochemistry at Vanderbilt University. After holding 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. He later became the Tobacco Inorganics Group Project Lead responsible for development of methods within the ISO 17025 framework for analysis of toxic metals in tobacco, smoke, electronic cigarette liquids, and aerosols. During the 2019-2020 CDC E-Cigarette and Vaping Associated Lung Injury emergency response, he was responsible for method development and analysis of aerosols from nicotine and cannabinoid delivery devices. Steve has earned three National Center for Environmental Health group honor awards for Excellence in Laboratory Research, and a CDC Innovation award for characterization of particles in electronic cigarette aerosols. In addition to authoring application manuscripts, Steve has written Annex 1, Toxic Metals in Tobacco and in Cigarette Smoke in World Health Organization Technical Report Series 967, a Metallomics review, "Toxic elements in tobacco and in cigarette smoke: inflammation and sensitization", and the metals section in "A Report of the Surgeon General: How Tobacco Smoke Causes Disease (2010)."

ST-12 Validation assessment and ISO/IEC 17025 – an interactive session. Sunday, January 16, 1 pm, Rob Ritsema, robritsema@gmail.com, RR Quality Consultancy, Amersfoort, The Netherlands; Petra Krystek, petra.krystek@vu.nl; Vrije Universiteit (VU), Amsterdam, The Netherlands

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. Crucial aspects of the ISO/IEC 17025 (2017) will be discussed too. This course will be held as an interactive session.

Keywords: Validation, performance characteristics, quality, ISO/IEC 17025

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 three years, he started his own company RR Quality Consultancy. Since 1998 he is a freelance assessor at the Dutch Accreditation Council (RvA) performing approximately 20 ISO/IEC 17025 technical assessments on a yearly base at accredited laboratories in mainly the Netherlands. 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 25 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 TNO in the Netherlands as well as in industries as Thermo and Philips. She is a visiting scientist at the Department of Environment & Health at the Vrije Universiteit (VU) Amsterdam, The Netherlands, and since 2018, she is a part-time lecturer at the

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

ST-13 Uncertainty of Measurements: Practical Approaches to Determine Measurement Uncertainty Budgets Thomas Prohaska, Sunday, January 16, 7 pm, Chair General and Analytical Chemistry, Montanuniversitaet Leoben, Franz Josef-Strasse 18, 8700 Leoben, Austria, thomas.prohaska@unileoben.ac.at

Metrology in chemistry is defined as the science of measurements. Even though we do take care about the best measurement results with respect of precision or the deviation from the 'true value', the validity of these results is determined by their uncertainties. Thus, a proper understanding of uncertainty budgets and the sources of error is crucial for providing validated measurement results. This short course provides the basic understanding for building an uncertainty budget and provides different approaches for doing so with a main focus on Monte Carlo calculations. Working on practical examples, the participants should be able to transfer the knowledge to their own measurement results.

Keywords: Uncertainty budget, metrology, errors, calculations

Thomas Prohaska is Chair for General and Analytical Chemistry at the Montanuniversität Leoben, Austria. He studied technical chemistry at the Vienna University of Technology and received his PhD with summa cum laude in 1995. In the same year he became scientific researcher at the University of Natural Resources and Life Sciences (BOKU), Vienna and was in charge to set up a laboratory for elemental trace analysis. From 1998 to 2000 he was researcher at the EC joint research center IRMM in Geel, Belgium. He returned to BOKU with a new focus on isotope ratio analysis in 2000. In 2004 he received the FWF-START award to setup a new research laboratory (VIRIS) for isotope research. He was associate professor at the BOKU from 2002-2018 before moving to Leoben. His current research focus is based on elemental and isotopic analysis using mass spectrometry, chemical imaging techniques and metrology with more than 150 peer-reviewed publications.

ST-14 Nanomaterials: Advances in Standardization, Measurement Methods, Reference Materials and Remaining Challenges Imposed by Regulation, Monday, January 17, 7 pm, Heidi Goenaga-Infante, heidi.goenaga-infante@lgcgroup.com, LGC Limited, Queens Rd, Teddington, Middlesex TW11 OLY, UK

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-15 Metrology Concepts in Plasma Spectrochemistry, Saturday, January 15, 8 am, Zoltan Mester, zoltan.mester@nrc.ca, and Paramee Kumkrong, paramee.kumkrong@nrc-cnrc.gc.ca, National Research Council of Canada (NRC), 1200 Montreal Rd, Building M-58, Ottawa, ON K1A 0R6, 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.

Paramee Kumkrong holds a PhD (2002) in Environmental and Analytical Chemistry from Aberdeen University, UK. She worked at a Thai government research organization for 23 years. In 2016 she joined National Research Council Canada as a Research Officer. She experienced in analytical laboratory management, metrology, laboratory quality system as trainer, mentor and technical assessor (ISO/IEC 17025) and in certified reference material production (ISO 17034). She is currently working on method development to support mining and environmental research, metal speciation, sensor development.

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