SAS SPECTRUM eNEWS

Award Nomination Solicitations

The Coblentz Society's Williams–Wright Award

The Coblentz Society's Williams–Wright Award is presented annually to an industrial spectroscopist who has made significant contributions to vibrational spectroscopy while working in industry. The work may include infrared and/or Raman spectroscopy, and instrumental development, as well as theory and applications of vibrational spectroscopy. Government labs are not considered industry in this definition. No restrictions are placed on the selection of the awardee because of age, gender, or nationality, but the awardee must still be working at the time the award is presented. The award consists of a framed certificate and an honorarium. In order to ensure that the award is based on an independent evaluation of the candidate's achievements, the selection is made by a committee chosen by the Coblentz Society.

This award is presented each year at the Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon). The Williams–Wright Award Symposium is held in honor of the awardee and immediately follows the presentation.

The nomination should clearly state the significance of the contribution made by the nominee, e.g., the introduction of novel methods, techniques, or theories; innovative work in the field of vibrational spectroscopy; significant improvement on existing methods, theory or techniques; or important impact on the field of vibrational spectroscopy arising from the volume of contributions in a specific area. The nomination packet should include a resume of the nominee's career including a publication list. Seconding letters to the nomination are useful, but not necessary. Files on nominees will be kept active for three years. Please send nomination packages (email is preferred) to: nominations@coblentz.org

Gordon F. Kirkbright and Edward Steers Bursary 2020 Awards

The Gordon F. Kirkbright bursary award is a prestigious annual award that assists a promising early career scientist of any nation to attend a recognized scientific meeting or visit a place of learning. The fund for this bursary was established in 1985 as a memorial to Professor Gordon Kirkbright in recognition of his contributions to analytical spectroscopy and to science in general.

Owing to the generosity of one of our former trustees, an eminent atomic spectroscopist, Professor Edward B.M. Steers, we are now, from 2020, in the position of being able to award an Edward Steers bursary, in addition to the long standing Gordon Kirkbright bursary, to similarly assist a promising early scientist engaged in or utilizing analytical spectroscopic techniques.

The ABS Trust defines early career as being either a student, or an employee in a non-tenured academic post or in industry, within seven years of the award of a PhD, excluding career breaks. The same conditions apply to each bursary.

Applications are invited for both the 2020 Gordon Kirkbright Bursary and the 2020 Edward Steers Bursary. Although both funds are administered by the ABS Trust, the Kirkbright award is not restricted to spectroscopists, but is open to all involved with or utilizing analytical science-based techniques.

Application Forms can be downloaded from:
http://www.abstrust.org/kirkirkbright-bursary-award-application-form and
http://www.abstrust.org/steers-bursary-award-application-form,
or for further information visit: http://www.abstrust.org/, or contact abstrustuk@gmail.com.
The closing date for entries is 30 November 2019.

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Past SAS Sponsored Sessions and Talks

The Society for Applied Spectroscopy (SAS) continued its tradition of organizing and sponsoring technical symposia at Pittcon with two sessions at the 2019 conference. The first session, "New Frontiers and Challenges in Clinical Spectroscopy", was organized by Ji-Xin Cheng of Boston University. It explored the latest advances and remaining challenges on the topic of spectroscopic examination of specimens and human patients in a clinical setting. Talks in this session included:

- "Pharmacokinetic Tomography", Conor Evans (Wellman Center). The title technique, which combines coherent Raman and/or fluorescent imaging with machine learning tools for image analysis, is leading to the analysis of the uptake and action of smaller pharmaceutical compounds.
- "Autonomous Dynamic Sampling for Hyperspectral Raman Image Reconstruction", Garth Simpson (Purdue University). The timeframe for image analysis decreases seven-fold through weighting the analysis by previously obtained spectra for the sample. The technique is applicable to all imaging methods where single-pixel measurement time is the limiting factor in image reconstruction.
- "Biomedical Spectroscopic Tools for Rapid Analysis of Disease Specific Changes Using Novel Raman and IR Techniques", Nick Stone (University of Exeter). Recent developments and challenges are described for the use of Raman and IR tissue analysis for near-patient ex vivo and in vivo applications.
- "Co-Registered Photoacoustic and Ultrasound Tomography for Non-Invasive Diagnosis of Ovarian Cancer", Quing Zhu (Washington University, St. Louis, Missouri). The two techniques are used in vivo to differentiate between malignant and benign ovarian tumors through observed differences in relative total hemoglobin concentration (indicative of higher vascularity in malignant tissues) and mean oxygen saturation.
- "High-Speed Label-Free Vibrational Microscopy Allows Signature Discovery and Signature-Based Precision Diagnosis of Human Diseases", Ji-Xin Cheng (Boston University). Nonlinear optical techniques, such as CARS and SRS microscopy, allow video-rate imaging and the determination of a spectrum of metabolic signatures that drive cancer aggressiveness, stemness, and drug resistance. The authors have also developed a catheter to map lipids inside blood vessel walls at video rate.

The second session, "Current and Emerging Methods for Optical Trace Gas Analysis", was organized by Robert Lascola of Savannah River National Laboratory. The talks in this session described a variety of techniques for, and applications of, high sensitivity measurements of trace components in small gas volumes. The presentations were:

- "Fabry–Perot Photothermal Interferometry: A New Concept for Trace Gas Sensing in Ultrasmall Gas Volumes", Bernhard Lendl (TU Wien). The technique amplifies the signal from a QEPAS-type measurement by putting the tuning fork in an optical cavity, to achieve single-digit parts per billion detection limits for SO2.
- "Infrared On-Chip Photonics for Breath Diagnostics", Boris Mizaikoff (Ulm University). Several innovative waveguide technologies, combined with efficient IR lasers, facilitate compact yet robust MIR-infrared diagnostic platforms for label-free chem/bio sensing and medical diagnostics.
- "MRR Spectrometers in Chemical and Pharmaceutical Analysis: Identification and Quantification of Isomers in Complex Mixtures", Justin Neill (Brightspec, Inc.). Molecular rotational resonance spectroscopy is shown to be an exceptionally powerful method for differentiating between molecular isomers, as the changes in moments of inertia are much more significant than changes in vibrational frequencies for these molecules.
- "Broadband, High Resolution Dual-Comb Molecular Spectroscopy in the Mid-Infrared and THz Spectral Regimes", Gerard Wysocki (Princeton University). Detection of the heterodyne interactions of two frequency combs with slightly different periods allows for broadband, high-resolution spectroscopy without the need for additional spectrometers or tunable lasers.
- "Novel Improvements and Applications Using Tunable Infrared Laser Direct Absorption Spectroscopy", Scott Herndon (Aerodyne Research Inc.). TILDAS has the spectral resolution and dynamic range to distinguish molecular isotopologues over many orders of magnitude. The significance of this property for applications such as emissions characterization, photochemistry, and biosphere interaction studies are described.

(L to R) *Speakers in the optical trace gas analysis session: Justin Neill, Bernhard Lendl, Boris Mizaikoff, Scott Herndon, and Gerard Wysocki.*

Microplastics Workshop Event

Focused on Building Best Practices for Sampling, Extraction, and Analysis

Organized at the Southern California Coastal Water Research Project (SCCWRP) from 4–5 April 2019 in Costa Mesa, California, this workshop focused on addressing the threat of microplastics to our environment. The two day meeting was organized by Dr. Steve Weisberg, and Shelly Moore from SCCWRP, Dr. Chelsea Rochmann from the University of Toronto, and our very own Marketing Chair Dr. Andrew Whitley. Attended by over 130 regulatory and analytical methods experts, the workshop addressed the need for microplastics research and development, standardized collection methods, and data management and sharing, designed to provide a better understanding, to drive regulatory policy and reporting.

Andrew stated that, "it is clear from the September, 2018 SB-1422 California Safe Drinking Water Act and the SB-1263 Ocean Protection Council: Statewide Microplastics Strategy that studies and strategies aimed at developing screening and identification for microplastics in waste and drinking water would need to be accelerated. This workshop was formulated to kick start this process."

As a result of the workshop there will be a designed study plan launched using microplastic standards to help understand the reliability of developed methods and standard operating procedures. As a further follow up to the workshop the organizers are guest editing a special issue of Applied Spectroscopy focusing on the best practices for microplastics analysis. If you are interested to submit a paper for the special issue, there is still time, the call for papers is open until August/September. To register your interest and intent please contact Andrew at the email below. Andrew is also organizing two special SAS sessions on microplastics at SciX in Palm Springs in October.

Additional information on the workshop and SCCWRP can be found here:
http://www.sccwrp.org/about/research-areas/additional-research-areas/trash-pollution/measuring-microplastics-workshop/

Contributed by Andrew Whitely
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Upcoming Talks and Events of Interest

Optical Society of America (OSA) Agri-Photonics Incubator: Advanced Spectroscopy in Precision Agriculture
12–14 May 2019
OSA Headquarters
Washington, DC, United States
www.osa.org/agriphotonicsinc

This meeting, as part of the OSA Incubator Program, will bring together experts in plant biology and precision agriculture technology development, regulatory work, and industry to discuss how modern optical sensing technologies, especially current spectroscopic techniques, are being applied in agriculture. The successful completion of this event leads to establish strong collaboration between participants and their institutes in spectroscopy, industry, and biological sciences communities and possibly initiate follow-up topical and nationwide conferences and workshops. While this is an invitation only meeting, a limited number of spots have been set aside for interested individuals to apply. Please send a brief letter of interest along with a CV to the hosts at osaincubator@osa.org.

Contributed by Gombojav O. Ariunbold
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Colloquium Spectroscopicum Internationale XLI

We kindly invite you to participate at Colloquium Spectroscopicum Internationale XLI (CSI-XLI) and the First Latin American Meeting on Laser Induced Breakdown Spectroscopy (LAMLIBS), which will be held on 9–14 June 2019 in Mexico City, Mexico. Both conferences are organized by the Institute for Applied Sciences and Technology of the National Autonomous University of Mexico (UNAM) and have the endorsement and support of the Mexican Physical Society, the Mexican Chemical Society and IUPAC. The conferences will be held at the UNAM. For more information, please visit the website: http://www.csi2019mexico.com/

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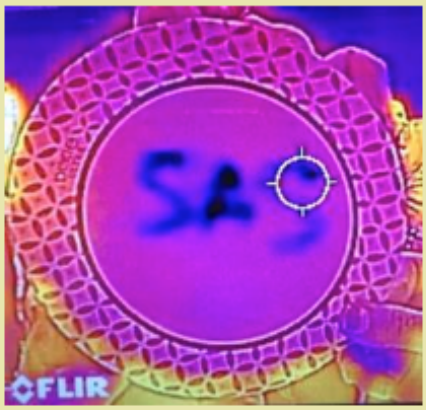
The State University of New York at Buffalo Section of the Society for Applied Spectroscopy Ellicott Science Night



Attendees: María Rivera, Emily Sekera, and Kelsey Williams

On 28 March 2019, the State University of New York at Buffalo (UB) section of the Society for Applied Spectroscopy attended Science Night at Ellicott Road Elementary in Orchard Park, New York. Ellicott's Science Night is an event that allows children, from kindergarten to grade 5, to engage in hands-on scientific activities. Booths ranged from showing live reptiles to making the ever-so-popular slime. The UB section of SAS brought a thermal-imaging camera to teach students about temperature and how spectroscopy can be used to measure temperature. Activities at the booth involved mixing methanol and water to show heat-of-mixing, as well as using the methanol-water mixture to make secret messages on paper plates that can be seen due to the cold nature of methanol. The activities at the booth brought both fun and education to children, parents, and the members who attended the event.

(L to R) *Emily Sekera, María Rivera, and Kelsey Williams*

An Overview of Intellectual Property Protection of Biopharmaceutical Compounds via Natural-Abundance Stable Isotopes

The March 2019 meeting of the New York (New Jersey) Regional Section of the Society for Applied Spectroscopy (NYSAS) was held on 27 March 2019 at the Horiba Optical Spectroscopy center in Piscataway, New Jersey. The guest speaker was John P. Jasper, Ph.D., Chief Scientific Officer of Molecular Isotope Technologies LLC / Nature's Fingerprint Authentication, Niantic, Connecticut (www.NaturesFingerprint.com).

John P. Jasper is an analytical organic and stable-isotope chemist who has worked in marine paleochemistry and in pharmaceutical sciences. He received his B.A. in Geophysical Sciences and Biological Sciences from the University of Chicago in 1981. He earned his Ph.D. from MIT and Woods Hole Oceanographic Institution in marine organic chemistry in 1988, where he assessed the quantitative relationship between paired specific biomarker compounds and contemporaneous carbon-isotopic of bulk organic matter for organic geochemical purposes. He was a Postdoctoral Fellow and Scientist at the Department of Chemistry at Indiana University at Bloomington from 1988-1994 where he employed the newly-developed gas chromatograph/isotope-ratio mass spectrometer (GC-IRMS) to reconstruct paleo-chemical CO2 levels. He served as an analytical organic chemist at Pfizer from 1994–1997. Since then, he founded and serves as the CSO of Nature's Fingerprint/MIT LLC. Last year, Dr. Jasper was elected as a Fellow of The Explorers Club for that work on the global greenhouse effect spanning the last 500 Myr.

All chemical compounds have distinctive ratios of stable isotopes. Regional variations in naturally occurring isotopes provide an intrinsic way to authenticate manufacturer's products and processes. "Every batch of manufactured product represents a slice of nature". Local and regional variations in raw materials generate unique isotopic ratios that can be used to identify the origin of manufacturing. Thus, the multiple isotope fingerprint of products is a highly effective way to identify, track, and classify batches based on origin of manufacturer. This analysis can be used to mitigate counterfeiting, diversion, theft, patent infringement, and liability issues. The presentation included three cases of process authentication: one of false advertising and two of process patent infringement. The presentation also included an overview of molecular isotopic engineering for product identification and of product security, and also for intellectual property considerations.

Fourteen people attended the meeting at Horiba. If you missed the meeting and would like to hear a replay of the presentation, send an email to debperu@outlook.com and we will send you a link to the webinar.

For more information about the NYSAS organization and a schedule of meetings, please go to our website www.nysas.org.

Contributed by Debbie Peru

Do you have something spectroscopy-related you want to discuss in the newsletter?
Or something that will help our membership such as career tips or application tips?
Please let us know by emailing xchen4@dow.com.

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