SAS SPECTRUM eNEWS

New Integrated Sampling Systems

SAS 2015 National Meeting in Providence, Rhode Island

Providence provided the setting for this year's national meeting at SciX. Set at the edge of the newly renovated downtown and the historic Federal Hill neighborhood, and close to the Brown and Rhode Island School of Design (RISD) campuses, the location provided for entertainment, Society planning, and the exchange of scientific ideas.

The SAS sponsored member social events at the Union Station Brewery, the Student Event, and the Wine and Cheese Awards reception. All events were a great success. The Union Station was filled to capacity, as was the Student Event. The Wine and Cheese Reception was remarkable this year for the fundraiser for the 2020 Initiative featuring the star attraction—Ian Lewis' beard! Reports on the social events will appear in an upcoming issue.

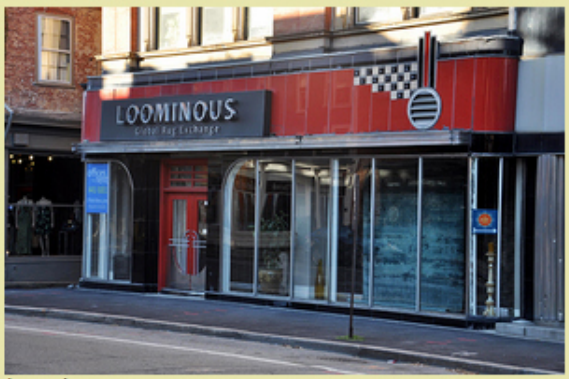
Society Officers meet at SciX to present semi-annual and annual reports to the Executive Committee and the Governing Board. Full reports are available for viewing by contacting the SAS office (sasadmin@s-a-s.org) or by visiting the Society website (www.s-a-s.org). Summary reports will be presented in the Newsletter. The highlight of the reports was that this year the Society has a balanced budget and the transition of the Journal to Sage Publications platform. The balanced budget has been achieved mostly through cost-cutting, advertising revenue, and small increases in membership fees. The full transition to Sage Publications on January 2016 is expected to both ease and speed the publication process for the Journal.

This issue of the Newsletter is dedicated to reports from the SAS-sponsored sessions at SciX. Member-contributed articles are the lifeblood of society newsletters. This is reflected by part of our Newsletter mission statement to publish "items of interest to the membership [and] personal notes concerning members." Sharing news about yourself and colleagues is part of building and maintaining our community.

A Visual Overview of SciX

Providence is filled with references to color and spectroscopy. Loominous is a textile gallery in the Downtown area. The Color Run is an informally organized 5K run to promote fun and fitness. The RISD specializes in the visual arts and architecture.

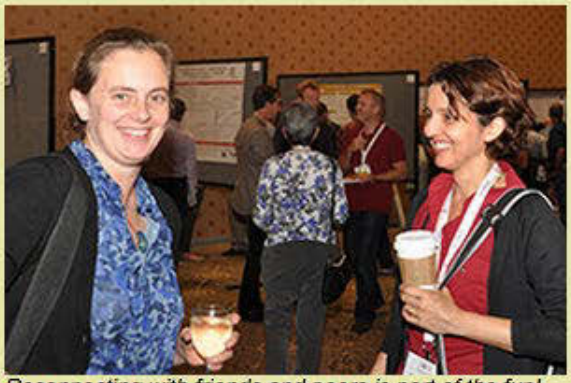
Early morning at the SciX convention center.

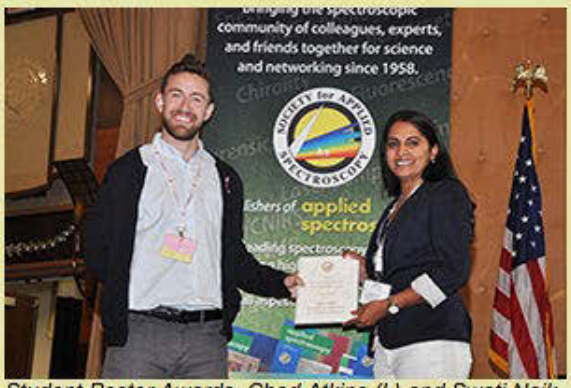


Loominous

Color run

Rhode Island School of Design

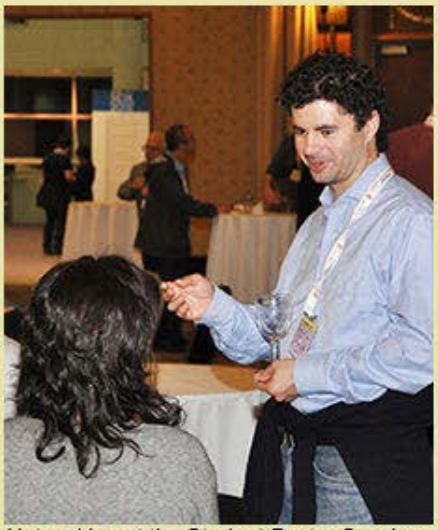

Reconnecting with friends and peers is part of the fun!



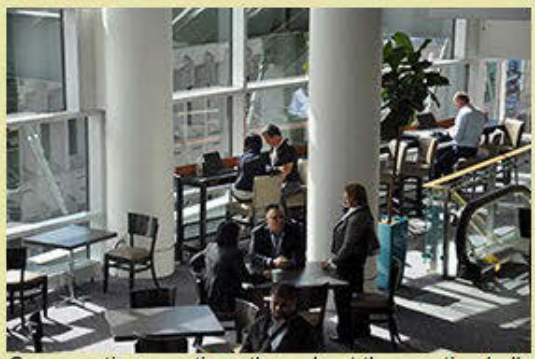
Student Poster Awards, Chad Atkins (L) and Swati Naik (R) pictured. (See text for full list of awardees.)

The SAS Student Poster Session was a great event to network with other conferees. FACSS, Coblentz Society and SAS Student Undergraduate Award, Undergraduate Student Travel Grants, and Poster session awards were presented. Congratulations to Liesl Krause, John Orlet, Collen Riordan for receiving the SAS Travel Grant, Jason Becker, Patrick Skrodzki, Michaella Raglione, and Allen Walker for receiving the SAS Undergraduate Student Award and the four Poster Award winners David Surmack for Self-Absorption Measurements of Resonant Aluminum Lines, Liesel Krause for Cold Atmospheric Plasma: An Inside Look Through Optical Diagnostics, Jason Becker for Absorption Spectroscopy of Uranium 238 in Laser Induced Plasma, and Swati Naik for Non-Hydrolytic Processing of Transition Metal-Doped TiO2 Nanostructures for Photocatalytic Applications.

Networking is one of the great advantages of the SAS. Meeting and discussing professional and personal topics before, after, and between sessions is valuable.


Networking at the Student Poster Session.

The Wine and Cheese Reception presented the various awards for the Society. A full list can be found on the website (http://tinyurl.com/SAS2015Awards) and in the previous Newsletter issue. The event ended with a fundraiser for the 2018 Strategic Fund.


Conversations continue throughout the meeting hall.


The 2018 Strategic Fund. Ian Lewis' beard is a proud supporter!

SAS Sponsored Sessions

Each year at SciX and Pittcon, the SAS sponsored a number of sessions that we believe are important to all of our members. At this SciX, the SAS supported: "Beyond PCA and PLS: New Frontiers in Chemometrics," "Women in Spectroscopy," "Advocating for Women in Science," "Analytical Chemists Easing World Poverty," "Kowalski Award Honoring Thomas Bocklitz," "Lester Strock Award Symposium Honoring R. Kenneth Marcus," and the "Meggers Award Symposium Honoring Dr. Eric Brauns." Some of the session organizers have been kind enough to provide reports on their symposia for those who were not able to attend the sessions.

Meggers Award Address and Symposium

The Meggers Award is presented to the author who is deemed by an SAS committee to have published the most outstanding paper in Applied Spectroscopy each year. This year Professor Eric Brauns of the University of Idaho was chosen for his 2014 paper entitled "Mid-Infrared Diffuse Reflection on Ultrafast Time Scales" (Appl. Spectrosc., 68[1], pp. 1-4).

As is known to most members of the SAS, diffuse reflection (DR) is a fundamental optical phenomenon in which light penetrates a translucent scattering solid and re-emerges after undergoing numerous instances of reflection and refraction. As a result, photons can travel long distances through semitransparent samples. In some cases this is advantageous, e.g., where the long effective path lengths can increase the net absorption of a weakly absorbing analyte. In other cases it is undesirable, e.g., in imaging applications where DR degrades spatial resolution and contrast. Despite its significance, relatively little is understood about the underlying mechanism, particularly for mid-infrared DR. A direct determination of the effective path lengths that photons travel requires time-resolved measurements on ultrafast time scales that, especially in the case of mid-infrared DR spectroscopy, poses unique challenges. Brauns developed an instrument in which femtosecond mid-IR pulses are generated by difference frequency, mixing the output of an optical parametric amplifier that is pumped by a regeneratively amplified Ti:sapphire laser. Time resolution is achieved by upconverting the diffusely reflected photons with pulses from the Ti:sapphire oscillator. The result is an instrument capable of studying mid-IR DR with femtosecond time resolution. In his award-winning paper, Brauns described the instrument in detail and presented experimental data on a series of powdered KBr samples containing varying amounts of carbon black. His results suggested that, contrary to most beliefs, mid-IR photon transport on ultrafast time scales is not diffusive, but can be explained by a bimodal distribution. Brauns described his instrument and results in a beautifully presented plenary address. In the Meggers Award symposium held later in the day, five spectroscopists described various theoretical and experimental applications of mid-infrared DR spectroscopy.

Arnold Kim of the University of California, Merced, gave a systematic derivation of the Kubelka-Munk equations from the equation of radiative transfer. In doing so, he derived an intermediate approximation, which he called the generalized Kubelka-Munk equations. These equations are better, and only slightly more difficult to solve, than the simple Kubelka-Munk equation, especially for strong absorbing and anisotropic scattering media. Kim then introduced their use in modeling diffuse reflectance. He then extended this theory to model time-resolved diffuse reflection. He proposed the use of this model for interpreting measurements of mid-infrared DR on ultrafast time scales of the type measured experimentally by Eric Brauns.

The remaining talks in the symposium covered various experimental aspects of mid-infrared DR spectroscopy. Thomas Blake of the Pacific Northwest National Lab discussed the accurate measurement of DR spectra. Past laboratory and field work by, for example, researchers performing thermal infrared sensing of geological surfaces, has shown that for most materials a laboratory measurement of the total directional-hemispherical reflectance, RT, of a target surface and the use of Kirchhoff's law gives a good approximation to the emissivity, ε, of that surface: $\varepsilon = 1 - RT$. Using a FT-IR spectrometer and a commercial off-the-shelf integrating sphere with a matte gold coating, the group at PNNL have begun to construct a quantitative database of infrared directional-hemispherical (specular + diffuse and diffuse-only) reflectance spectra covering the wavelength range 1.3 to 16.7 μm for materials relevant to long-wave infrared field sensing. Results for measurements of standard materials as well as data from several materials of interest were presented and excellent agreement with previous data measured at NIST was obtained.

Francisco Calderon of the Agricultural Research Service of the USDA in Akron, Colorado, described attempts to characterize organic matter present on mineral and soil surfaces by mid-infrared DR spectroscopy. He reported the results of attempting to remove the absorption features caused by the inorganic materials by spectral subtraction. His results demonstrated that only when absorption by the mineral components was very weak could bands assignable to organic components be observed. In the spectral regions where strong bands of minerals appeared, the non-linearity of Beer's law for mid-infrared DR measurements led to the conclusion that spectral subtraction was usually ineffective. Unfortunately, Calderon's talk was given at the same time that the management of the Providence Convention Center had scheduled a fire alarm test that continued for 15 minutes of this 20 minute presentation. The alarm could only be switched off by the Providence Fire Department. Dr. Calderon is to be congratulated for giving his talk under the most trying of circumstances.

Samuel Hernández-Rivera of the University of Puerto Rico-Mayaguez described how stand-off (SO) mid-infrared reflection spectroscopy using quantum cascade lasers (QCL) sources could be used to tackle various analytical problems involving detection of hazardous threat chemicals, biological threat simulants, landmine explosives in soils, the content of active pharmaceutical ingredients in formulations, and the detection of oil residues in soils. The high collimation and spectral radiance (brightness) of the QCLs used made some previously impossible measurements feasible. In other cases, results were as good as those that can be obtained using ATR FT-IR spectroscopy with the added capability of sensing at a distance. Research with SO-QCL spectroscopic systems has allowed the detection, discrimination and quantification of highly energetic materials and homemade explosives present as trace residues on metal substrates (neat or painted) and on non-reflective substrates such as travel bags, cardboard and wood was possible when combined with various chemometric techniques such as principal components analysis and partial least squares regression.

Michael "Micky" Myrick of the University of South Carolina discussed detection limits of blood on forensic samples. The factors affecting detection limits are often not well understood, and some of the best-known methods for detecting blood have literature values for detection limits that vary by many orders of magnitude. Furthermore, the units in which detection limits are cast have mainly been units of convenience that are not readily converted to the kind of units that an analytical chemist would recognize. Detection limits using mid- or near-infrared spectroscopy are at best crude estimates to date. Myrick and his co-workers studied the factors that determine the detection limits for blood on fabrics via mid-infrared DR spectroscopy measured under simple conditions (i.e., well-controlled laboratory samples with no additional interferences). They showed that the system is quite nonlinear working in the reflectance mode, but that models are not appreciably better in the log(1/R) mode. They found that high order derivative processing works gave a number of beneficial outcomes. For example, because of the effect of smoothing, spectra processed with high-order numerical gap derivatives can have signal-to-noise ratios greater than the original spectra and work as well or better than traditional Savitzky-Golay derivative processing. The high-order gap derivative can behave like a matched filter for improving recognition of the analyte. Detection limits for different spectral windows on four different fabrics were given, with the best being in the range of 0.01 ‰w/w.

In summary, the speakers both in the award address and in the associated symposium described both approaches to better understanding mid-infrared DR spectroscopy and some unusual and effective ways in which this technique can be applied to a variety of unusual analytical problems.

Contributed by Peter R. Griffiths

Beyond PCA and PLS: New Frontiers in Chemometrics

The standing room only crowds of each of the five Chemometrics Symposia demonstrated the resurgence of chemometrics at SciX, as well as the other five contributed chemometric sessions. There were a significant number of international presenters from Australia, Canada, Denmark, France, Germany, Italy, The Netherlands, and Spain. Topics ranged from state-of-the-art developments in chemometric methods, such as topological modeling of data spaces and homeopathic independent components analysis to practical applications in the forensic and food sciences, medicine, and the pharmaceutical industry. There was a preponderance of presentations and posters in the other sessions that also had a healthy dose of chemometrics.

Contributed by Peter Harrington

Kowalski Award Honoring Thomas Bocklitz

The SAS-sponsored session honoring the Bruce Kowalski Award brought in speakers from all career stages within academia to present and discuss their research. The goal was to allow researchers from all career levels, from younger researchers to well-established scientists, to learn from each other. Another goal was to show how many different data types and applications can be tackled by chemometrics. Prof. Max Diem and Prof. Martin Hedegaard presented the preprocessing and analysis techniques for Raman and IR imaging-based diagnostics. Prof. Steven Brown presented a method to construct hierarchical models for evaluating complex data and Brett Brownfield showed a combination of different dissimilarity merits in order to detect outlier in datasets. To conclude Dr. Thomas Bocklitz, the 2015 Bruce Kowalski awardee, described an analysis workflow for multimodal imaging. Altogether, the symposium featured great talks, fruitful discussions, and a coming together of generations of chemometricians.

Contributed by Peter Backlit and Juergen Popp

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