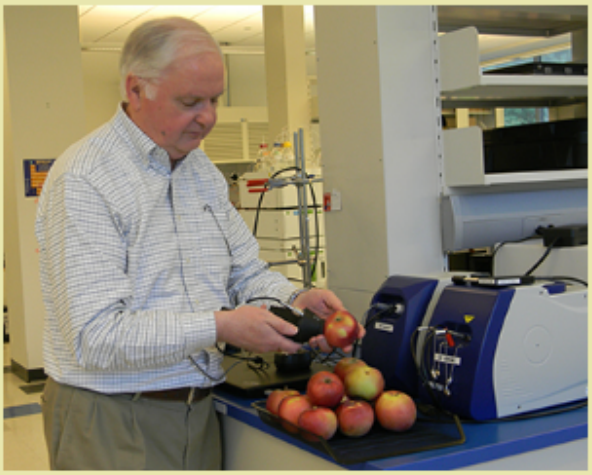
SAS SPECTRUM eNEWS

Editor's Note and SciX Diary

Returning from SciX 2018, I got home around 11:00 P.M. after catching my connecting flight with only one minute to spare. Reflecting on the previous four days of the meeting, I felt that it has been a very exciting and productive SciX on all fronts: There were interactions with the next-generation of spectroscopists, numerous activities with the various SAS meetings, technical programs and exhibits, and last but not least, lots of networking. Since I am already three days overdue with the newsletter for this issue, many of the formal reports from the various SAS sessions will have to wait until next month. I did keep a diary recording my various encounters and all of the fun events I participated in at SciX. If you are interested in seeing it published in our next issue of Newsletter, please let me know by sending an email to xchen4@dow.com. If I get more than five requests, then I will share it with our readers. Of course if there is any particular topic that you want our Newsletter crew to investigate and to include in our newsletter, please email me anytime. I have also got a lot of constructive feedback on how to improve our Newsletter, which we plan to implement in the next few months.

In this month's issue, we introduce the researchers whose contributions to spectroscopy and SAS have earned them SAS Meggers Award, the inaugural SAS/NASLIBS award for the best paper published in Applied Spectroscopy in 2017, the Bruce R. Kowalski Award in chemometrics, the SAS Fellows Award, and the SAS William J. Poehlman Award.

Richard Crocombe, Author of the December Issue Focal Point Review



The Society for Applied Spectroscopy and Applied Spectroscopy are pleased to announce Dr. Richard Crocombe's upcoming Focal Point Review paper entitled "Portable Spectroscopy" in the December 2018 issue of the journal. What follows is a brief interview with Dr. Crocombe in which he outlines his background and interest in the topic of portable spectroscopic technologies. As always, Focal Point Review papers are free to view and can be found at http://journals.sagepub.com/home/asp on publication.

1. Tell us about yourself
My academic background was in inorganic chemistry and vibrational spectroscopy in the pre-data system era, where you had to rely on pen recorders, and computational tasks involved daily trips to the computer center carrying a tray of punch cards. However, I became interested in application and instrumentation development, and joined an instrument company, and have spent my career in that milieu. I spent about twenty years in the laboratory FT-IR business, including running both commercial instrument development and applications developments like step-scan FT-IR and FT-IR hyperspectral imaging. For the past fifteen years I've been working in the field of miniature and portable spectrometers, with techniques ranging from GC-MS, XRF, Raman, mid-infrared and near-infrared. I left the corporate world in 2017 and set up my own consulting company, focusing on portable spectroscopy.

2. Do you own any portable spectrometers?
Not personally! But I use a lot of them, made by my clients.

3. Who should buy portable spectrometers?
Anybody who needs actionable screening answers in the field, and where it's costly or inefficient to send samples to the lab. That field is huge, ranging over areas like field geology and mining; explosives and hazardous materials; pharmaceuticals and street narcotics; metal fabrication and recycling; food fraud and adulteration; precision farming and crop heath.

4. Compared to conventional benchtop spectrometer market, is the portable spectrometer market larger or more profitable?
a. There are more portable Raman systems in the field than there are laboratory Raman spectrometers, and more portable XRF instruments in the field than in the lab. That's impressive given that portable instruments have only been available recently. A portable instrument sold to the military or hazardous materials teams can actually cost more than a low-end lab instrument. Technology is moving very rapidly, and for instance 'mouse-sized' Raman and near-infrared instruments are now possible or available, sometimes at very low cost. These have the potential to expand the market dramatically, so the questions of larger market size and profitability are moving targets.

5. What caused you to become so interested in portable spectrometers?
a. The very rapid technological developments in that area, spurred by telecom optics, consumer electronics, etc., along with the possibility of widespread new applications.

6. When will we have accessories that can convert our smart phones into spectrometers? Give us an estimation for NIR, mid-IR, Raman, XRF, LIBS, etc.
There's a lot of work being done in this area, especially in the visible to 1µm region, accessible via very low cost silicon-based detectors. The area that may have most impact in the future is the ability to do clinical diagnostics using the smartphone as a detector. This could have a huge impact on human health in remote and low resource areas of the world. For developed countries, Apple and Garmin have "smart watches", and both tissue hydration and blood oxygenation can be measured. In addition, there are products already released (e.g., NIR, Raman) which are very small and use the smartphone as a data system. Mid-IR is more difficult, as you need reasonable-sized optics (e.g., ½" diameter) to get decent throughput and signal to noise. XRF and LIBS both have intrinsic hazards (radiation safety), and will probably remain more specialized. An area to watch out for is low cost hyperspectral imaging, again in the silicon detector region, enabled by technologies like scanning Fabry-Pérot and linear variable filters. These make low-cost and very compact devices. One organization has already shown a smartphone-based hyperspectral imager.

7. How fierce is the competition? Is it too late to enter this market now?
Many of the traditional instrument companies already participate in these markets. But because the instruments are very application specific, the door remains open for those targeted at specific markets, where the company really understands the applications, and has an existing channel to market. The low-cost area is wide open, with many start-ups entering the field. The key to success is not so much technology, as it is deep market and applications knowledge, coupled with turnkey applications development to give actionable results to non-spectroscopist customers. And then all the sales and marketing connections to reach those markets. One company has a handheld spectrometer that will analyze stains on garments, and then program their washing machine to take that stain out!

2019 Gold Medal Award: Society for Applied Spectroscopy (SAS), New York Section

Nominations are being sought for the 2019 Gold Medal Award of the New York Section of the Society for Applied Spectroscopy. This coveted award was established in 1952 to recognize outstanding contributions to the field of applied spectroscopy. The Gold Medal will be presented at a special award symposium, arranged in honor of the awardee, at the 2019 Eastern Analytical Symposium. A nominating letter describing the nominee's specific accomplishments should be submitted along with a biographical sketch by January 15, 2019. Please e-mail all materials as well as questions and inquiries to Dana Garcia at dana.garcia@arkema.com.

Society for Applied Spectroscopy Meggers Award

The Megger's award recognizes the author(s) of an outstanding paper(s) appearing in Applied Spectroscopy. This year it was presented to S. Michael Angel, Patrick D. Barnett, Nirmal Lamsal, Kelly C. Paul, and K. Alicia Strange Fessler for five related papers on the topic of spatial heterodyne spectroscopy applied for Raman and laser-induced breakdown spectroscopy in 2017, Volume 71.

S. Michael Angel

Mike Angel is a professor of chemistry at the University of South Carolina where he has held the Fred M. Weissman Palmetto Chair in Chemical Ecology since 2005 and was named a Carolina Trustee Professor in 2013. He received his PhD from North Carolina State University in 1985 and carried out postdoctoral work with Tomas Hirschfeld at the Lawrence Livermore National Laboratory. Angel's research group works mainly in the areas of remote and in situ laser spectroscopy with a focus on deep ocean, planetary, and homeland security applications of Raman and LIBS. Recent work includes developing the spatial heterodyne Raman spectrometer (SHRS) which was awarded the 2012 Meggers Award, and exploring the SHRS for deep UV Raman, remote Raman, and for use on future planetary landers and SmallSats.

Patrick D. Barnett

Patrick received a BS in chemistry at the University of Central Missouri in 2011, and a PhD in analytical chemistry at the University of South Carolina in 2016. His graduate research focused on the development of a miniature spatial heterodyne spectrometer (SHS) for Raman spectroscopy and laser-induced breakdown spectroscopy (LIBS) for planetary exploration and other extreme environments. In early 2017, Patrick started a postdoctoral fellowship with Shiv Sharma at the Hawaii Institute of Geophysics and Planetology. His work has focused on spectroscopic studies of minerals under pressure and temperature conditions similar to the surface of Venus to provide data necessary for planning and designing spectroscopic instruments for future Venus lander missions. In late 2017, Patrick was hired as a postdoctoral appointee at Sandia National Laboratories in the Advanced Remote Sensing group.

Nirmal Lamsal

Nirmal Lamsal received a master's degree in physical chemistry in 2008 from Tribhuvan University, Nepal. After spending two years teaching chemistry at a private college in Kathmandu, Nepal, Nirmal joined the University of South Carolina in 2010. He obtained his PhD in analytical chemistry in 2015 under the supervision of Dr. S. Michael Angel. His PhD research focuses on designing and constructing a novel deep-UV FT Raman spectrometer, known as the SHRS for standoff measurements. During his time at USC, Nirmal has written three papers and has presented his results at several meetings and conferences, including SciX, Pittcon, and the Lunar and Planetary Science Conference. After graduation, Nirmal moved to Austin, Texas, to join the IMACC, LLC as a senior scientist. In his time at IMACC, he worked extensively in the field of optical analytical instruments and designed a new type of FT-IR-Raman system for fast fuel gas analysis in stacks and process applications. Currently, he works at ChemImage Corporation in Pittsburgh, Pennsylvania, with a focus on the development of instruments for chemical imaging using Raman spectroscopy.

Kelly C. Paul

Kelly C. Paul earned her BS degree in chemistry (ACS certified) from the University of South Carolina in 2015. She completed an extended undergraduate research project with Dr. S. Michael Angel, focusing primarily on Raman spectroscopy. In 2016 she joined Shakespeare Company, LLC, a division of Newell Brands, where she is currently employed in the polymer analytical lab.

K. Alicia Strange Fessler

K. Alicia Strange Fessler (Dr. Strange) received her BS degree from East Carolina University in 2008, an MSc from the University of Manchester in 2010, and PhD from the University of South Carolina in 2016. PhD research conducted under Dr. S. Michael Angel characterized and demonstrated standoff and one-dimensional imaging using visible SHRS for the detection of solids and solutions related to planetary exploration and high explosives applications. Her research also demonstrated and quantified the larger field-of-view and throughput of the SHRS for transmission Raman spectroscopy measurements in comparison to an f/1.8 dispersive system. After completing her doctoral degree, she took a postdoctoral position at Savannah River National Laboratory (SRNL) in the Global Security group, and she was hired as a Senior Scientist into the Analytical Development division at SRNL in 2017. Her research at SRNL applies optical spectroscopic methods and techniques to applications concerning nuclear nonproliferation, safeguards, and process analysis.

SAS-NASLIBS Award

The inaugural SAS-NASLIBS award for the best paper published in Applied Spectroscopy in 2017 on the topic of laser induced breakdown spectroscopy was presented to S. Michael Angel, Patrick D. Barnett, and Nirmal Lamsal for "Standoff Laser-Induced Breakdown Spectroscopy (LIBS) Using a Miniature Wide Field of View Spatial Heterodyne Spectrometer with Sub-Microsteradian Collection Optics", Volume 71, Issue 4, pp. 583–590. The biographic information of these authors is not repeated here as they were a subset of the authors who received the Meggers Award above.

Bruce R. Kowalski Award in Chemometrics

The Kowalski award, administered by the Society for Applied Spectroscopy, is presented in honor of the legacy of Professor Kowalski by recognizing outstanding young researchers in the field of chemometrics and by extension, for advanced mathematical and/or statistical methods in chemistry.

Andrew T. Weakley

Andrew (Andy) T. Weakley graduated in 2014 with a PhD in chemical engineering from the University of Idaho. As a graduate student, Dr. Weakley developed several model-free baseline correction algorithms applicable to vibrational spectra containing uni- and bi-directional bands, quantified the hard and soft segment fraction of mixed thermoplastic polyurethanes using partial least squares (PLS) with Raman spectroscopy, and developed a variable selection algorithm known as backward Monte Carlo unimportant variable elimination (BMCUVE). Presently, Dr. Weakley is post-doctoral fellow at the Air Quality Research Center (AQRC) at the University of California, Davis, where he continues to advance chemometric techniques in the atmospheric sciences by developing and implementing source-sensitive multilevel PLS methodologies to quantifying organic and elemental ("soot") carbon in ambient particulate matter. Dr. Weakley also collaborates as an independent contractor (Weakley Consulting), most notably supporting occupational health studies that aid in the cost-effective implementation of portable infrared spectrometers to determine filter-bound respirable silica in US coal and non-coal mines. Other research and interest areas include the near-infrared analysis of agriculture samples, mid-infrared forensic analysis, PLS latent variable interpretation, and chemometric education.

Society for Applied Spectroscopy Fellows Award

The Society for Applied Spectroscopy Fellows award recognizes individual members for their outstanding service to the field of spectroscopy and the Society for Applied Spectroscopy.

Linda McGown

Linda Baine McGown is the William Weightman Walker Professor of the Department of Chemistry and Chemical Biology at Rensselaer Polytechnic Institute. She received her BS from the State University of New York at Buffalo in 1975 and her PhD from the University of Washington in 1979. She was a faculty member at California State University, Long Beach, Oklahoma State University, and Duke University before joining RPI in 2004. She is a Fellow of the American Association for the Advancement of Science since 2001, and recipient of the 2018 Eastern Analytical Symposium Award for Outstanding Achievements in the Field of Analytical Chemistry and the 1994 New York Section of the Society for Applied Spectroscopy Gold Medal Award. She was included in the 2016 Power List: The Top 50 Most Influential Women in the Analytical Sciences, and she was featured in the Future of Women in Chemistry and Science in honor of the UNESCO declaration of 2011 as the International Year of Chemistry. She has served on numerous editorial boards including Chemical and Engineering News, Analytical Chemistry, Applied Spectroscopy, Analytica Chimica Acta, and Life.

A common thread through Dr. McGown's research is the recognition of the analytical potential of new discoveries and emerging technologies, beginning in her early career with frequency-domain fluorescence lifetime techniques. She enjoys pursuing unconventional pathways to overcoming existing challenges, such as her genome inspired approach to aptamer discovery. Other current research interests include molecular self-assembly (particularly G-quadruplex DNA), bioseparations, and the prebiotic chemistry of early Earth.

Michael (Micky) Myrick

Michael (Micky) Myrick received his PhD from New Mexico State University in 1988 and was a postdoctoral associate of S. Michael Angel at Lawrence Livermore National Laboratory (LLNL) from 1989–1990. He was a staff member at LLNL from 1990–1991 and has been a member of the Department of Chemistry and Biochemistry at the University of South Carolina from 1991–present. He is the author of 170+ publications and 33+ patents.

His work in multivariate optical computing lead via a startup to the ICE sensor system commercialized by Halliburton Energy Services for petroleum exploration and carbon sequestration, in use worldwide. His work has featured on the covers of Analytical Chemistry, Applied Spectroscopy, Laser Focus World, and the Reservoir Innovations Technical Journal. His work in infrared chemical imaging and adsorption thermography was publicized on CNN, Fox, NPR Science Friday, SC Radio Network, Popular Science, and elsewhere. He received the Outstanding SC Chemist Award from the SC Section of the ACS in 2018.

As an educator, Micky teaches general chemistry, both physical chemistry laboratory courses, and a graduate course in molecular spectroscopy. He has published five papers on new spectroscopy experiments for physical chemistry laboratories in the Journal of Chemical Education, and has received several teaching awards at USC, including the Michael J. Mungo undergraduate teaching award and the SC Honors College Outstanding Professor of Science award.

David Schiering

Dr. David W. Schiering is a founder and principal of Czitek, a small company dedicated to the development and marketing of vibrational spectroscopy products. He has more than thirty years of experience in the business of instrumentation for chemical measurements. Prior to Czitek, Dr. Schiering has held numerous roles in management, science and technology, product development, and product management at Smiths Detection, SensIR Technologies, Thermo Electron Corp., and PerkinElmer. In his career Dr. Schiering has either been a key contributor or leader in the development of ground-breaking vibrational spectroscopy technologies in the fields of infrared microspectroscopy, portable and hand held FT-IR and Raman instruments and methods, vibrational spectroscopy applications in security and defense, Raman spectroscopy for threat detection in airport screening.

Dr. Schiering, who has authored more than 25 publications on various aspects of vibrational spectroscopy, holds a PhD in analytical chemistry from Miami University, where he is also an adjunct Assistant Professor of Chemistry. Dr. Schiering has served the Coblentz Society as a member of the Board of Managers from 1993 to 1997, and as secretary from 1991 to 2010. In 2011, Dr. Schiering was made an Honorary Member of the Coblentz Society and in 1983 received the Coblentz Society Student Award. Dr. Schiering has been a member of the Society for Applied Spectroscopy since 1981. He is a member of the Coblentz technical section and the New Jersey-New York affiliates.

Society for Applied Spectroscopy William J. Poehlman Award

The SAS William J. Poehlman award recognizes an outstanding SAS Regional Section that has met the goals and ideals of the Society over the past year:

SAS Cleveland Regional Section

The SAS Cleveland Section is being recognized as this year's outstanding section for maintaining a consistently high level of activity throughout the year and completing a large number of projects that has furthered the mission and goals of the Society.

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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