May 2021

Portable Spectroscopy and Spectrometry Literature

John Wiley and Sons Publishing has just published a two-volume book, *Portable Spectroscopy and Spectrometry*, edited by Richard Crocombe, Pauline Leary, and Brooke Kammrath. Volume I covers “Technologies and Instrumentation”, and Volume II covers “Applications”. The two volumes provide a thorough treatment of the subject, with over 40 chapters and 1200 pages in all. Many of the chapter authors are SAS and Coblentz members, and also familiar faces from SciX and Pittcon.

Volume 1 (ISBN: 978-1-119-63641-0) includes chapters on FT-IR, NIR, Raman, UV–Visible, microplasmas, LIBS, mass spectrometry, GC-MS, ion mobility spectrometry, X-ray fluorescence, NMR, DNA, and biological analyzers. Additional special topics include MEMS and MOEMS, optical filter technology, smartphone, and stand-off spectroscopy.

Volume II (ISBN: 978-1-119-63642-7) focuses on applications, with coverage of industrial, pharmaceutical, forensic, military, hazardous materials, food, geochemistry and astrobiology, field geology, cultural heritage, and archeology. Additional special topics include chapters on algorithms, libraries and calibrations, calibration transfer, specific Raman and NIR applications, and applications of smartphone spectroscopy in the clinical field.

You can see the contents of these books and sample chapters by viewing Volume 1 and Volume 2.

These books are available to SAS members at a 20% discount. Log-into the SAS website, navigate to this page and then use the discount code found on that page.

In addition, John Wiley and Sons Publishing, in association with SAS and Coblentz, is planning a number of webinars based on book chapters and presented by the chapter authors. The provisional schedule for these webinars is:

Thursday, 27 May 2021
Pharmaceutical, Industrial, and Counterfeits

Thursday, 24 June 2021, 2.30 pm
Clinical, Bio and DNA

Thursday 22 July 2021, 2.30 pm
Forensic and Law Enforcement, Safety, and Security

Final details of these events will be posted on social media, including the SAS web site, as we get closer to those dates.

SciX 2021 Invitation

FACSS PRESENTS SCIX2021 The Great SCIentific eXchange

The Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) invites you to come together with its fourteen member societies at the SciX 2021 conference to be held at the Rhode Island Convention Center on 26 September–1 October 2021 in Providence, Rhode Island. SciX attendees will enjoy a vibrant downtown venue that is close to hotels, restaurants, and entertainment. SciX 2021 is the first in-person analytical chemistry conference in over a year. We are committed to providing a world-class experience that brings together the best technical program, cutting-edge technologies, and opportunities for career development. To see our program preview and learn how we are planning for COVID-19, please visit our website: www.scixconference.org.

The SciX conference is recognized for the strength and diversity of the technical program and this year is no exception. The Sunday keynote speaker will be Professor David Walt of Harvard University who will speak on “Measuring Scientific Impact”, drawing on examples from his illustrious scientific and entrepreneurship career. Professor Walt pioneered the use of microwell arrays for single-molecule detection and analysis, which has revolutionized the process of genetic and proteomic sequencing, enabling the cost of DNA sequencing and genotyping to plummet nearly a million-fold in the last decade. This technology is now the gold standard for sequencing in a wide variety of applications including screening embryos for genetic defects before in vitro fertilization, studying disease in preserved/frozen tissues, improving crop disease resistance, and identifying individuals’ metabolic profiles to ensure proper drug dosage.

SciX 2021 will contain scientific sessions and workshops covering all fields of analytical chemistry. The program theme in translating analytical sciences will run through the spectroscopy, biomedical, biopharmaceutical, chemical, polymer, and separation sciences technical oral and poster sessions. In addition to these exciting topics, SciX will host sessions on the topical themes of remote teaching chemistry, spectroscopy-based sensing for COVID-19, and sessions honoring some of the pillars of our field including Ramon Barnes, Bob Hannah, and Peter Griffiths. Workshops will complement the world-class technical program. Taught by experts in the field, introductory, advanced, and/or hands-on technical short courses will be offered onsite encompassing the areas of molecular spectroscopy, atomic spectroscopy, and multivariate analysis. Three exciting workshops will be offered for the first time this year: Innovations in Beer Quality through Instrumental Analysis, Grant/SBIR Writing, and 3D Printing. Space is limited for all workshops.

SciX is also the venue for a large number of internationally renowned award presentations. Unique to SciX is the Charles Mann Award for Applied Raman Spectroscopy, the FACSS Student Award, the Tomas B. Hirschfeld Scholar Award, and the FACSS Distinguished Award. The flagship FACSS award is the FACSS Innovation Award session, held on Thursday afternoon featuring a lively interactive format. Up to four abstracts will be selected based on novelty to compete in this session for the $1000 cash award. Previous winners have presented groundbreaking research in optical reflection and waveguiding of sound, infrared theory and instrumentation, portable spectroscopy, 5D single particle tracking in live cells, and inexpensive medical devices. What will be the groundbreaking innovations in 2021? Submit yours and come to SciX 2021 to find out!

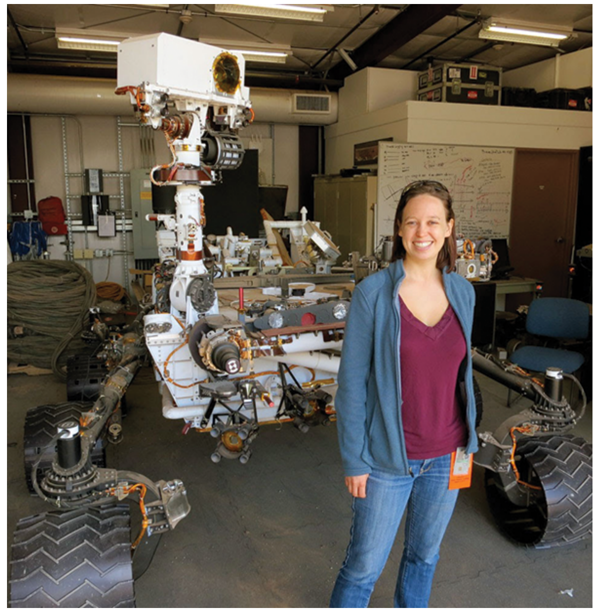
The Exhibits feature the latest in instrumentation from the leading vendors in the analytical sciences. Special events are designed to spotlight the important technology work of analytical vendors, bring attendees and exhibitors together for technical and networking discussions, and allow exhibitors to share their industrial perspective with the SciX community. We are pleased that the exhibit hall will also hold a career fair, a new vendor technology award, and a special session on entrepreneurship.

By design, SciX remains a great conference for students. We feature a large number of student awards, special conference hotel rates for students, the opportunity for travel grants, and networking events. There are also numerous volunteer opportunities that students can participate in to increase their involvement in the conference, as well as earn discounted registration.

As we think about what SciX looks like in the new normal, we draw upon our nearly 50-year history and remember why people attend SciX. We have built a meeting where we hear the world’s best analytical scientists exchange scientific progress, see the latest in technologies, and build our professional network. It is that combination that makes SciX a unique conference, and the experience simply cannot be replicated in a virtual environment. Thus, FACSS is committed to delivering an in-person SciX experience that you have come to expect.

We also recognize constantly evolving circumstances in the new normal, and the importance of flexibility to address these circumstances. We are continually monitoring travel alerts and working with partners towards minimizing the impact on our event, and we are preparing for a variety of scenarios for not only our annual meeting in October 2021, but year-round activities. We invite you to join us and set your science sailing at SciX 2021! To learn more about SciX, visit our website www.scixconference.org or follow us on LinkedIn.

Interview with Dr. Melissa Rice, Western Washington University



Melissa Rice, a planetary scientist at Western Washington University, stands alongside a Curiosity testbed rover at the Jet Propulsion Laboratory" (Photo credit: NASA / JPL Photo via WWU)

Dr. Melissa Rice (MR) is an Associate Professor of Planetary Science at Western Washington University, where she has held a joint appointment in the Geology Department and the Physics and Astronomy Department since 2014. Dr. Rice received her Ph.D. from the Department of Astronomy at Cornell University in 2012 and was a NASA Astrobiology Institute Postdoctoral fellow at Caltech from 2012–2014. Her research focuses on the sedimentology, stratigraphy and mineralogy of Mars. She is a collaborator on the active Mars Exploration Rover *Opportunity* missions, a Participating Scientist on the Mars Science Laboratory rover mission, and a co-investigator for the Mastcam-Z investigation in development for the Mars 2020 rover mission.

The interview was carried out by Michael Blades (MB) and took place on 19 March 2021. The interview has been lightly edited in the for clarity.

MB: What is your role on the *Perseverance* mission?

MR: On *Perseverance*, I have two distinct roles and one of them is as a co-investigator for the Mastcam-Z instrument, which means that I was part of the group of scientists who proposed the Mastcam-Z instrument, which was selected to be built and fly on the rover back in 2014. And as one of those co-investigators, I've been part of the Mastcam-Z investigations since the beginning. Very early on, right after we knew that the instrument was selected and we would be building this pair of cameras for *Perseverance*, we established a set of working groups among the team to divide and conquer the different aspects of what the camera investigation was going to be about. And so we have, for example, a stereo digital terrain modeling working group which has been deeply involved with developing tools for how we can take images from the two stereo imagers and create 3D models of the surface. Also, colleague of mine, Jeff Johnson and I, were tasked with leading the multispectral working group and so we have been leading the team in discussions about what the specific spectroscopic capabilities of Mastcam-Z would be, what kind of software tools we would need to do the analysis with the filter set once we got to Mars, what types of analyses we needed to do to make the best decisions about which specific wavelengths we wanted to build into the spectroscopic capability. Now we're spending a lot of time talking about what rocks on Mars we want to acquire multispectral images of—so that's a big role, a big part of what I've been involved with.

The other hat that I wear on *Perseverance* is called a long-term planner. And there was a group of us, about a dozen scientists, on the mission who are in this long-term planning group. We are the ones tasked with leading the team to decisions about not so much what the rover is going to do tomorrow or next week, but the big picture, where are we going to drive to over the course of the next month? What do we want to have accomplished a year from now and how are we going to achieve all of these objectives in what really is a very limited amount of time? So in that role, I make sure that the day-to-day activities match these big picture science objectives that we have for the mission. And when I'm on duty, in that role, I help lead discussions from the team about how we are going to implement our bigger picture goals and come up with that long-term plan for what *Perseverance* is going to do.

MB: So I have to ask, why is it called Mastcam-Z?

MR: It's because the predecessor for this instrument was called Mastcam, which is for the Mast Cameras. And those are the two stereoscopic, multispectral cameras that are on the *Curiosity* rover. Now, when we were writing the proposal for this next set of cameras that would go on *Perseverance*, they were as close to build to print as we could make them of the previous Mastcam cameras, but the big difference was that we wanted them to have a zoom capability. So, unlike Mastcam, which has essentially one of the cameras zoomed all the way in and one of the cameras zoomed all the way out, Mastcam-Z has two identical cameras that have a zoom mechanism in each camera. So they both can zoom all the way in and out. Because it was the zoom that was the big improvement over what came before, we started, just as a nickname, jokingly calling the new cameras, the Mastcam Zooms, and then Mastcam-Z wound up sticking.

MB: So is this an optical or digital zoom?

MR: Optical. And so this is why we didn't end up having a zoom previously because it's another motor—another moving part on each of these cameras. And anytime you introduce an additional moving part, that's a point of failure, something that can go wrong. So it's a big deal to have zoom lenses on the surface of Mars for the very first time.

MB: And I was about to ask you what's special about the cameras, but obviously the zoom is what's special about these cameras.

MR: The zoom is the big improvement, and the zoom was something that had been originally planned for *Curiosity*'s cameras, the Mastcams, but because of budget cuts and related to flight delays that zoom capability got "descoped". So, the desire to have zoom lenses on Mars has been around for decades, and we're just getting it enacted on Mars now.

MB: What are the primary science objectives for the cameras you've been talking about?

MR: We have a number of objectives and some of the most important ones are providing the geologic context for the landing site. Now, we have a number of instruments such as SHERLOC [Scanning Habitable Environments with Raman and Luminescence for Organics and Chemicals], which Luther Beegle is involved with, and PIXL [Planetary Instrument for X-ray Lithochemistry] instruments that are on the end of the rover's arm that are going to do very detailed characterization of the chemistry and mineralogy and the organics at very small scales. And ultimately, one of the major objectives of the mission is to collect rock samples that will eventually be brought back to earth. Mastcam-Z is intended to be a step back, a bigger picture view of the surrounding landscape and the objective is to provide the context that's going to help us understand where those rocks came from and what their depositional environment was once we get those rocks back here on earth.

MB: I read through an article in Space Science Reviews that was published recently, and it talked about the geologic diversity and the potential habitability of the field site, which implies that people are going to end up going there at some point or another. Is that part of the assessment using the cameras?

MR: Well, when we say habitability we're thinking about the ancient habitability of 3.5 to 4 billion years ago. Was this an environment on Mars that microbial life might have found habitable.

MB: Right. I see. Okay.

MR: Now paving the way for future human exploration at Mars is another objective of *Perseverance* more broadly, but we're interested in characterizing the surface environment of Mars more broadly and not necessarily characterizing this spot as a future human exploration site.

MB: There's also a Raman system and a LIBS system on the mast. Are those integrated into a single unit?

MR: Yeah, they are. A single instrument called SuperCam.

MB: Okay.

MB: And there's a LIBS, there's a Raman, and there's also a visible and near infrared spectrometer. And those are all using the same bore-sight, I believe. And so they can all do remote analysis. I think the Raman and the LIBS can observe rocks that are a few meters away. And then with the visible and near infrared spectroscopy, as well as the imager, there's essentially a telescope incorporated into that camera. We can see things that are several kilometers away.

MB: How did you get involved in planetary spectroscopy? Is that something you've always wanted to do or it came on one day, what's the story?

MR: I don't know that any small child says they want to be a spectroscopist when they grow up. If they do, I'm impressed. But what brought me here was an interest, first, in astronomy. That was my major in college, astrophysics. And then as I started doing my first research experiences in the larger field of astronomy, I kept finding that what was most interesting to me were the things that were closer and closer to home. So I started, in college, doing research on planetary nebulae. And what was the most interesting to me was research opportunities that I had to study the planets. And so I kept finding these interests that were a little more Earth-like, a little closer to home and then I realized that if I really wanted to study the planets I was going to need to essentially get another degree and become a geologist.

So I went to graduate school specifically to study Mars. And this was at the time when the Mars exploration rovers, Spirit and Opportunity, were having their heyday on Mars. And I wanted to be a part of that and to be part of a mission that was actively collecting data on the surface and be part of the team at NASA that was telling these rovers what to do every day. The science team was based out of Cornell University and that's where I decided to go to grad school and wound up becoming a PhD student of Jim Bell. And Jim, now 15 years later, is the principal investigator of Mastcam-Z and so that was my direct connection to become one of the co-investigators for Mastcam-Z.

MB: You must be pretty stoked.

MR: I am. Yeah. As a graduate student, I got to work with data from Spirit and Opportunity, but I just parachuted into that mission after those rovers had already been exploring Mars for two years. And now, this time around, I've been part of the development of this mission since it was just a twinkle in its father's eye. And we got to design the cameras from scratch, bringing in all that experience from Spirit and Opportunity. And so I've had a long, deep personal investment with these cameras for about a decade now.

MB: The paper I read was basically on calibration of the multispectral system and had 44 coauthors.

MR: Yep.

MB: How did you manage to work with so many people who were involved in that, especially during the time of COVID?

MR: Well, most of the work that went into that paper was done pre-COVID, very thankfully. We had a couple of furious weeks of calibrating those cameras at Malin Space Science Systems and we had a good number of us from the science team and a bunch of the engineers from Malin down in San Diego in-person. And there'd be a handful of people at a time in their full bunny suits in the clean room with the cameras, and then a couple dozen of us in a control room analyzing the data in real time, documenting every one of hundreds of thousands of images that we were taking for this calibration sequence. I can't imagine how that would have happened in a remote environment like we're in now, although we probably would've done that same work just over Zoom, like we're so familiar with now, but most of that actual work with the hardware and the planning and the operations of that calibration set of activities that, very fortunately, was all in person about a year before COVID hit.

MB: Okay. That's fortunate in some ways. You did say that you started in 2014, working toward this end.

MR: Right. By the time COVID hit, the cameras had long been delivered to JPL and integrated onto the rover already. And actually the rover at that time, by the time we all went into lockdown about a year ago, the rover had already been delivered to Cape Canaveral in Florida.

MB: So have any images come back yet? I mean, obviously I've been following the news stories about *Perseverance*, but have you got multispectral imaging?

MR: We have just a couple images with the full filter set of rocks on the surface. And those at this point have mainly been commissioning activities just to check out that our filter wheel is spinning and every filter is returning good data. And the vast majority of the multispectral images we've taken so far were of the calibration target. And actually just yesterday, we put out a blog post about all of these calibration images.

MR: Something that is brand new for this mission, being the zoom on the cameras, we need to figure out in large part with trial and error, which combination of zoom and focus settings are going to be the best for us to use on the calibration target. Every time we take an image of the surface of Mars, we want to take an image of the calibration target almost immediately before or after we take an image of the surface of Mars so that we can get spectra from the calibration target at the same time of day under the same atmospheric conditions. And so this calibration target here is going to end up being the most photographed object on Mars by the end of this mission.

About the spectroscopic capabilities of Mastcam-Z. We have eight filters in front of the camera optics, or rather behind the camera optics, so a big part of what we needed to decide in designing Mastcam-Z was what would the specific band centers of these filters be and what wavelengths of light would we tune these eyes to? And so Mastcam-Z has been specifically attuned to the iron oxides and distinguishing oxidized iron from reduced iron in minerals, and also to distinguishing the presence of hydration in different minerals. And so that's a big part of what's coming up next for Mastcam-Z, is using these cameras to help distinguish different types of mineralogy on the surface.

MB: So these are reflectance spectra, right?

MR: Right. Exactly.

MB: Okay. And they're using the sun as a source, is it?

MR: Yep. So, the sun is our light source. And so depending on what time of day we're acquiring these images, that's our incidence angle. And depending on the geometry of where the rover is and where it's looking on the ground, that's our admission angle. So we essentially have a goniometer on Mars where we can acquire a full suite of different viewing geometries. And with the CCD that's on the cameras, we're sensitive to about 1050 nm.

MB: And you said seven windows?

MR: We have eight windows in each eye and in each eye we've reserved one of those slots for just a clear filter and one of those slots for a solar filter. So we can look directly at the sun and do astronomical imaging as well. And so that leaves six filters in each eye, 12 wavelengths for narrow band spectroscopic imaging.

MB: Well, that's great. So you said that you were on a planning group. What do you see as the future for future Mars missions?

MR: For future Mars missions, well, the next step is very clear because one of *Perseverance*'s big goals is to prepare for sample return. Meaning *Perseverance* is preparing samples, it's extracting little rock cores, putting them into sealed sample tubes and leaving them on the surface of Mars but *Perseverance* isn't actually going to return those all the way to earth. So the next step in Mars exploration more generally has to be going back to the same site to pick up those sample tubes and then launch them back to earth. And then the next step after that is also very clear because we can't launch the samples all the way back to earth from the surface of Mars in one go. So it's going to require those samples being launched into orbit around Mars, and then a third stage in this sample return process grabs those samples quite literally from thin air in orbit around Mars and brings them all the way back.

MB: If you do obtain those samples, what would you learn about them that you couldn't learn from the robotic part of the mission?

MR: Yeah, that is the big question, why do we need to get these rocks back here on this planet to do the work we want to do? And the big things that we need to do are things that require bigger instrumentation and more involved sample preparation than we can do with a set of miniaturized instruments on the rover. We really want to understand the isotopic compositions and the rock. We need a big mass spectrometer. *Curiosity* has a mass spectrometer, but it's miniaturized. And we really want to get a much higher precision than we can with *Curiosity*'s mass spec. We also want to do things like scanning electron microscopy, and other analytical techniques that are going to require just bigger instrumentation and also more advanced instrumentation. The time frame for getting an instrument to the surface of Mars? I said Mastcam-Z, we were laying the blueprints in 2013, 2014 and so all of our instruments that are on *Perseverance* are almost a decade old now, their technology is. So if we want to keep pace with technology, we need to be working with rocks here on earth, because everything we send to Mars is always obsolete by the time it lands on the surface.

MB: That's interesting. Okay. I don't want to use up too much of your time. I'm sure you're very busy, but I was curious, just to finish up with, what do you do in your spare time when you're not heavily engaged in this mission? And I guess you also have a position at the university and you teach and so on, so how do you relax?

MR: Well, when there's not a global pandemic going on, I travel. And that's been hard this year, but when the weather has been nice I've been enjoying taking road trips and camping and getting to know my backyard in Western Washington here. I'm an avid hiker and backpacker and have been becoming a kayaker as well. And I think it's not a coincidence that I wound up in a landscape that is as different from Mars as you can get. I sought out rain and green and water and lush landscapes. It was bizarre when I was working at Caltech, which is a desert arid landscape and studying very similar looking landscapes on Mars, and then coming home to the same landscapes, I find it very refreshing to go outdoors in the Pacific Northwest and be in a very non-Mars like world.

MB: Thank you very much Dr. Rice.

May 2021 Focal Point Overview

"Can I See Your Passport Please?" Regulating and Protecting Cells at Their Borders
Michael Blades

Regarding the May 2021 Focal Point Review, “Single-Molecule Fluorescence Techniques for Membrane Protein Dynamics Analysis“

I live 50 km from the US–Canada border. Before COVID, 300,000 people a day crossed the border between the USA and Canada. Every one of those people were stopped at the boundary to be interrogated by an immigration/customs agent. Their purpose is to check permits and allow the flow of people and goods and to prevent the movement of undesired people and illicit goods between the two countries.

Like the borders between countries, the boundary between the inside and outside of the cells of our bodies acts as a barrier that both facilitates and prevents movement of material back and forth across it. The immigration agents are membrane proteins that sit at the border and decide on what goods can pass across and what is denied.

These membrane proteins represent over a third of all the proteins in our bodies and are targets for a large number of therapeutic drugs. Membrane receptor proteins bind to external ligands causing a conformational change that allow the movement of ions (e.g., Ca^{+}) small molecules (glucose, amino acids) and proteins that are vital for the functioning of the cell, and our bodies, through the membrane. Membrane proteins can also act as binding sites that are used by viruses to invade cells. For example, the deadly COVID-19 virus that has plagued the world for the past year, gains entry to cells through its’ spike-protein that binds to a membrane receptor protein called ACE-2 [Front. Cell. Infect. Microbiol., 05 June 2020; https://doi.org/10.3389/fcimb.2020.00317]. It gains entry using a “fake” passport. The study of membrane proteins is critical for better understanding how viruses infect cells and how drugs can be designed to prevent them from doing so.

> “The powerful ability to discriminate subpopulations with different FRET efficiencies and to display the time trajectories of dynamic events has made it an elegant tool to analyze biomacromolecule structures”.

Professor Meiping Zhao, Peking University

In the feature article in the May 2021 issue of *Applied Spectroscopy*, “Single-Molecule Fluorescence Techniques for Membrane Protein Dynamics Analysis“, Meiping Zhao and members of her group in the College of Chemistry and Molecular Engineering at Peking University, review how one can better understand the movements of the cells immigration agents using state-of-the-art spectroscopic methods like fluorescence correlation spectroscopy (FCS) and single-molecule fluorescence resonance energy transfer (smFRET). These methods are used to study the dynamics of conformational change, the movements, in membrane proteins.

Professor Zhao is a full professor at Peking University. She has served as an Associate Editor for *Applied Spectroscopy* and is currently on the Editorial Advisory Board.

Dr. Zhao and her group also published the Focal Point Review, “Nucleic Acid Fluorescent Probes for Biological Sensing”, in *Applied Spectroscopy* in 2012 [Appl. Spectrosc. 2012. 66(11): 1249–1262; doi: 10.1366/12-06803].

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 luisaprofeta@gmail.com.
