SPIE.DCS Next-Generation Spectroscopic Technologies XIV

Join SAS members virtually starting 12 April 2021 for the Next-Generation Spectroscopic Technologies XIV conference at the SPIE Defense and Commercial Sensing (DCS) meeting. For a full list of talks at the meeting and to register, please follow this link.

April NJ/NY SAS Monthly Meeting

Please join us on 29 April 2021 at 12:00pm EDT for an exciting virtual presentation by Peter Larkin, PhD, from Cytec/Solvay Research Labs in Stamford, Connecticut.

The title of his presentation is, "At-Line Reaction Monitoring of a Water-Soluble Polymer with a New Generation Raman Spectrometer: Circumventing Fluorescence and Developing Robust Chemometric Analyses".

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MS Teams Link

About the Speaker

Peter Larkin received his PhD from the University of Pittsburgh in 1990 from Sanford Asher employing resonance Raman and vibrational circular dichroism to study heme proteins. Since that time, he has worked in analytical departments both in the specialty chemical and pharmaceutical industries using vibrational spectroscopic techniques to solve industrial problems.

While at American Cyanamid/Cytec Industries Stamford, Connecticut, labs, Peter received comprehensive training in the IR interpretation of a wide variety of structural problems in organic and polymer chemistry from Dr. Norman B. Colthup. He subsequently worked at Wyeth Pharmaceutical at Pearl River, NY, had a brief stint with Pfizer in Groton, Connecticut, a rewarding and productive tenure at Bristol Myers Squibb in New Brunswick, New Jersey, and returned back to where he started at the Cytec/Solvay research labs in Stamford, Connecticut. Peter presently leads the spectroscopy, thermal analyses, and chromatography groups there and continues to focus his efforts on vibrational spectroscopy. He has published and presented extensively and his book, entitled *IR and Raman Spectroscopy: Principles and Spectral Interpretation*, second edition (Elsevier) was published in November 2017.

Peter has been a long-time member of both the Society of Applied Spectroscopy (SAS) and the Coblentz society. He has served on the Megger's Award committee (2012–2013, Chair 2013), Lester Strock Award committee (2016–2017, Chair 2017), the William Wright Award committee (2019–2020, Chair 2020), the Coblentz Society board of managers (2019–present), as a delegate at the SAS governing board meeting (New England section representative 2019, 2020 and 2021) and as a secretary for the New England SAS section (2020–present).

For additional information please see my LinkedIn profile, or contact John.Wasylyk@bms.com

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Upcoming Mars Interview Features in the SAS Newsletter and Website!

On 18 February 2021, the NASA Perseverance rover gently touched down in Jezero Crater on Mars. NASA scientists believe that 3.5 billion years ago the area where the crater is located was filled with water, a lake

about the size of Lake Tahoe, which created an ancient river delta. According to NASA, the Perseverance mission is to "seek signs of ancient life and collect samples of rock and regolith (broken rock and soil) for possible return to earth".

Central to the Perseverance mission is an array of spectroscopy instruments that have been designed to "survive" the landing, stay aligned, and function in the harsh Martian climate which can have daily temperature extremes of –70 to +20 C. The instruments are marvels of science and engineering.

High atop the Rover is "SuperCam", a remote analysis instrument consisting of Raman and LIBS spectrometers that allow soil and rocks to be sampled and assayed at a distance. Just below SuperCam is the Mastcam-Z, a stereoscopic camera that can be zoomed and is designed to take hyperspectral images of the Mars surface and atmosphere at different wavelengths. At the end of the Perseverance robot arm is the Scanning Habitable Environments with Raman and Luminescence for Organics and Chemicals (SHERLOC) instrument. SHERLOC is a combination fluorescence and UV resonance Raman spectrometer whose function is "fine-scale detection of minerals, organic molecules, and potential biosignatures". Adjacent to SHERLOC on the robotic arm is an X-ray spectrometer called PIXL, which will be used to "measure the chemical makeup of rocks at a very fine scale". Five spectroscopy instruments mounted on a roving platform have brought the laboratory to the sample —255 million kilometers from Earth!

Behind each of these instruments is a team of scientists with many years of spectroscopy experience. Over the past two decades many of these scientists, some members of the SAS, have published papers in Applied Spectroscopy and other journals describing the design and testing of components and concepts that have led to these instruments being deployed on Perseverance (see the SAS collection of Mars papers).

We have decided to highlight the contributions of a few of the hundreds of scientists who are members of the Perseverance mission through their involvement with the instruments mentioned above. Accordingly, we have interviewed Roger Wiens (Los Alamos National Labs, Supercam Principal Investigator), S. Mike Angel (University of South Carolina), and Shiv Sharma (University of Hawaii), members of the Science team for the Rover SuperCam instrument; Joseph Hollis (postdoctoral scholar in the Planetary Sciences Section at JPL), who works on the SHERLOC instrument; Sandy Asher (University of Pittsburgh), a principal in the design of the SHERLOC spectrometer; Melissa Rice (Western Washington University), a principal member of the Mastcam-Z team; and Abigail Allwood and Christopher Heirwegh, members of the PIXL team. We will be publishing these interviews in the Newsletter and on the SAS website and highlighting their roles in the mission and identifying key publications that are the foundation of the exciting science currently taking place on Mars.

Stay tuned for these interviews in future issues of the newsletter and on the SAS website!

Michael Blades
Luisa Profeta
Adam Hopkins

Interview with Dr. Sandy Asher, University of Pittsburgh

Our first interview was with Dr. Sandy Asher, a Professor in the Chemistry Department at the University of Pittsburgh. Sandy received the Chancellor's Distinguished Research Award at the University of Pittsburgh in 1996, the Bomen-Michelson Award of the Coblenz Society in 1998, and the American Chemical Society Pittsburgh Award in 2003. Sandy is a pioneer in the development and application of ultraviolet resonance Raman spectroscopy for analytical, physical, and biophysical chemistry. He is also an honorary member of the Society for Applied Spectroscopy, a recipient of an SAS Fellows Award and a regular contributor of cutting-edge research papers in *Applied Spectroscopy*.

Sandy (SA) was recently interviewed by Michael Blades (MB), Editor of *Applied Spectroscopy*. The following is an edited version of that interview.

MB: Thank you for taking time from your busy schedule to talk to us about your connection to the current Perseverance mission. Can you tell is a little bit about your role on the SHERLOC team.

SA: Basically, we've been working for a very long time in developing UV Raman methodologies to study protein structure and function and a little bit of nucleic acid studies. So, we've had a long-term interest in this. One of the things that was required was developing new UV sources and that's something my lab has been very active in, and we've also been entrepreneurial looking for opportunities to build UV lasers and finding ways to fund deeper UV lasers for Raman. That's been an activity where I've interacted a lot with some of the people in SHERLOC, and especially with Bill Hug from Photon Systems, who developed the first robust deep UV laser source. In fact, he and I collaborated, wrote some papers together, and talked about what opportunities exist for UV lasers. That's been my major interaction.

It turns out that I had a postdoc who's quite interested in meteorites and things like that, and so, because of his particular interest, we found that the UV Raman measurements of meteorites were easy to obtain and that they also had a lot of information content. This gave some real opportunities and we never worked in this area very seriously, but we demonstrated proof of concept. So, basically, as time evolved and people thought about

putting a UV Raman instrument on a Mars lander or rover, this became more and more serious—it nucleated and grew. I was asked if I was interested in somehow participating. Of course, I was interested, but at the same time, my interest was finite in this area. I think one of the things we did was we kept track of who worked in UV Raman and its applicability to the SHERLOC work.

MB: You said [in a separate interview] that you'd always been interested in looking up at the stars, and so on, when you were a young child and so you were pretty excited to participate.

SA: Actually, that's absolutely true.

MB: Yeah. I think most of us did. Your contribution is related to the UV resonance Raman system/fluorescence system, so I imagine that there is interest in looking at aromatic amino acids and nucleic acids on Mars as a probe of life. Is that right or is that hoping for too much or is that it's primary function?

SA: It's probably all of those things. It's almost certain that life on Mars evolved separately. If it didn't, that's going to be very exciting. Whether it's going to be carbon nitrogen based, it's really unknown. We will look for materials that could be the basis of life that maybe we've seen before or have never seen before. We don't know where it's going to be. As I look at the pictures coming from Mars, it looks pretty desolate to me. And so, [chuckling] there's not a lot of bars open with little green ladies and men having drinks.

MB: Those scenes from *Star Wars*!

SA: That's right. So maybe we have to wait a little bit.

MB: I'm assuming that you participated in some way, as you said earlier, in the design of the spectrometer, or at least had some input into the design. There must have been some special design considerations that went into that. So how is it different from one on Earth? I mean, to ruggedize, I would think for one thing.

SA: Well, ruggedize is everything. Basically, what you need is a UV Raman instrument that can cycle down to liquid nitrogen temperature up to room temperature and stay aligned. I have trouble keeping them aligned on an optical table, floating on nitrogen. So, to ask it to bounce off Mars a couple of times is a big deal. And one of the things that was so important in SHERLOC was the fact that Bill Hug's laser had the capability of being able to stay aligned. And that's what really was the big enabling feature, I think. I could be wrong about this. So, you should ask other people as well.

MB: Anything else you wanted to say you think the people, readers, *Applied Spectroscopy*, and people in general would like to hear or know?

SA: Well, I mean, spectroscopy is moving out the frontiers or moving out. There are lots of advances. The Mars trip looked so easy that there's going to be a lot more searches for life on other planets.

MB: Yeah. It really is a profound technical achievement. I mean, it's just amazing and spectacular that you can, with such accuracy and precision, put something down on a planet and have it run the way it runs on Earth.

SA: It's amazing.

MB: Yeah. I know, it is, especially since you've got 14 minutes between sending and receiving, so you don't really know what's going on for 14 minutes.

SA: That's right.

MB: It's pretty astounding, really. So, I mean, when you go to sleep at night, you must be pretty satisfied with your contribution to that.

SA: Well, we've got pretty good rocket scientists too! [smiling]

MB: Yeah. I know. I'm talking about the whole project. And one of the things I'm trying to do is get some feel for the scope. I've seen interviews with individuals, but I haven't really gotten a feel for the scope, how many people are involved?

SA: There are hundreds, and it depends. "Involved" is a funny term. I mean, some people are really interested in particular issues of taking photographs of a particular resolution and adding to that other measurements of physical properties, combining them to get insight into the planet on Mars itself. Other people are more engaged in engineering. Some people are interested in the science, a small cadre of people. And it's an interesting human part of this to see who's involved, what their questions are, how can they start to work together. Most of these people never really worked together very much before. And I'm playing a very small part of this.

MB: Well, you have a strong connection to this society and to the journal. And I mean, that's one of the reasons we wanted to talk to you because you have your foot in both sides. And we wanted to talk to people who were involved in the mission and knew something about the mission, and contributed to the mission but also had a strong connection to the society as well so we can feature that part of it. So, this is great that you've spent some time with me. Thanks very much.

SA: Let me just mention something else. One of the other challenges in looking for life or the looking for the chemistry of Mars is that it has been bombarded with solar wind for billions of years. And this solar wind is not redirected because Mars doesn't have a significant magnetic field. And so, basically, there are some people who think that Mars is just a fully oxidized planet and so, if you really want to see what was on Mars at some

geologically relevant time period going back, you probably have to dig, and we have that capability at SHERLOC to drill some holes. So, you drill a hole. If you can put the laser beam down there and collect the scattered light, and there's so many things you don't know yet. The excitation wavelength that was chosen for the SHERLOC Raman spectrum is probably not the perfect wavelength. The choice was what was available from the Bill Hug's enabling laser.

MB: Right. It was around 250 if I remember, somewhere in that range.

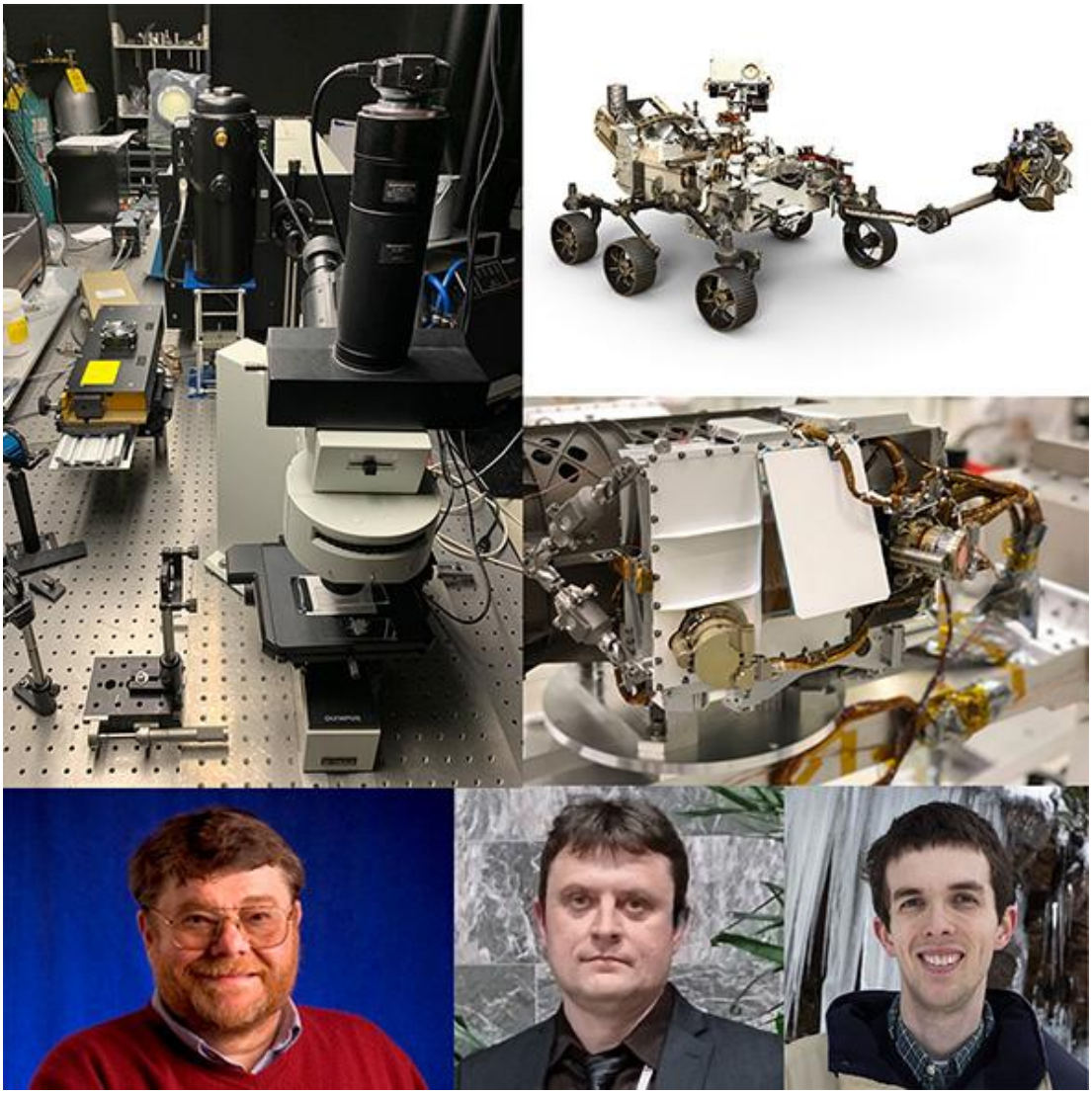
SA: Yeah, something like that.

MB: I hadn't really thought about that. I guess I imagined that there was some single cell organism that washed down the river and fell on the soil and sat there for the next two or three million years, if not a billion years, and then you just find it and you get a spectrum from it. Hey, are the rest of us going to get to see the spectra at any point or another?

SA: There's a process by which information is shared within the community working on it and then further out. There's a lot of attention to how do you do that efficiently and how do you make sure that the science wins. If we've discovered something, we should talk to more senior people involved to make sure it's transmitted in a reasonable way. But everything, it's all open. Unless the Martians have developed new weapons we've not heard about, I don't think there's anything classified.

MB: Yeah. Okay. That makes sense. All right. Well, I'll look forward to it. Thank you so much again.

Note: See, M.C. Sparrow, J.F. Jackovitz, C.H. Munro, W.F. Hug, S.A. Asher. "New 224 nm Hollow Cathode Laser–UV Raman Spectrometer". *Applied Spectroscopy*. 55(1): 66–70, for a seminal paper describing the deep UV laser similar to the one discussed by Sandy in the interview.



Clockwise from top right: SHERLOC on the extended arm of the Perseverance rover; close-up view of the SHERLOC instrument at JPL; graduate student Ryan Roppel; Research Assistant Professor Dr. Sergei Bykov; Distinguished Professor Dr. Sanford Asher; SHERLOC-like UV Raman microscope utilizing a Photon Systems 248 nm laser in construction in Asher lab at Pitt. Rover and SHERLOC photo credit: NASA/JPL-Caltech.

ABS Trust: 2022 Gordon F. Kirkbright and Edward Steers Bursary Awards for Promising Early Career Scientists

The Gordon F. Kirkbright bursary award is a prestigious annual award that assists a promising early career scientist of any nation to attend a recognised 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 able to award an annual 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 an untenured academic post or in industry, within seven (7) years of award of PhD excluding career breaks. The same conditions apply to each bursary.

Applications are invited for both the 2022 Gordon Kirkbright Bursary and the 2022 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 here.

For further information visit: http://www.abstrust.org/, or contact abstrustuk.kirkbright@gmail.com.

The closing date for entries is 30 November 2021.

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www.SciXconference.org

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.

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