July 2021

2021 SAS Officer and Governing Board Election

The Annual Election of SAS Officer and Governing Board Delegates has started and will be available for all members in good standing to vote between 21 June–23 July 23 2021.

Those eligible to vote will receive an email with voting instructions and login information from our online election provider Elections Online. Please check your spam folders for this email. If you do not receive it, please contact the SAS office at sasadmin@s-a-s.org or 301-694-8122.

Click here to read candidate profiles.

Third Summer Wiley and SAS/Coblentz Webinar

The third seminar in the Wiley-SAS collaborative series will be held on 22 July 2021 at 9.30am EST, 2.30pm BST, 3.30pm CEST. Registration for the webinar can be found here. The following speakers and topic areas will be discussed:

Dave Schiering, RedWave Technology: Portable IR
Shawn Chen, Dow Chemical: Industrial Applications
Richard Crocombe, Crocombe Spectroscopic Consulting: Counterfeit Pharmaceutical

---

Award Announcements from SAS Technical Section: The Coblentz Society

The Coblentz Society is pleased to announce that Professor Dr. Sandra Luber of the University of Zurich has been selected as the recipient of the 2021 Coblentz Award. The Coblentz Award is presented annually to an outstanding young molecular spectroscopist and is the Society's original and most prestigious award. Due to complications arising from the COVID-19 situation, the date and place of the award presentation has not yet been determined. To read more, visit https://www.coblentz.org/awards/the-coblentz-award/.

As a reminder, the 2020 Coblentz Award was presented to Dr. Benjamin P. Fingerhut of the Theory Department, Max Born Institute, at the 2021 International Symposium on Molecular Spectroscopy (ISMS, https://isms.illinois.edu/). ISMS was virtual, and the award was presented on Tuesday, 22 June, followed by Dr. Fingerhut's plenary award lecture "Noncovalent Interactions of Hydrated DNA and RNA Mapped by 2D-IR Spectroscopy".

The 2021 winners of the Coblentz Student Awards are Isabella Goodenough (Eric Borguet, Temple University), Paulina Koziol (Tomasz Wrobel, Jagiellonian University), and Chris Warkentin (Renee Frontiera, University of Minnesota). Pauline Koziol has also been recognized with the 2021 William G. Fateley Student Award. Watch for our July Newsletter for more details. Congratulations to all our student awardees!

Call for 2022 Award Nominations

2022 Coblentz Award

The Coblentz Award is presented annually to an outstanding young molecular spectroscopist under the age of 40. Nominations for the 2022 award are due by 15 July 2021. More information may be found on the Coblentz Society's website.

2022 Emerging Leader in Molecular Spectroscopy Award

Selected by an independent scientific committee, the Emerging Leader in Molecular Spectroscopy Award recognizes the achievements and aspirations of a talented young molecular spectroscopist who has made strides early in his or her career toward the advancement of molecular spectroscopy techniques and applications. The winner must be within 10 years of receiving their Ph.D. The submission deadline for the 2022 award is 3 December 2021.

New Coblentz Society Website Launched

The new Coblentz Society website (Coblentz.org) went live the week of 7 June 2021. A tremendous thank you goes to Mary Carrabba for all the hard work she put into it. We hope that Coblentz and SAS members find the website useful and easier to navigate compared to our old design. We do ask members to help us populate it with new content, and we need to maintain the site. Anyone interested in helping with either of these efforts should contact Mary Carrabba or Ellen Miseo.

Next NY/NJ SAS Regional Meeting

July 21st at noon

Join us for Part Two on SERS. This will be an exciting set of two presentations.

Professor Amanda J. Haes, Ph.D. from the University of Iowa.
Title: "Nanoparticles for SERS – From Stability to Beyond"

Lamyaa M. Almehmadi, M.S. from the University at Albany, SUNY, Lednev Laboratory.
Title: "SERS for Single-molecule Detection, a Tool for Developing New Technologies"

Perseverance Mars Mission Interview: Abigail Allwood and Chris Heirwegh

The Society for Applied Spectroscopy is pleased to present this interview with Abigail Allwood (AA), an Australian geologist and astrobiologist at NASA Jet Propulsion Laboratory (JPL) who studies stromatolites, or [the] layered sedimentary formations that are created by photosynthetic cyanobacteria, detection of life on other planets, and evolution of early life on Earth. Chris Heirwegh (CH), is a Canadian scientist working at NASA JPL whose expertise is in fundamental physics of X-ray fluorescence, spectroscopy, and ion-beam analytical techniques. Both are involved in the Planetary Instrument for X-ray Lithochemistry, which goes by the acronym PIXL. The interview was carried out by Michael Blades (MB), Editor of *Applied Spectroscopy*. The transcript has been edited for content and clarity.

MB: Thank you to you both for joining me today. You both must be very excited since February 18th, when the first *Perseverance* "touched down." Things seem to be going very well. I wanted to ask each of you about your roles in this mission.

AA: I'm the principal investigator for PIXL. I was responsible for development and delivery of the instrument to the Rover. Now I oversee PIXL's functioning and investigation on the surface of Mars, as well as get involved in the general science decisions (when I get a chance!) and data interpretation.

CH: My role is working on elemental calibration of PIXL. When PIXL starts doing its work and measuring rocks, it's going to return lots of spectral data. My job is to convert that data into elemental weight percentages of the composition of the rock, then informing geologists, astrobiologists what that rock is made from. If there are potential chemical signatures, bio-signatures, that might be in the rock, being able to distinguish those, and give quantities of elements that might be in the signatures, because those can be useful tools to tell what has happened to that rock through its history.

MB: OK, there are two facets here. One is the geology that people are interested in and the other is the technology that's being used to study that geology. So, tell me about the interest in the geology.

AA: I am a geologist and astrobiologist first and foremost. Compared to most principal investigators, I think that makes me a bit of a black sheep because I'm more like a user of the data that is produced by PIXL rather than an expert in the development of the instrument or the measurement technique. I leave that to Chris and Tim. I am their very, very, ultimate picky customer.

I started using micro-XRF, a commercial lab instrument, over a decade ago to investigate stromatolites, a kind of biosignature created by microorganisms. It turned out to be incredibly powerful for revealing tiny, texture-specific compositional variations in the rocks, and thought it would be a great tool to have on Mars.

PIXL doesn't really have an analogue instrument on earth. There was never a micro-XRF that we could take into the field. So, apart from converting a hefty, power-hungry, liquid nitrogen-guzzling, possible-to-fix-when-it breaks lab instrument into a lightweight, low power, highly robust flight instrument (which was hard enough!)—more fundamentally, we also had to think about the science of how we would use it "in the field", which had never been done before. So, it's a really weird situation to be in. It's also very, very exciting.

MB: I'm sort of somewhat familiar with XRF [X-ray fluorescence] and PIXE [proton induced X-ray emission], but tell me about this particular instrument.

CH: Sure. This instrument doesn't use any of the PIXE components, so there are no charged particles like we had with alpha-particle X-ray spectrometers used in the previous missions. This is 100% XRF. It actually utilizes an X-ray tube design that would be not too different from what you would find in a dental X-ray unit. We have the benefit of making use of the very light Martian atmosphere, which allows us to see more elements down to some of the other major constituents that are found in rocks that we couldn't necessarily see as easily on Earth if we just took a similar instrument out to the field. That sets another advantage [because of atmospheric absorption]. If we were to do a similar measurement on Earth, we would miss a few key elements. So, Mars is actually a really good ground area for us to do this sort of work.

AA: It's interesting too that PIXL, as it is, can't be picked up from Mars and taken and used directly on any other planet. On Earth, for example, you've got one atmosphere of pressure for electrical insulation; that makes the high voltage needed to power the X-ray tube easier to do. Likewise, the vacuum, if you go to an asteroid or the moon or just out into space, that's insulating too. But the Martian atmosphere is a unique thing—it's about the worst possible scenario for electrical insulation. So, PIXL uses a design that is unique for Mars, but is not directly translatable to any other planet. You would have to basically start from scratch.

CH: That's right. That was a part that I always found fascinating how the Martian atmosphere is actually pretty volatile at high voltage. That just the very nature of the exact pressure and the gas composition, mostly CO2. It represents a real instability point for operating [at] high voltage. So, it has to be really expertly insulated and sealed in our power supply. That represented a pretty huge engineering challenge.

AA: It was threatening to be fireworks on Mars!

MB: I have a friend who's in charge of an X-ray crystallography lab at UBC [University of British Columbia] and his instruments are the size of my kitchen stove. I'm looking at the instrument at the end of the robotic arm. How did you do that?

CH: That sort of design part predates my arrival to JPL, but really I think it just took a lot of different expertise at JPL to put together such a compact system. So that's probably something Abby can speak toward maybe a little better than I.

AA: The mechanical design of the instrument was an incredibly long and difficult process. Reducing the volume to fit to the available space out on the rover's arm was just one aspect. We had to start with a miniature, micro-focus X-ray tube from Moxtek, Inc. and a polycapillary focusing optic from XOS. Those were the enabling technologies at the heart of PIXL. Fortunately, they were already small and robust. We had to modify the X-tray tube to make it a side-window design as opposed to an end-window, which was going to make the X-ray path a bit too long. That pushed us into what turned out to be the extreme cutting edge of X-ray tube design! But fortunately, it all worked out.

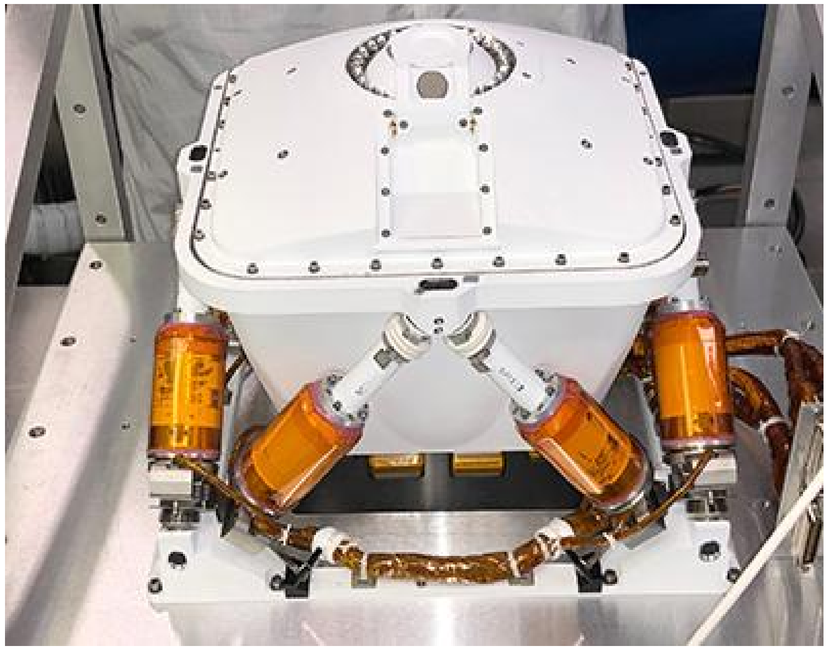
As well as reducing the volume, we had to make it very robust because, for example, if you break one of those little beryllium windows, that's it—you're stuck. There wasn't much room for redundancy because again, trying to fit into such a small envelope prohibited that. In the end, we built something that went from about, I think, a 60 kilogram beast that's as big as your stove, plugs into a power outlet, has a big appetite for liquid nitrogen, and which relies on [the] provision of a flat geological sample being placed on a scanning stage at just the right standoff distance, etc., to something that is about 20 centimeters cubed, operates off the power of a light bulb, doesn't rely on a human maintenance crew, and scans the instrument relative to the stationary target. And that was just the start.

Perhaps our greatest challenge wound up being positioning and placing PIXL. We couldn't rely on the robotic arm to do the movement because you need such fine-scale movement, consistent placement, and steady positioning. The X-ray beam is only 100 microns in diameter, then you have to move that in tiny 100 μm steps. And that's pretty difficult for a two-meter-long arm with a 100-kilo weight on the end. We ended up inventing the hexapod, a positioning device with six struts that go on the outside of the instrument sensorhead box. By extending and contracting, they effectively enable the instrument head to be scanned across the surface in *x* and *y*, and also to be placed at very precise *z*-distance from the target as well.

CH: And it comes down to using some fairly sophisticated mathematics and computer algorithms to get all six of these struts to start to move together, to just give us a nice uniform scanning pattern, line by line by line.

MB: Have you gotten any data back yet from the PIXL spectrometer?

CH: We have oodles of data from pre-launch. So, we've seen how it performed and it performed really quite beautifully. I mean, making the steps very nicely. The data from Mars so far is pretty limited. We are not quite at the stage of exercising our legs. Some of the other instrument checkouts are still going on, but we do have some data just from the X-ray tube itself. Mostly we're just seeing that everything there is working okay. We took a measurement of the inside of the cover door, nothing too interesting, but it tells us that the spectrometer is working exactly as we thought it should.



PIXL's sensor head before being integrated with the robotic arm at NASA's Jet Propulsion Laboratory in Pasadena, California. In this image, four of the six legs of the sensor head's "hexapod" are visible. The adjustable legs of the hexapod allow minute adjustments so the sensor head can point its X-ray beam exactly at tiny structures in the rocks on Mars. Credit: JPL/Caltech https://mars.nasa.gov/mars2020/spacecraft/instruments/pixl/

MB: It's on the opposite side of Sherlock, is that right on the robotic arm? So, you had to work together with the Sherlock group to talk about placement and who's going to do what, when?

AA: All the instruments must operate separately, so we all work together to figure out what to do and when.

MB: Whenever I see X-ray florescence data from a place like Mars, it's always elemental ratios. Does that have to do with calibration? Or is there something intrinsically interesting about the ratios? Or is that a different question?

CH: It's probably more of a geologist's question to answer. The ratios are probably a little more strongly correlated to mineral and rock identification than just knowing what the element concentrations are themselves. So that is coming at it as more of a physics, spectroscopist point of view. That's something I've just kind of learned through osmosis working with many geologists for a few years; they really do like to look at ratios of this element to that element.

AA: We are going to use all sorts of different ways to look at the data with PIXL. Elemental ratios are one of them, but more exciting and less well known are the elemental maps. It will be like having thin sections and a microscope in the field.

CH: That's one of the real powers of PIXL, the two-dimensional, spatial ability to look at the composition of the rock. The two-dimensional map is almost like a contour map, something that could not be realized with any of the other [Mars] spectrometers.

MB: I was wondering about, for example, the strange green rock has been in the news lately. This strange green rock that has LIBS holes in it already. So, I assume they've been looking at the elemental composition of it. How does PIXL, the PIXL team and the spectrometer work together with all the other spectroscopic systems? There are five spectrometers in total. Well, I include the Mastcam-Z as a spectrometer. How do you work together with everybody? One person wants to go over and look at the green rock and then someone else wants to go over and look at the turquoise rock... Who decides what to do?

AA: It's all theoretical at the moment because our PIXL's not actually running; we are actually the last instrument to be deployed. Instruments have to go through a lot of checkouts just to make sure that everything's working properly before you go deploy it to do science and PIXL is the last instrument to finish going through that. But this was all part of the plan that our checkouts would not complete until well after the helicopter test flights, which require a lot of data downlink volume.

MB: I hadn't thought about the bandwidth of data going back and forth.

AA: Yes, it is a little frustrating having to wait, but the good thing is there's a sort of sense of anticipation of PIXL getting some data down, but that's not going to be for a while yet.

MB: I'm still curious about once it does get up and running and how, or what to do it, there's a lot of people who want to shine light at material up there. So, who decides how to proceed? Is it a big team, a planning team?

AA: It is a big team and that might make it sound more difficult. But I don't think there's any sense of like, "mine is going to have to go first." Or, "my instrument is going to find the evidence that we need". There is not going to be any sort of single smoking gun that one instrument is going to find that constitutes evidence of life or anything else. It's going to be assemblage of evidence. Like here's an environment that was seen yet over here and it's all going to be contributed to by every single geological instrument on the *Rover*. So that's how we all help each other. There's no sense of "we want to get out there first".

CH: I was also thinking earlier too, and Abby correct me if I'm wrong, but some of the instruments like SuperCam are going to be able to scan a little more readily anyways, because these are more remote-scan instruments while our instrument is a contact science instrument. It takes a few extra Sols really for the team to plan if we find something interesting like taking an image, to know where we're going to measure on the next Sol, then we're measuring. And then on the next Sol all after that making decision on whether or not we like our data. It takes a little more time to do all that. So PIXL might not be deployed as much as let's say SuperCam.

AA: SuperCam I'd expect would be doing dozens more experiments in a given area or a given timeframe than PIXL would be. PIXL's going to be fairly resource intensive.

CH: Actually, that gets back to one of the earlier challenges Mike had mentioned too. If we are hoping to, get at minimum a postage-stamp sized map, mission constraints and practicalities of getting data on, say days that are very warm, could limit operation time. Which means if our instrument is in danger of heating, you can't run as long. We might have to settle with a much smaller map or maybe just a sparse grid, spotty map data set. So, there's a lot of practical considerations that I've learned on this team over the past couple of years that we're going to be working through when we start taking data.

AA: We have our version of quick draw or shotgun approach, but it's not going to be as fast as SuperCam or Mastcam-Z.

MB: I was wondering, what do you see as the next step? The next Mars mission, what's going to be different on that one compared to this one?

CH: There is not really a next *Rover* type mission being planned at present. The next big mission would be the sample return mission. One of the big aspects of 2020 is to go around collecting samples, caching them, and eventually storing them at one, maybe two depot locations where a potential future lander might come pick all this up and bring it back to Earth. This would be the first Martian material that we would have on Earth, other than Martian meteorites, which are highly altered and not necessarily as indicative of the natural surface as these samples would be. So those samples would be brought back sometime around 2026, 2028, and measured in labs around the world, probably to figure out what is what. As far as XRF on Mars, it's hard to say what that future is. Could be XRF on another planet, for example.

AA: It could be XRF toted by helicopters.

MB: Briefly, how each of you became involved in this project. Did you, for example, Abigail, when you were a little girl, did you say, "Oh, I want to explore Mars".

AA: I did my graduate thesis project, out in the Pilbara region of Western Australia studying stromatolites. That culminated with a paper in *Nature* in 2006 that's based purely on the field evidence claim argued that these stromatolites were actually biologically formed. But Harvard paleobiologist Andy Knoll said, "if they are microbial, where is the microbial scale evidence?" I came across Horiba XGT for the first time at Penn State University where Hiroshi Ohmoto was using it to map the elemental chemistry of some drill cores. By chance, there was one at JPL and the owner of it, Mark Andersen, allowed me access to it during my postdoc. It ended up providing some really unexpected, amazing insights, just totally out of left field. It really kind of nailed that microbial scale evidence and that wound up being published in a paper in 2009 (DOI: 10.1073/pnas.0903323106) providing evidence of microbial formation of Archaean rocks.

CH: Well, for me, my early days, I didn't really know that I was going to get into planetary science. I had no idea even that I would go into physics, but I always liked science. As I went through university, I started to realize I really liked physics and applied physics. When I started a master's degree, I got in with a group that looked at in vivo elemental abundance. So, element constituents in a person, it could be bone lead, bone strontium, arsenic in skin, and using XRF to look at elemental exposure related problems. When I finished my master's, I realized that for all the applied work I'd done, I didn't really understand a lot of the physics that went into that. I hadn't really studied a ton of physics that would really bump up my math ability. And so, I realized that I'd like to branch out a bit and I found this group at the University of Guelph and did an applied physics degree for my PhD that looked at using, again, XRF and PIXE techniques to do applications. But I also looked at the fundamental physics used as part of translating X-ray data into useful quantified weight percentages.

This group was also involved with the APXS [alpha particle X-ray spectrometer] devices on MER [Mars Exploration Rover] and MSL [Mars Science Laboratory] through Ralph Gellert. Just by proxy, some of my work ended up being beneficial to helping out that team and this was work that I enjoyed doing very much during both my PhD and post-doc at the University of Guelph. Later, I was looking for work and I first asked Tim Elam, a spectroscopist on PIXL, if he knew of anything. I think he at that point talked to Abby and, as I didn't mess up my job interview too much, she brought me onto the PIXL project at JPL in 2016 as a postdoc. I worked as two years as a postdoc and then found myself fortunate to be hired on at JPL in 2018 as a scientist where I still work, I work primarily on the PIXL project.

MB: That's great. Well, I want to thank you both for spending time with me this morning, and we look forward to the data and the successful mission for you both.

For more details on the PIXL instrument see, A.C. Allwood, L.A. Wade, M.C. Foote, et al. "PIXL: Planetary Instrument for X-ray Lithochemistry". Space Science Reviews. 2020. 216: Article number 134. DOI: 10.1007/s11214-020-00767-7.

Dr. Abigail Allwood (AA), Geologist and Astrobiologist at NASA JPL. Picture by Sonja de Sterke.

Dr. Christopher Heirwegh (CH), Scientist, Planetary Chemistry and Astrobiology at NASA JPL.

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.