SAS SPECTRUM eNEWS

Report from the Applied Molecular Spectroscopy Lab at the University of Puerto Rico-Mayaguez (UPRM): Situation Critical
Professor Samuel P. Hernández-Rivera, PI

On September 20, 2017, Hurricane María hit Puerto Rico unleashing all its destruction power. Not only have personal lives been disrupted as discussed in the media, but also education and academic research. While academic duties have resumed as of October 30, eight weeks later the laboratory remains closed and unavailable to continue research or teach students. Our current situation is unique—the tropical environment destroys instrumentation and the students are distracted by fundamental needs in their families' communities. We do not have immediate access to the resources required to rebuild the laboratory fast enough. Claims to the insurance companies will take long to pay out and there will be lasting effects, impacting both education and research. Help is needed in terms of replacing optical and optomechanical components, spectroscopic equipment, and general lab equipment with used or refurbished equipment. With this help, we will be able to mentor our students and provide part of the services we have provided for the last 20 years.

In the past, our research group at the Chemistry Department of the University of Puerto Rico, Mayaguez Campus (UPRM) and the many students and professors from chemistry, bioloy, physics, chemical engineering, mechanical engineering materials science and engineering provided support locally, in island-wide academic communities, as well as pharmaceutical and biotechnology industries. Three teaching labs remain inoperable, even 20 days after academic duties resumed on October 30, 2017. Damage to our facilities, which took more than 30 years to build, remain without a full account of the damage because we can neither access or turn on equipment, but it is clear that at least three labs and the infrastructure within, will have to be completely replaced or rebuilt.

For over two decades, the research, education, and training efforts of the Applied Molecular Spectroscopy Lab at UPRM have concentrated in investigations in support of the national defense and security infrastructure. The lab has had a complex history and a broad national and international impact.

Initial funding to establish our facilities was provided by the FAA from 1998 to 2001. At the time, our interests centered on explosives detection using vibrational spectroscopy and ion mobility spectrometry as well as explosives characterization. Several research and education endeavors resulted in highly successful ventures, such as a course in explosives synthesis, properties, and modern methods of detection (that has been taught continuously for 18 years at UPRM), several reports and publications (six peer-reviewed papers), several summer/COOP internships at the FAA (TSA) Trace Detection Lab, Atlantic City International Airport, New Jersey, sponsored by the Hispanic Association of Colleges and Universities (HACU), and Gordon Research Conferences on Detecting Illicit Substances: Explosives and Drugs (from 2001 to 2009).

After 9/11, we focused on working for the DoD under a Multidisciplinary University Research Initiative (MURI) grant from 2002 to 2008, a collection of instrumentation grants, and Historically Black Colleges and Universities–Minority Serving Institutions (HBCU-MSI) grants. These fund efforts that are still ongoing. Starting in 2002 and working funder the support of Night Vision and Electronic Sensors Directorate, Fort Belvoir, Virginia, we began presenting the results of our investigations at the annual SPIE Defense and Security symposia. Since 2003, we have presented a total of 89 papers at SPIE DSS. The number of peer-reviewed papers in that period is: 80, the number of chapters in books is: 21, and the number of MS degrees granted is 24, all within the same time span. The relationship with DoD and Night Vision Labs resulted in the establishment of our first centralized facility, The Center for Chemical Sensors Development (CCSD), dedicated to serve the UPRM Chemistry community and its graduate and undergraduate programs. Services for research support extended to the whole campus and chemical analysis also served the local pharmaceutical, biotechnology and electronics industries (including Pfizer, Abbott, AbbVie, Bristol-Myers Squibb, and Hewlett Packard). Work in sensors development included nanosensors (SERS based) to laser-based standoff detection sensors (Raman and IR based). A visible light (532 nm) Raman telescope was developed from COTS (custom off the shelf) components.

In 2004, the doctoral program in Applied Chemical Sciences began. In the last 17 years, I have directed 17 successful Ph.D. degree candidates, hosted four visiting professors, trained five post-doctoral candidates and established the second centralized facility: The Chemical Imaging and Surface Analysis Center (CISAC). This second research, education, and training center was established based on instrumentation acquired from DoD and NSF programs (including a DoD Defense University Research Instrumentation Program grant, fully backed by the Central Administration of the UPR). Part of the instrumentation included: a CISAC AFM-Raman, four Raman microspectrometers (Renishaw and Horiba), with excitation lines from the UV to the NIR (10 diode lasers), a Cary 5000 UV-Vis-NIR high-resolution spectrophotometer, a Bruker Optics IFS-66/v: FAR-MID-NIR vacuum interferometer equipped with ATR, grazing angle, variable angle diffuse reflectance (both macro and micro chambers), four QCL laser spectrometers, sample deposition devices (thermal inkjet, electrospray, spin coating, and others).

In 2008, we teamed with Northeastern University (Boston, Massachusetts), and the University of Rhode Island (Kingstown, Rhode Island) to form part of DHS sponsored ALERT Center of Excellence for Explosives Research. For the last 9 years we have mentored more than 20 REU (research experiences for undergraduates) under the DHS-ALERT-COE, and three summer visiting professors, each with two undergraduate students and have developed a wide variety of applications of mid infrared laser detection, quantification and identification of explosives, biothreats (or simulants), chemical warfare agents simulants, toxic industrial compounds, and others. We have extensively incorporated chemometrics and multivariate analyses routines to couple with our spectroscopic measurements and even disclosed two inventions consisting in hyphenated techniques based on quantum cascade lasers (for a total of one patent and four additional invention disclosures in the last five years).

When Hurricane Maria came along our labs were partially flooded, left without electric power for over a month, and experienced an ambient humidity of over 97% RH for nearly two months. Presently, three of our five labs are severely affected by water condensation and uncontrolled fungal growth that led to condemnation of the facilities until cleanup and decontamination can be accomplished by a private company. Our belief is that all the equipment, materials, and supplies in the three mentioned laboratories (including our largest equipment facility) are all damaged beyond repair and that the cleanup and decontamination process will affect all our optical components, including several of the lasers. Please look closely at the condensation on one of the PCs and the "goose bumps" on the video monitor caused by water dripping on the desktop computers (10 units) and three workstations that formed our data analysis and modeling lab.

We know that Puerto Rico, UPRM, and our research and education facilities will not be the same as before September 20, 2017, but our efforts will not be lessened in any way and we will continue striving for the excellence that we have professed in the last 35 years of service to UPRM and to the scientific and industrial community of Puerto Rico. We also know we can count on our colleagues and friends from DHS-ALERT and from Northeastern University. Help will also be available from insurance companies of the UPR. This help will take time, and we need to keep supporting, mentoring and training our students, and cannot wait for the insurance claims to be disbursed. Many students who still do not have water, electric power, or communications in their hometowns and even locally, but even so, they have joined our efforts to restore our facilities and our name. To them, I bow in deepest respect.

Desktop computers damaged by rain drippings and by water condensation.

East side Ground Floor corridor condemned by the UPRM Safety Office.

UPRM Chemistry Department personnel removing equipment and movable optical table from labs on the right side of the corridor (two labs) less affected by contamination and humidity.

Research and teaching will continue, as soon as possible in a colleague's lab.

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Perspectives from the SAS Newsletter Team: SciX 2017

In the previous issue, we covered the various technical sessions sponsored by SAS at SciX 2017 in Reno, Nevada. In addition to serving its membership by providing such avenues of technical knowledge exchange, SAS also offers its membership many other benefits, such as camaraderie, recognition, networking opportunities, and certification programs. In this issue, we will focus more on these less technical, but equally important, aspects by sharing the perspectives from several of our Newsletter committee members.

I arrived in the afternoon on Sunday, October 10, just in time to check into my room and then get to the members' events. While the original plan to visit Tesla Gigafactory did not materialize as originally hoped, the hypnotist's show turned out to be an eye-opening experience to me. Even though I did not appear to show enough talent to be selected to participate on stage, I witnessed several of our fellow spectroscopists become deeply hypnotized. Two of them (both experts in Raman spectroscopy, one for archaeology and one for food study) clearly demonstrated their multifaceted talents in music, singing, and dancing. Seeing is believing and the follow-up talk with the hypnotist convinced me beyond reasonable doubt that this performance was not staged and that hypnosis is a genuine psychological phenomenon.

My experience at SciX continues to evolve with every meeting. This year, the main highlights for me were several technical sessions. One of them turned out to be unexpectedly relevant to my own work, even though most of the audience in that talk might have found that topic mundane or irrelevant. For me, it clearly showed why a similar quick-and-dirty experiment I tried just a week ago failed, and the newly gained knowledge has rekindled my hope to try the experiment one more time. In fact I am proud to say that SciX2017 has helped me overcome a sampling bottleneck to progress that project to the next stage.

It is also nice to re-connect with many friends from various industries, universities, and vendors. This year was the third time for me to chair a session. My session related to how optical spectroscopy techniques are used in the chemical industry. It is great to see good attendance and general interest in the session. One challenge I always face is to find enough industrial speakers who can get approval to speak externally, and often speakers may have to cancel at the last minutes due to all kinds of reasons. I truly think that it is important and valuable for such sessions to continue to forge collaboration and understanding.

I always feel like an extrovert during technical sessions, but often will switch to an introvert at members' events. I am curious whether there are others who may experience similar personality switching. Regardless of your personality, it is clear that SAS will need more volunteers to help out with all kinds of activities. If you are interested, please send an email to SAS President-Elect Rob Lascola at robert.lascola@srnl.doe.gov.

— *Shawn (Xiaoyun) Chen, SAS Newsletter Editor*

This year, I had the pleasure of participating in the Coblentz Society Speed Mentoring event, held Monday at lunchtime. While the number of students was smaller than in previous years, it was no less interesting, nor rewarding to give back to those students. Hearing their questions, and then seeing their enthusiasm as they realized potential ways to go about approaching graduate school, finishing school or starting their careers was enjoyable. I highly recommend that those of us further along in careers help out and encourage the up and coming scientists in future meetings by participating in this event!

As someone involved in several organizations that converge at SciX each year, most of my free time is spent "behind the scenes" with those planning committees and other events that help allow SciX run smoothly from meeting to meeting. For those not involved, I encourage you to get involved with SAS, Coblentz, NASLIBS, and other professional organizations that help contribute to the technical and social success of SciX and applied spectroscopy at large.

— *Luisa Profeta*

SAS-Sponsored Sessions at Pittcon 2018, Orlando, Florida

"SAS—Frontiers in LIBS Imaging" is scheduled for Wednesday afternoon, February 28, 2018, beginning at 1:30 PM. This session is organized by Matthieu Baudelet from University of Central Florida National Center for Forensic Science.

"SAS—Leading-Edge Women in the Field of Applied Spectroscopy: Future Frontiers and Directions" is scheduled for Thursday afternoon, March 1, 2018, beginning at 1:30 PM. This session is organized by Karen Faulds from the Centre for Molecular Nanometrology, Department of Pure and Applied Chemistry Technology Innovation Centre, University of Strathclyde, Scotland.

Measure Venture: SAS Crowdfunding

SAS is now providing an online, science-focused crowdfunding venue to inventors and investors interested in measurement instrumentation, sample handling, science training, and other SAS-related entrepreneurship. By scientists, for scientists, Measure Venture fills a gap for entrepreneurial measurement scientists. Measure Venture also provides crowdfunding options for scientific events and charitable activities. Jump in and give it a try! https://crowdfund.s-a-s.org/

Contributed by Diane Parry

Memorable SAS pictures from SciX 2017

Exhibit floor.

Student event.

SAS = Science Across the Spectrum.

Duncan Graham at the Charles Mann Award Ceremony.

Folks enjoying the SAS Wine and Cheese Award Reception.

Duncan Graham receives the FACSS Charles Mann Award from Ian Lewis

SAS Barbara Stull Graduate Student Award: David Bryce

SAS Meggers Award: Presented to Naoto Nagai, Yuta Kijima, and Makoto Okawara.

SAS William J. Poehlman Award: SAS Cleveland Regional Section

SAS Lester W. Strock Award: Frank Vanhaecke

Bruce R. Kowalski Award in Chemometrics: Joseph P. Smith

SAS Distinguished Service Award: Geoffrey Coleman

SAS Distinguished Service Award: Brian Perry

SAS Honorary Membership Award: Terry Miller

SAS Fellows Award: Franklin E. Barton, II, Richard Crocombe, Karen Faulds, Kathleen Gough, Terry Miller, Linda Kidder

Frederick Haibach, past SAS Newsletter editor

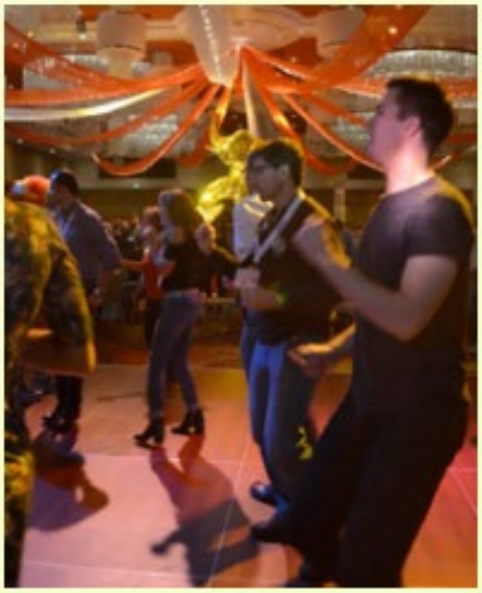
Rob Lascola, past Chair of Regional and Technical Section affairs

SAS gives back to the community

Wednesday night party pictures

Wednesday night party pictures

Luminescent SAS members



SAS members dancing the night away

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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