

SAS SPECTRUM eNEWS



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Editor's Note

Historically, April to August tends to be a relatively quiet time for the SAS Newsletter. At present, however, many political events are occurring, including the conclusion of President Trump's first 100 days in office, UK starting its Brexit process, and France in the middle of an election cycle. Some of these events may even impact the field of applied spectroscopy, though I have not personally experienced much impact yet. We will be interested in hearing your perspective on how such global events impact your work and our broader community.

In this issue, we provide links to two very interesting lectures recorded by the Infrared and Raman Discussion Group (IRDG) in the UK. It just so happens that the SAS Newsletter Committee recently completed an interview with Professor Peter Griffiths, who gave one of the IRDG lectures. We believe many members, especially the younger generation of spectroscopists, will benefit from the lectures and the perspectives offered by Peter. To quote Peter, "You'll find that even the best known spectroscopists are delighted to talk to people who are relatively new to the field." We encourage the junior spectroscopists reading this to reach out to the experienced members within SAS to maximize historical information inheritance.

Contributed by Xiaoyun (Shawn) Chen (xchen4@dow.com)

Two Great Lectures on the History of IR and Raman Spectroscopy

The IRDG has recorded the following two lectures of great value to all members, especially those who want to know about the historical developments of IR and Raman spectroscopy. Links to these two lectures are included here:

Lecture 1: The Early Days of FT-IR Spectroscopy: Strong-men, Connes-men, and Block-Busters, by Peter R. Griffiths: <http://www.irdg.org/meetings/irdg-200-250/irdg-216/>

Lecture 2: IR and Raman in the Dark Ages, by Pat Hendra <http://www.irdg.org/meetings/irdg-200-250/irdg-212/>

Contributed by IRDG <http://www.irdg.org/>

Interview with Professor Emeritus Peter Griffiths

With numerous awards to his name, Professor (Emeritus) Peter Griffiths is one of the most well-known names in vibrational spectroscopy. He is also a valued long-standing member of SAS and has served as the Editor-in-Chief/Editor of Applied Spectroscopy. Interested readers can find more of his biographic information on his website: <http://www.webpages.uidaho.edu/ftir/cv.htm>

In this interview, the SAS Newsletter Committee got Peter's perspective on the current status of vibrational spectroscopy, and various ways for members to improve themselves.

Has SAS been your #1 professional society? How long?

Since 1970. Yes, it has been my number one professional society throughout my career.

The SciX (formerly FACSS) Conference on average attracts approximately 1,100 attendees, while ASMS attracts 6,000. Does this reflect the impact/importance of vibrational spectroscopy and MS?

Many people use IR and Raman as routine tools and they (or their managers!) often don't feel that it's necessary to go to conferences. I suspect that a good number of people who use MS consider it a more sophisticated tool and can justify attending the ASMS meeting. SciX is trying to get different groups together to make it a more generalized meeting.

How can we avoid making vibrational spectroscopy "routine" and how do you suggest for scientists to hone their skills in spectral interpretation?

Relying solely on computer interpretation of vibrational spectroscopy is a dangerous practice. A combination of library searching and visual interpretation of the spectra of unknowns is a better way. Short courses may be helpful, but you cannot expect to become an expert simply by sitting through a two-day short course.

Can you discuss your experience as the Editor of Applied Spectroscopy? Benefits of the position? Wisdom for potential authors?

The biggest benefit for me was that it broadened my own interests. The journal covers more than just vibrational spectroscopy. It spans a wide range of subjects. You get to see new technology before it becomes commercially available.

Finding knowledgeable reviewers for each article is one of the bigger challenges. We receive more than 400 articles each year and need to find two reviewers for each. I use Google and other references such as Web of Science to find reviewers. Sometimes I luck out, but sometimes I cannot find anyone appropriate. As the number of papers submitted increases year by year, top scientists are inundated by review requests. For myself, I have used the following rule of thumb—I review three papers for each manuscript that I have submitted to a given journal.

Did the experience change your own research direction?

Not really. However, I have noticed that reviewers sometimes miss a key error in a manuscript and it finds its way into "spectroscopic lore". I would stress to my own students that just because something is being published doesn't mean that it is right.

How important is the ability to fix an instrument nowadays for applied spectroscopists?

It's far less important than, say, 20 or 30 years ago. In general, you probably do more harm than good if you try to realign optics yourself. However, knowing how an instrument works is very important so that when something goes wrong, you know what signs to watch for.

Many Ph.D.s with spectroscopy training are graduating doing work in nonlinear spectroscopy, ultrafast spectroscopy, with limited "application", that is, limited use of those techniques outside academia. What's your advice on transitions into the "applied" side of spectroscopy?

Make sure that you read about the instrumentation you are going to use. Attend as many training courses as possible. Simply having a Ph.D. in second harmonic generation does not guarantee that you know how to interpret a simple infrared or Raman spectrum. The need for training courses has become even stronger nowadays, because in-depth courses in interpretation and instrument design are no longer taught in universities.

What's your philosophy on working with vendors?

Most instrumental developments in IR and Raman spectroscopy today are driven by vendors. Today's FT-IR and Raman spectrometers and their associated software are amazingly powerful and allow a plethora of new applications, so I try to maintain a good working relationship with all vendors.

What are your thoughts about SAS? How should SAS recruit new members to the organization? How can SAS remain relevant?

The SAS works hard to bring new students into the fold both by technical and social means. The journal and the newsletter cover different materials. The journal covers state of the art developments in spectroscopy. Short application notes highlighting "we are using this for this" are rarely accepted for publication in the journal, but could be included in the newsletter. This type of paper can be really useful for people in industrial labs.

What do you consider more important for an applied vibrational spectroscopist, a solid grasp of group theory and origin of vibrational modes, or a phenomenological understanding of the correlation between types of functional groups and group frequencies for frequently-encountered materials?

I strongly believe that an understanding of the theory of vibrational spectroscopy (but not necessarily group theory) and a phenomenological understanding of IR and Raman group frequencies are of about equal importance, but I would also include an understanding of how instruments work and the strengths and limitations of the accessories that are installed, as exemplified by the following example. I am a member of a team of four experienced scientists who teach a week-long workshop in the interpretation of vibrational spectra that is offered each July at Bowdoin College (www.ircourses.com). In this course we start by spending the first morning immersing the attendees in the theory of vibrational spectroscopy (hopefully in a way that doesn't leave them in the dust!). Although much of the rest of the course is mainly spent on the practical interpretation of IR and Raman spectra, we come back over and over again to the concepts taught in the first morning. We also discuss the theory and practice of attenuated total reflection (ATR) spectroscopy in this course since ATR has become the most used (and sometimes abused) technique for the measurement of infrared spectra of condensed-phase materials. Many users of this technique don't recognize that ATR spectra are different from transmission spectra or understand the cause of this difference. Thus in this course, we recognize that not only is a solid grasp of the theory and origin of vibrational spectra critical to the effective application of IR and Raman spectroscopy but also that an understanding of the measurement process is similarly important.

Having said that, you have probably realized that I haven't answered the part of your question that concerned group theory. In the early days of vibrational spectroscopy, when the pioneers of the field were developing an understanding of the spectra of small molecules that possessed additional symmetry elements to the identity operation, the application of group theory was tremendously important. Today, most molecules that are being studied by IR or Raman spectrometry are larger and less symmetrical than those studied in the past and therefore an understanding of group theory is less critical. Nevertheless, a comprehension of group theory can occasionally still lead to a more enhanced solution of difficult problems.

We have talked about how to become a professional applied spectroscopist above for a student freshly coming out of college or graduate school. Can you talk about how you as an experienced spectroscopist and SAS in general can help mentor the youngest generation of spectroscopists?

This is a difficult question to answer as, unlike the situation 20 or more years ago, there are very few companies that now employ specialists in vibrational spectroscopy. Nonetheless, new employees who are interested in IR and/or Raman spectroscopy and want to turn this interest into a career should attempt to glean enough training in vibrational spectroscopy that they become the guru in this area for their company. Frankly, it is unlikely that today's new graduate will start work with a really strong training in vibrational spectroscopy. Although many universities and colleges offer a course in the interpretation of molecular spectra, these courses are almost invariably taught as a relatively small component of the organic chemistry curriculum and don't cover much theory. Over the years, the percentage of the time in such courses that is devoted to the interpretation of infrared spectra has diminished significantly. (Raman spectra are almost never covered!)

Organic chemistry instructors now devote more time to MS and multi-dimensional NMR spectroscopy because these techniques are of pre-eminent importance in their own organic research labs. As a result, today's undergraduates and graduate students tend to have a weaker understanding of vibrational spectroscopy than their peers of 20 or 30 years ago. Undergraduate students who wish to become specialists in vibrational spectroscopy should get involved with a research group for which IR or Raman spectroscopy plays an important role at least a year before graduating. Otherwise, after starting work with a new employer, graduates should read books and journals on different aspects of vibrational spectroscopy, attend conferences such as SciX, and take professional development courses.

I would strongly recommend any recent graduate find a project in his/her workplace in which the application of IR or Raman spectroscopy plays an important part. Talk informally to the project manager suggesting areas where the application of vibrational spectroscopy could help. Even if your advice is ignored, it will let your manager know of your interests. Membership of professional societies is also important. I would especially recommend joining the SAS. Relative to, say, the ACS, membership in the SAS is a bargain and over the course of my career, I have benefitted enormously from my membership in the Society. Membership gives access to Applied Spectroscopy as part of the packet. It is not a bad idea to set up a file that holds papers from the journal that are, or could be, relevant to projects that are active in your company. New employees should also try to attend a conference at which you can meet both recent graduates and more experienced scientists. The SAS always holds a reception for its members at SciX. Come to this reception with a couple of technical questions that you can pose to the gurus of the field, possibly followed up by more general questions. Not only will you get some useful answers, but it's a great way of getting known. Don't be afraid to introduce yourself or ask to be introduced to some of the "names" in vibrational spectroscopy. You will find that even the best known spectroscopists are delighted to talk to people who are relatively new to the field.

SAS Information

- The deadline to apply for the SAS Certification Program has been extended to May 31. Please [click here](#) for more information on the certification program and application process.
- Reminder that award nominations deadline is May 15 for the SAS GRADUATE STUDENT, UNDERGRADUATE STUDENT, KOWALSKI, and REGIONAL SECTION AWARDS. [Click here](#) for information on these awards and how to submit your nominations.
- SAS is seeking a new Student Representative to the SAS Executive Committee and Governing Board

The term of the current student representative to the SS Executive Committee and Board of Governors, David Bryce, is up at the end of this year. As such we are going to be conducting a student-only election for this representative who serves as a student voice in the Society.

The student elected will serve a two-year term and will be required to attend the Executive Committee and Governing Board meetings at both PITTCON and SciX in 2018 and 2019 (we will also be requesting your presence at the 2017 SciX meeting in Reno, NV for transition purposes). Travel expenses, except meeting registration, will be reimbursed at a set rate for the time that the elected student is required to be at the meeting for SAS purposes (travel will not be covered for the transition meeting at SciX 2017). Generally this will cover most travel costs, but not all depending on how you budget for the trip. The student representative is responsible for coordinating student-related activities at SciX and PITTCON and for generating new ideas related to student needs and issues.

In order to qualify for this position you must be a member in good standing of the Society and you must maintain that status throughout your term. You must be a student for at least one of the two years that you will serve in this position. You must be able to attend the above stated meetings. You must have an interest in Society activities.

We will be accepting your self-nominations for this position until May 15. Elections will be held shortly thereafter. To nominate yourself, please email the following information and question answers to exdir@s-a-s.org.

Name
Address
Phone
Email
Years remaining as a student

Please answer the following questions:

1. What are the top issues facing students of spectroscopy and how can SAS help?
2. How does being a student member of SAS help in your career preparation?
3. What ideas do you have for recruiting and retaining student members?

**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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