ACA RefleXions

American Crystallographic Association
Structure Matters

Number 2 Summer 2017

The winner of the Elizabeth Wood Science Writing award is James O'Brien. The title of his talk is 'Famous Mad Hatters'. Welcome to Wonderland!

2017 ACA Annual Meeting
New Orleans, Louisiana

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ACA RefleXions

Summer 2017

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What's on the Cover

The idea for this cover came from James O'Brien, the winner of the 2017 Elizabeth Wood Science Writing Award.:

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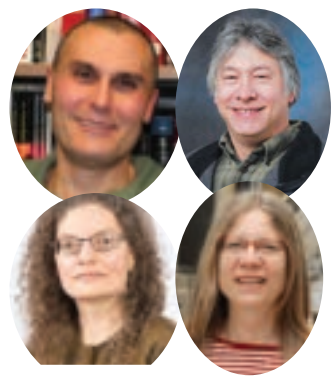

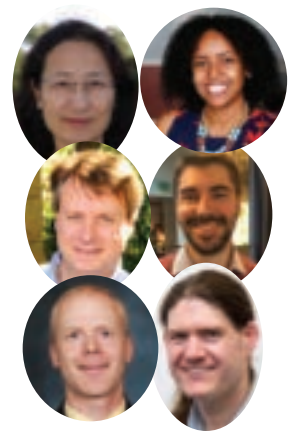

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From the President's Desk
Lassiez les bon temps rouler!

Here we are on the other side of our 2017 Annual Meeting – and what a great time it was! Well over 500 of us convened in New Orleans for four days of science, collaboration, networking and just good fun. From the standing-room-only crowd at the opening ceremony that stayed in rapt attention as Nobel laureate Sir Fraser Stoddart spun stories of research and life lessons, to the stand-out *Transactions Symposium* on Cryo-Electron microscopy, this meeting was an unqualified success. We had as many attendees as the 2016 meeting in Denver and about 100 more than we anticipated for this IUCr year. We're excited to have this meeting's abstracts archived by the IUCr. Our vendors showed amazing support, both financially and scientifically with contributions to many sessions and some fabulous exhibits. We presented the first-ever Rognlie Award to Helen Berman. This award, made possibly by a posthumous donation, honors Dave Rognlie and his many contributions to the ACA. And of course, who could forget the wedding of Allen Oliver and Jeanette Krause right in the middle of the expo! I can't think of any other society that would stand as witness to two of its members' lifelong commitment.

During the meeting, we were fortunate to have representatives from our journal, *Structural Dynamics*, including editor-in-chief Majed Chergui. Council had an update from the journal which shows some excellent statistics: a 3.67 Impact Factor for 2015, an average time to publication of 55 days, and a 3-fold increase in submissions since the journal launched in 2014. There have been several special issues, including last year's *Transactions Symposium* which is now published and, don't forget, ACA members get a 40% discount on the submission fees.

If you happened to miss the All-Members Business Meeting in New Orleans, I offer this brief recap: The ACA is continuing to plan for the future. We've hired Kristin Stevens as our new Assistant Director of Administrative Services, and she did a fantastic job keeping the show on the road in New Orleans. Financially the ACA continues to face challenges with declining membership and meeting attendance. Raising dues helped stem the tide, but we are still in need of more members – both new and renewing – to fund the ACA's activities. To this end, we've launched a Membership Drive; the individual who succeeds in bringing in the most new members to the ACA will receive a free membership for one year, in addition to the people's ovation and fame forever. We've also formed two *ad-hoc* committees to address the membership experience and meeting reorganization. We anticipate having some actionable data from these two committees by the time our fall council meeting rolls around. Committee chairs Allen Oliver (Membership) and Kristin Stevens (Meetings) welcome your feedback. We have launched a Website Redesign fundraiser and before leaving New Orleans, obtained pledges for over $7500 towards our $20,000 goal. Check our website for the many ways you can donate to support the ACA's general activities. We closed the business meeting with a challenge to our members: Given that the scientific content of our meetings is changing to reflect a broader range of structure determination techniques, should we consider a new name for the society that would speak to this wider demographic? We'd love to know what you think this new name should be!

Even though the 2017 meeting has just finished, we're already planning for Toronto. Thanks to all the SIG officers who gave us valuable feedback on our new session proposal process. We're already considering ways to improve communication among your SIG members. We left New Orleans with a solid program in place including sessions on Hybrid Methods, Mineralogy, and Diversity and Inclusion. Our *Transactions Symposium* "Shining a Light on Structure-Based Drug Design" promises to attract a broad range of talks from Cryo-EM structure determination to small molecule ligand design. Mark your calendars for July 20-24, 2018; you truly don't want to miss this meeting!

Finally, I'd like to end this column by recognizing a dedicated volunteer to the ACA community and by raising a call for volunteers across the board. As you may know, Tom Koetzle has been co-editor of *RefleXions*, since 2014. His attention to detail and turn of phrase help make *RefleXions* the quality publication that the ACA community consistently ranks as one of the top benefits of membership. Tom will be stepping down from his co-editorial position after producing the fall issue, and as we thank him for his efforts, we call to members for a volunteer to take up this position. If you're interested in the task, please let us know. It's not just *RefleXions* that requires volunteers, though. We rely on our active and engaged members to keep the society running and we can always use an extra set of hands. We'll be adding volunteer information to our website in the coming weeks so you can see where we need the most help. After all, the ACA can only be as strong and vibrant as the members who pitch in and help us with the many things that make this organization such a great place to call home.

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET - December 31, 2016 and 2015

CURRENT FUNDS (2016)		TOTALS	
		2016	2015
ASSET4			
Current Assets:			
Cash	100,972	100,972	131,807
Investments (unrestricted)	580,789	580,789	578,713
Investments (restricted)	524,053	524,053	544,182
Accounts Receivable	0	0	0
Total Current Assets	1,205,814	1,205,814	1,254,702
Fixed Assets:			
Computers and Printers	0	0	0
Office Equipment	0	0	0
Accumulated Depreciation	0	0	0
Total Fixed Assets	0	0	0
TOTAL ASSETS	1,205,814	1,205,814	1,254,702
Liabilities:			
Unearned Revenues	73,876	73,876	75,624
Other Liabilities	22,133	22,133	0
Total Liabilities	96,009	96,009	75,624
Fund Balance			
Unrestricted	585,752	585,752	634,896
Restricted	523,053	524,053	544,182
Total Fund Balance	1,127,805	1,127,805	1,179,078
TOTAL LIABILITIES & FUND BALANCE	1,205,814	1,205,814	1,254,702

*** Current Balances in individual restricted funds -** ***as of December 31, 2016***

Bau Neutron Award	36,494
Buerger Award	38,978
Rognlie Award	60,000
Etter Award	68,783
Fankuchen Award	71,343
Patterson Award	48,786
Pauling Award	38,780
Supper Award	12,661
Student Travel Fund	21756
Trueblood Award	40,459
Warren Award	31,299
Wood Science Writing Award	54,221

A more detailed report on the ACA finances may be obtained by sending a written request to the ACA office in Buffalo, PO Box 96, Ellicott Station, Buffalo, NY 14205-0906.

History Fund (unrestricted) *www.amercrystalassn.org/history_home*

ACA History Project News

Have you subscribed to the ACA YouTube Channel? There are 24 videos of Award and Historical lectures at previous ACA meetings on our channel. The most recently added: Brian Toby's 2014 Transactions lecture, "Powder Diffraction Crystallography: 98 Years as Plan B?" and Elspeth Garman's 2016 Fankuchen Award lecture, "Travels in Protein Crystallography".

If you would like to take on a technical challenge, volunteer to help us turn more of the raw video files we have from past ACA meetings into finished movies on YouTube. Contact Virginia Pett for more information and assistance in getting started.

Two articles in this issue of *RefleXions* magazine illustrate some of the work of the History Committee: encouraging structural scientists to write their Living History and researching the careers of those who have passed on but whose contributions have not yet been recorded in depth. In his Living History Mike Glazer, Vice-President of IUCr, describes his 66 years of fascination with crystals. He gave the 2017 Bragg Lecture at the Royal Institution, "The Wondrous World of Perovskites". The link to his video is online at ACA History/Impact of Structural Science.

The biography of Rose Mooney-Slater that appears in this issue was researched and written by Frank Fronczek. Following the trail from Dick Marsh's recollection of Mooney-Slater as the person who introduced him to crystallography, Frank wove together information from a number of sources to portray the life of the first female x-ray crystallographer in the United States. If you have suggestions for other crystallographers who should be remembered in more detail, contact Virginia Pett.

Virginia Pett, pett@wooster.edu

66 Years in Crystals!

*A. Michael Glazer is currently the vice-president of the IUCr and one of the founders of Oxford Cryosystems. Mike obtained his Ph.D. with Kathleen Lonsdale followed by a post-doc in Helen Megaw's laboratory. He is well known for his research into structure-property relationships in perovskites. He's also taken an interest in the history of crystallography: "There ain't nothing like a Dame: a commentary on Lonsdale (1947) 'Divergent beam X-ray photography of crystals'" [*Phil. Trans. R. Soc. A ***373****: 20140232] and* Crystal Clear: The Autobiographies of Sir Lawrence and Lady Bragg *(co-edited with Patience Thomson). Mike has been an ACA member for over 40 years.*

I must have been 7 or 8 years old when, walking home from school, I picked up a spherical pebble, and as little boys are apt to do, I threw it on the ground to break it open. I saw that inside there were colored bands, and when I got home I showed it to my mother. She then went and bought me a copy of the "Observer Book of Geology" and I identified the pebble as agate or banded flint. I saw in the book many pictures of crystals and thus began my love of crystals. So, I soon learnt that one could see crystals in the Geological Museum in London, and despite my young age I took the underground train by myself into London each Saturday to take a look. I was so captivated by their huge collection that I became a regular visitor, touring all the showcases, learning about minerals and making friends with the curators, who from time to time slipped me some specimens. This became my regular routing virtually every Saturday for several years after.

I also used to go on schools' visits to the Royal Institution (RI) to listen to and watch the great Sir Lawrence Bragg. He loved teaching science to children, especially by showing them demonstrations. During his time at the RI something between 100,000 and 200,000 children passed through that famous lecture theater. The photo (at the top right) shows Bragg demonstrating how to make voice-like sounds with a tube, air and modelling clay. You can see his delight in his expression. Also, there I am (circled) in my school uniform laughing my head off. I guess I must have been about 14 years old then.

The result of spending so much of my time with crystals was that I did very badly at high school, failing some of my key examinations. At the time in Britain there were not as many universities as there are now, and so I found it difficult to be accepted for a university degree. Finally, I was accepted to read chemistry at Dundee in Scotland, which at that time was considered to be a college of the University of St. Andrews. I recall that to gain entry I had to have an interview. They asked me one question: tell us what you know about aluminium. Well, just the week before I had been to a lecture on aluminium at the Science Museum in London and came away with a booklet all about its history, methods of preparation and chemistry!! That was indeed a stroke of luck.

Right: W.L. Bragg demonstrating the Paget voice synthesizer. Left: Audience of school children in 1957. The young boy ringed is me!

Before going up to university I had some time to kill and so I went for an interview with a local military research company, Elliott Automation in Borehamwood. I recall that I was interviewed for this job on a Friday afternoon. I was asked just one question: do you know Ohm's Law? I said yes and they said, OK you start on Monday. And on Monday I found myself working on three top-secret projects: the Verdan computer for the Hawker-Hunter aircraft, the Blue Steel missile and the aircraft TSR2! In those few months, I learnt a lot about how British industry worked (or rather didn't). A great deal of money was being wasted and I was not surprised when the government finally cancelled Blue Steel and TSR2.

The city of Dundee then was very poor with huge amounts of unemployment, drunkenness and crime. It seemed to me then to be like a scene from a Dickens novel, with children sitting outside pubs after ten at night waiting for their parents to come out and feed them. (I have to say that today Dundee is hugely improved.) The chemistry school was very small, consisting of only 18 final honors students, and in such a small environment and because there was so little else to do, I immersed myself in my studying and eventually came out with a good degree. Now, while I was there I carried out some projects with the local crystallographer John Iball, and was fascinated with taking x-ray powder photographs of various compounds. It was he who then recommended me to do a PhD at University College London in the research group of Professor Dame Kathleen Lonsdale.

My first impression of Kathleen Lonsdale was of a tiny frail looking figure, with a reddish nose suggesting a cold, a huge shock of curly white hair (reminding me of the man on the Quaker Oats package). However, I soon began to appreciate that this was no weakling but a tough and clever person who did not tolerate fools gladly. In October 1965, she asked me to carry out research into organic mixed crystals and so I began the search for the materials that I would have to study. I was given a desk in a small room right next to the area where the group used to make its tea and coffee. Starting at the same time, and seated next to me was the late Howard Flack, and we soon became good friends. He was assigned to work on diffuse scattering in crystals of anthrone and anthroquinone. I finally discovered the topic for my research in June of 1966, the study of phenazine and phenazine-N-oxide mixed crystals, and it turned out that this showed diffuse scattering quite similar to that being studied by Howard. And so we worked closely together. During our first year Mrs. L. (as we used to call

her) sent Howard and me to evening classes in crystallography at nearby Birkbeck College. This was a fantastic introduction to the subject. The lecturers there included Harry Carlisle (x-ray camera geometry, direct methods and the Patterson function), Jim Jeffery (crystal optics), Rex Palmer (space groups) and Alan Mackay (drawing crystal morphologies). On a couple of occasions we met with the great J. D. Bernal, who at that time was very ill after suffering some strokes.

Kathleen Lonsdale's group at that time consisted of about 30 people including Judith Milledge (working on diamonds), Marianne Ehrenburg and C.J. Brown (organic crystal structures), Robin Shirley (bladder stones), June Sutor (bladder stones), Jeff Harris and Richard Henriques (diamonds), and several visitors including Maureen Julian (nee O'Donell) from the USA, Terry Rummery from Canada and Eugene Hoff, a medic from New York. Every now and again Mrs. L would summon us upstairs to her room for a discussion on progress. It always began with a question: where are the Laue photographs? Woe betide any student who appeared in her office without the necessary set of Laue photos!

Two photographs of Howard Flack (wearing the suit) and me working on the Ferranti Pegasus Mark II computer. We often had to change the valve (tubes for you Americans!) boards.

We were very lucky in her research group as we had for our own personal use a real computer. I think we may have been the only scientific research group anywhere with its own computer. This was a Ferranti Pegasus Mark II machine with 8K of store on a magnetic drum, and 5-hole paper tape. Programming was in machine code. This actual computer is now on show in the Science Museum in London ***(blog.sciencemuseum.org.uk/the-pegasus-computer/)*** and still has a coffee stain on the chair that I left there one night. The photos show Howard and me working on the computer in 1966.

It was during my studentship in London that I finally got to meet in person the great Sir Lawrence Bragg a few times, as he visited from time to time. When he was just about to retire from the Royal Institution in 1965, Mrs. L. gave Howard and me a ticket to his retirement lecture.

In 1966 Howard and I went with Mrs. L. to Moscow to attend the IUCr Congress where she was standing in as president in place of Bernal, who was too ill to travel. She was able to pay our expenses in Russia because she had some money there from a book she had written on Quakers in Russia. I recall that we arrived at the wrong airport and had to wait for our host, Professor Zhdanov, to come across Moscow to meet us. It was at the height of the cold war, but we found everyone to be very friendly. On the ride into Moscow the interpreter, whose name was Valery Demidov, taught Howard and me several Russian swear words, and from that time most communications between Howard and me started or ended with one of those swear words! The picture shows me sitting in the lecture room at Moscow State University, next to Howard and Terry Rummery. By the way, I have attended every IUCr Congress since.

1966 IUCr Congress Moscow at Moscow State University. I am the second person from the left in the front row; Howard and Terry Rummery are sitting to my left.

In 1968 Howard and I published together six papers in *Phil. Trans. Roy. Soc.* and left University College. Howard went to the Cavendish Laboratory, Cambridge and I to the chemistry department at Harvard. There I worked in the group of Jack Gougoutas on a compound that tended to explode. The interesting thing about this was that you could follow a change in crystal structure that involved turning over of benzene rings without destroying the crystal's integrity. Two of the people there were Jon Clardy and Les Lessinger. In 1969 I attended the IUCr Congress at Stony Brook and there I met Helen Megaw from Cambridge. Mrs. L. had suggested that she should meet me and try to persuade me to work for her as a postdoctoral assistant. At first I was dubious about my ability to do this as she was interested in inorganic materials (perovskites mainly) whereas I only understood molecular crystals. Anyway, she was very nice and persuasive and in September 1969 I moved to the Cavendish Laboratory (a different section from Howard though). The head of the Crystallography Laboratory, which had originally been set up by Lawrence Bragg, was W.H. (Will) Taylor, a kindly white-haired gentleman, who had been the first person to solve one of the feldspar structures. The other senior staff members there were Helen Megaw and P.J. (Jane) Brown, with a research group of about 20 people. My first sight of Jane was interesting: I went into a lab to find Jane machining a piece of beryllium on a lathe with beryllium dust everywhere and no obvious protection!

Helen gave me the task of building a suitable apparatus to heat a crystal of sodium niobate in order to map out its phase transitions (there are about 6 phases at high temperature). To do this I built a special back-reflection single-crystal camera in which I could move the film while automatically raising the temperature. By careful selection of an oscillation range a plot of the spots at very high angle nicely showed all the phase changes, and Helen and I were able to publish a few papers around that. Now another interest of Helen at that time was in understanding what

happens if you take an octahedron in the perovskite structure and tilt it. Because each octahedron is linked to each other through its vertices the answer seemed to be impenetrable. Helen asked me to look into this. A previous visitor, Jim Brandon, had been looking at this I think with regard to calcium pyroniobate and he had sketched an approach to this problem in terms of tilting about a crystallographic axis. This suggested to me a way of generalizing the problem in a very simple way: tilting about each axis in turn. I discovered that in terms of the signs of tilt there were 10 possibilities and that when you allowed for different magnitudes this became 23 (some years later application of group theory showed that in fact there were 15 unique solutions). I devised a notation to describe the various tilts and this is now standard in the perovskite literature. In fact it has become so standard, that I often see papers that use it but no longer bother to refer to the original paper (so much for citation indices). I was very pleased at the time to discover in this way another cubic perovskite structure in which there were equal tilts about three axes.

There is a funny story attached to my 1972 paper on the tilt systems. I sent it into *Acta Cryst*. for publication and eventually received a referee's report: six pages of closely typed comments and criticisms! I was furious and went to Helen in a bad temper, cursing and using several choice words. (I was young and impetuous then, not the kind and loveable character I am today.) Helen calmed me down and offered to help me deal with the comments, and I had to say that at the end the paper was much improved. I sent it back to the editor and received two more pages of closely typed comments. Again Helen had to calm me down and help me. This was the paper that was finally published and is to date my most quoted publication. A few years later when Helen retired, she confided in me that she had been the referee!

After she retired I became the Head of the Crystallography Laboratory, but I did not hold a permanent position in the Cavendish Laboratory. This was a difficult time because we were under pressure to leave the Cavendish Laboratory and I had to learn how to head off actions by the Cavendish Professor who wanted to get rid of us. I discovered that the workshop personnel and the secretaries were always the first to know what was happening and so they used to tip me off regarding an impending action. Fortunately, in 1976 I was appointed to a Lectureship in Physics in the Clarendon Laboratory in Oxford and at the same time to an Official Fellowship and Tutorship at Jesus College Oxford. Kathleen Lonsdale, when she was in hospital with a terminal illness, wrote several letters of recommendation for her favorite students, and so I was able to use this to secure my position in Oxford.

So, in 1976 I moved the Crystallography Group to Oxford including all the records, people and equipment. At that time the Clarendon Laboratory was in a very poor state compared with Cambridge. I was the first person to be appointed from outside in 23 years and there were only two research groups that I could see were doing first-class research. A little later W. (Bill) Mitchell from Reading University was appointed as head of department and set about transforming the whole laboratory with considerable success. Most of the research done in my group then was on the relationships between crystal structures and physical properties and over the years up to my official retirement in 2000 there were a total of 30 research students, and following in the Bragg tradition, almost one half were women.

One topic that we worked on with colleagues in Kraków, Poland was on the relationship between optical activity and crystal structure. We were able to explain the link between the two for all the crystal structures studied in relatively simple terms. This was a most successful collaboration; however, in December 1981 martial law was declared by the Jaruzelski government and all connections between Poland and the rest of the world were severed. In May 1982 I was finally allowed into the country to visit my colleagues. Conditions were very bad, little food, empty shops, long queues everywhere, tanks in the streets and a curfew. There was little work that we could do except sit at a table telling jokes. Back in Oxford I was contacted by Professor Z. Pełczynski to set up the so-called the Oxford College Hospitality Scheme for Polish Scholars. The idea was to be able invite Polish academics to Britain for short visits. I was to deal with scientists while he and another person, Kathy Wilkes, were to deal with the humanities. We persuaded all the Oxford Colleges to agree to give a room and food for one or two months a year. The Foreign and Commonwealth Office agreed to fund the visits and somehow, Pełczynski managed to persuade the military government in Poland to allow us to invite academics without governmental interference. The result was that we were in the unique position for a while to make our own decisions on who could come from a communist country to the UK without the need for special permissions or visas! This scheme was later enlarged to cover the other socialist countries including the Soviet Union, and George Soros gave us money to support this venture. Ten years after establishing this scheme we were all invited to Warsaw for a celebration. The communist government by then was no more and we were received by Lech Wałęsa, President of Poland, and given the National Medal of Education.

In 1986 I wanted to construct apparatus for cooling crystals in an x-ray beam. The available techniques then were most unsatisfactory, with temperature oscillations of several degrees, a minimum temperature of about 150 K, massive use of liquid nitrogen and flimsy apparatus. I joined forces with John Cosier, whose expertise was in looking after the laboratory's low-temperature facilities, and we came up with a unique design, which we called the Cryostream. Suddenly we had a small device capable of going down to 77 K with a stability of 0.1 K, easy to use and thus making low-temperature crystallography hassle-free. We started to construct Cryostreams in the basement of our laboratory but such was the demand by customers that we then set up Oxford Cryosystems to the northwest of Oxford, and John left the Clarendon to carry on with construction and design. I dealt mainly with the business side, marketing, demonstrating and accounts. Looking back, I realize that we were extraordinarily lucky in coming out with the Cryostream when we did, because this coincided with the discovery of flash-cooling of protein crystals, and so sales rocketed. As of today, Oxford Cryosystems remains the primary distributor of equipment for low-temperature x-ray crystallography.

My research continued in Oxford, especially dealing with the structures and properties of an important perovskite piezoelectric material, PZT (I started this research some 45 years ago). Even

now that I have been retired nearly seven years I continue to work on this problem, and I think that we have finally reached a solution to explain how the piezoelectric activity arises from the structure. It turns out to be very complex involving elements of short- and long-range structure that vary with composition. In 2012 I was awarded the Czochralski Medal in Warsaw by the European Materials Research Society for my work on perovskites. I don't normally go in for honors personally but since my friends had worked so hard to propose me for this and it was, after all, in Poland, I decided to accept it. One of our publications (*Nature Comms*. **5**, 5231, 2015) on the structures of PZT was awarded the Spriggs Award by the American Ceramics Society in 2015. Throughout my career I have carried out a considerable amount of work for the IUCr, as a journal editor, main editor and as a member of the Finance Committee. I was pleased during the Montreal IUCr in 2014 to be voted in (though by one vote!) as vice-president, and now I am looking forward to the next IUCr Congress in Hyderabad.

Mike Glazer (Oxford, 2017)

Editor's note: Mike Glazer's 2017 Bragg Lecture, *The Wondrous World of Perovskites* is now online at ***tinyurl.com/nykch2k***. In the introduction he points out that both William Henry and William Lawrence Bragg were "quite competent artists". Glazer thinks that the combination of being scientists and artists led to the discovery that kicked off x-ray crystallography.

Ideas take shape

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Rose C. L. Mooney-Slater

"*Thank you, R. C. L. Mooney.*" So ends Richard E. Marsh's ACA Living History memoir, for it was she who introduced him to crystallography in 1945, launching him on his 70-year distinguished career. At the time of their meeting, she was a 42-year old professor of physics at H. Sophie Newcomb Memorial College, the sister school (coordinate women's college) of Tulane University in New Orleans. She was a Fellow in the American Physical Society, a Guggenheim Fellow, had served as Associate Director of the X-ray Structure Section of the Metallurgical Laboratory in the Manhattan Project, and had a distinguished publication record on the structures of inorganic compounds, complex ions formed by halogens and of synthetic fibers. She was the first female x-ray crystallographer in the United States, beginning her career shortly before Elizabeth Wood (1912-2006), and among the first in the world, being a contemporary of Kathleen Lonsdale (1903-1971), Dorothy Crowfoot Hodgkin (1910-1994) and Helen Megaw (1907-2002). She would go on to play a pivotal role in establishing a long tradition of x-ray crystallography at NBS/NIST, marry the noted physicist John C. Slater, and work as a research physicist at MIT and a research professor of chemistry at the University of Florida. She was an excellent teacher, well liked by students. Given that she was a pioneering female crystallographer and was influential in so many ways, it is remarkable that she is not better known today.

Early Life: Rose Camille LeDieu was born October 23, 1902 in New Orleans, to parents who were both Louisiana natives. At about age 20, she married a New Orleans pharmacist and WWI veteran eight years her senior, Carroll E. Mooney (1894-1965). She thus became R. C. L. Mooney, the name that she used on all her published work until 1961, when Slater was added. This marriage appears to have lasted at least eight years, perhaps quite a bit longer, but it seems unlikely that he accompanied her when she left New Orleans for graduate school.

Education: Rose studied physics as an undergraduate at Sophie Newcomb College, earning a BS in 1926. She remained at Newcomb as an instructor of physics until 1930, while working on her MS in physics at Tulane, a degree she earned in 1929. She then applied to graduate school at Caltech as R. C. L. Mooney. Dick Marsh best tells what then transpired: "*Mooney had … been accepted into graduate school at Caltech (my undergraduate school). But when Mooney arrived at Caltech, both sides were surprised: Caltech, because Mooney was a female (the "R" turned out to be "Rose"); and Mooney, because she did not know that Caltech, at that time, did not accept female students. What to do? My understanding is that Linus Pauling gave her a temporary appointment as research associate and helped arrange for her to transfer to the University of Chicago as a student of Will Zachariasen. She received her PhD there.*" (Note: Caltech's first PhD awarded to a female was in 1955, and undergraduate women were first admitted in 1970.) W. H. Zachariasen was four years *younger* than R. C. L. Mooney and just beginning his 44-year career at Chicago at age 24, but had been publishing excellent crystallographic work since he was 19. They had access to both Laue and oscillation cameras, and in 1931 she published the structure of potassium permanganate as sole author. In December of that year, she attended the New Orleans meeting of the American Physical Society and presented the structure of ammonium bicarbonate. The location of that meeting in her hometown was fortuitous for her, as funds for travel and particularly lodging were in short supply during the Great Depression, and she likely still had family, including a husband there. She would complete her PhD in physics the following year and return to Newcomb as an assistant professor of physics.

Rose Mooney in about 1938.

Career at Sophie Newcomb: Rose Mooney was a faculty member at Newcomb for 20 years, becoming associate professor in 1935, then professor and head of the physics department in 1941. Newcomb College was primarily an institution for the education of women, and Prof. Mooney was by all accounts an excellent teacher. Carrying out crystallographic research there was somewhat more problematic. Dick Marsh recalled that her "*…office-laboratory-classroom contained a single X-ray tube and a Laue film holder – period*" as late as 1945. However, she was quite adept at arranging to spend summers visiting institutions with better instrumentation and managing to do excellent crystallography. She did so at Johns Hopkins University, Caltech and the University of Michigan during the period 1934-38, publishing nine papers, most on structures of triiodide salts and those of related interhalogen anions. She was recognized by Linus Pauling for making significant progress in understanding the bonding in these ions, and in 1938, she was elected Fellow of the American Physical Society at the age of 36. Mooney would continue spending summers at other institutions, including Argonne and Oak Ridge National Laboratories, Polaroid, DuPont and the Massachusetts Institute of Technology (MIT). Besides giving Dick Marsh his start in crystallography, while at Newcomb, Mooney was mentor to Ruth R. Benerito (1916-2013), a noted chemist and inventor who spent most of her career at the USDA Southern Regional Research Center in New Orleans, where she invented wrinkle-free cotton fabrics. In an oral history, Benerito spoke warmly of Mooney, "*I earned my masters in Science and Physics from Tulane University. And it was because of Rose Mooney, who later became Rose Mooney Slater who taught me after school, and I earned my degree in*

1938 in physics and x-ray crystallography. . . . She was in physics and I understand she had something to do with the beginnings of the atomic bomb? . . . Well I graduated on ´35 and I came back to teach high school, she taught me the evening after school and I got my degree in ´38. Then in ´41 she went to the University of Chicago, she had graduated from there. . . . So that was an exciting time to be at the University of Chicago during the war years. And she was there when I was there."

Guggenheim Fellowship: In 1939, R. C. L. Mooney was awarded a Guggenheim Fellowship with chemistry as the field of study, for "researches into the structure of crystals, in particular by methods of x-ray analysis". The tenure of the award was for twelve months beginning September 1, 1939. Apparently, her intent was to study in Holland, but events in Europe were deteriorating as WWII approached. She had been in that country during the month the fellowship period began, but returned to the U.S. from Rotterdam, arriving on September 29, the same month that Germany invaded Poland. Germany invaded The Netherlands on 10-May-1940, and the country surrendered five days later. Mooney's obituary in *Physics Today* states that she spent a year in Leiden, however it appears that she had to abort her studies very soon after they began on account of the war. She apparently carried out her studies at MIT instead, as the MIT President's Report for 1939-40 states "*The X-ray branch had as a guest Professor Rose C. L. Mooney of Newcomb College, who was prevented by the war from carrying on research in Europe under a Guggenheim Fellowship*." During this visit, the chairman of the Department of Physics was John C. Slater (see later).

Manhattan Project: When the US entered WWII in December of 1941, preliminary research was already underway into the nuclear physics of uranium and the recently-discovered (May 1940) element plutonium. In 1945, this work would ultimately result in the plutonium implosion bombs exploded at the Trinity Site and over Nagasaki as well as the U^{235} atomic bomb used at Hiroshima. Only a month after Pearl Harbor was bombed, the Metallurgical Laboratory (Met Lab) was created at the University of Chicago, with emphasis on preparation of plutonium from uranium in nuclear piles, its purification, and understanding the chemistry of plutonium and other transuranium elements. The Met Lab was the precursor of Argonne National Laboratory. A number of scientists who would later become prominent crystallographers were involved in the Manhattan Project. Both Isabella and Jerome Karle worked as chemists in the Met Lab on the rather complex chemistry of plutonium. Joan R. Clark was a math assistant for the Manhattan Project in 1943, before she became involved in crystallography. There were likely others. A major problem with studying Pu metal was that it existed in six allotropes, and its chemistry was also difficult to study because only microgram quantities were available early in the project. William H. Zachariasen (1906-1979) was renowned for performing "X-ray miracles" in interpreting powder diffraction patterns from extremely small samples. He joined the Met Lab to establish an X-ray crystallography laboratory to study the crystal chemistry of transuranium compounds, and it is unsurprising that he chose his former student Rose Mooney to assist him. She took a leave of absence from Newcomb 1943-44 to become Associate Chief of the Met Lab's Structure Section, thus becoming one of the highest-ranking women in the Manhattan Project. Henrietta Anne Plettinger (1917-2012), who was a 1939 graduate of Sophie Newcomb, also came to the Met Lab and became an assistant to Will Zachariasen in 1943. She was also instrumental in the Structure Section, taking many if not all of the powder diffraction images for him. Plettinger would later spend 30 years at Argonne, become a renowned photographer, coauthor nine papers with Zachariasen and become an environmental activist after retirement to her native south Louisiana.

William Zachariasen, Rose Mooney, and H. Anne Plettinger.

It is not entirely clear to what extent Mooney and Zachariasen worked together in the Met Lab. The work at the time was of course top secret, and did not begin to see the light of publication until about 1948, after it was declassified. The two clearly collaborated on a very important study of the crystal structures of the oxides of plutonium. However, during 1948 and 1949, as sole author, Mooney published papers in the new journal *Acta Crystallographica* on the structures of $ThCl_4$ and UCl_4, "element 43" (technetium), and lanthanide phosphates. H. Anne Plettinger took the diffraction photographs for the actinide tetrachloride paper. The bismuth phosphate process, patented by Glen Seaborg, was used for separation of all the plutonium used in the Nagasaki bomb from other materials from the nuclear reactors. Mooney determined the structures of three polymorphs of bismuth phosphate as well as other bismuth compounds.

Mooney's marital status at this time is uncertain. In their book on women in the Manhattan Project, *Their Day in the Sun*, Howes and Herzenberg point out that there were very few female physicists at the time, and if married, they were "generally treated as talented amateurs." They incorrectly state that Mooney "married only after establishing her reputation as a crystallographer." It may not have been well known at the time that she was (or had been) married. From his WWII draft registration document, it appears that she was still married to her first husband as late as 1942. Carroll Mooney remarried in 1946, so they were certainly divorced by then.

By late 1944, the exploratory work of the Met Lab was essentially complete and the project shifted to the plutonium production phase. Rose Mooney returned as head of the Physics Department to Newcomb, where she would remain for another eight years.

National Bureau of Standards: In 1952, Rose Mooney left Newcomb College for a position as a senior physicist at the National Bureau of Standards (now National Institute of Standards and Technology), where she worked for four years with Howard F. McMurdie (1905-2004). The following year, he established the highly productive ICDD Research Associateship. NIST maintains no records about Mooney's activities at NBS, but Alan Mighell recalls McMurdie's comments that "*…she was well liked, highly respected and that she played a pivotal role in*

establishing a long tradition of crystallography at NBS/NIST." From her *Acta Cryst*. publications during this period, it is clear that she continued her work begun during the Manhattan Project on structures of phosphate compounds, including phosphates of scandium, indium, thallium, aluminum, and gallium. In 1954, midway through her tenure at NBS, she married John Clarke Slater of the Department of Physics at MIT, whom she had likely met during her summer work away from Newcomb early in the WWII years. Jenny Glusker recalls, "*I do remember that John Slater came to crystallographic meetings for a while and we all said it was because he liked to see Rose*." It was the second marriage for both, and both were in their mid-50s.

R. C. L. Mooney-Slater and John Slater.

Massachusetts Institute of Technology: In 1956, Rose Mooney-Slater left NBS to join her husband as a research physicist at MIT, where she would spend the next ten years. Her research there continued along similar themes to those in previous positions, particularly structures of phosphates. She published her Manhattan Project work on bismuth phosphate polymorphs while at MIT, as well as further work on gallium, indium and thallium phosphates and the structure of tetragonal uranium disulfide.

A glimpse into Mooney-Slater's MIT years, albeit not a terribly complimentary one, was provided in an AIP oral history by Elsa M. Garmire, who was a graduate student in physics at MIT in the early 1960s. Garmire was briefly assigned to Mooney-Slater's lab because she was "the one woman on the faculty." Later to become an accomplished laser expert, fellow in both the APS and Optical Society of America, she was not cut out for Mooney-Slater's brand of inorganic crystallography, and would have found Watson and Crick's DNA-related work or study of phase transitions more interesting. Garmire was distressed because Rose "didn't do any *physics*" and read only *Acta Crystallographica*. Interestingly, she was also under the impression that "she had never been married" before Slater.

Dedication of the Pepinsky X-RAC Synthesizer, Alabama Polytechnic Institute, April 21, 1949. Left-to-right are Martin J. Buerger, Carolina H. Mac Gillavry, David Harker, Rose C. L. Mooney, and A. Lindo Patterson.

In several of her publications from this era, Mooney-Slater acknowledges Raymond Pepinsky at Penn State for the use of his X-RAC analog computer for computing structure factors and Fourier maps. This revolutionary device, which displayed contours on a cathode ray tube and sped up crystallographic computations enormously was built in Auburn, Alabama and later moved to Penn State. Rose Mooney had been present at the dedication of this invention in 1949, along with a number of other notable crystallographers.

ACA and other Organizations: Rose Mooney was very active in the ACA and IUCr from the beginnings of those organizations. When the American Society for X-ray and Electron Diffraction (ASXRED) and the Crystallographic Society of America (CSA) merged at the beginning of 1950 to become the American Crystallographic Association, she was appointed as a member of the Data Standing Committee. She was present at the first congress of the IUCr (Harvard, 1948) and published two papers in volume 1 of *Acta. Cryst*. She was also one of the original members of the USNCCr in 1951. Mooney was a charter member of the Southeastern Section of the American Physical Society and served in many capacities in that organization while at Newcomb, including chairman (1946-47). Jenny Glusker recalls "*She was a delightful lady and whenever she went to a crystallographic meeting and found herself among students and others that she did not know, she would introduce herself by name and invite people to come and talk to her. She was greatly admired for her careful work. I was just a postdoc at the time but I will always remember her with admiration*."

Photo credit: AIP Emilio Sergre Visual Archives, Physics Today Collection

Florida: In 1965, when John Slater reached the retirement age of 65 at MIT, the Slaters moved to the University of Florida, where the retirement age was 70, he in the Physics Dept. as a Research Professor in the Quantum Theory Project and she as a research professor in the Dept.of Chemistry. Both spent the remainder of their lives there. She taught physics but published no further crystallography, being in the twilight of her career just as automated diffractometers were beginning to become available. Rose retired in 1974, John Slater died in 1976, and Rose died on 21 November 1981 at the age of 79. They are buried together in Evergreen Cemetery in Gainesville.

Further Material: Both John and Rose Mooney Slater were among the 235 signatories of the congratulatory scroll presented to Max von Laue on the occasion of his 80th birthday, at the Cornell ACA meeting, July 1959.

Mooney-Slater bequeathed her husband's papers to the American Philosophical Society, and the Slater estate also donated a collection of her diaries and letters. These include letters between the two before their marriage, her correspondence with H. Anne Plettinger (1944 - 1976), and correspondence with Ray Pepinsky, Will Zachariasen and others. The American Philosophical Society Library, is located at 105 South Fifth St., Philadelphia, PA.

Acknowledgements: Thanks to Jenny Glusker, Alan Mighell and Bill Fronczek for their assistance.

Frank Fronczek

The 2017 Elizabeth A. Wood Science Writing Award was given to **James O'Brien** for bringing science to the attention of a wider audience. Jim is a theoretical chemist who did molecular orbital calculations on Organometallic species. He retired from Missouri State University as a 'Distinguished Professor'. The idea for this cover came from Jim. Because the title of his talk is 'Famous Mad Hatters', it seemed natural to invoke Alice in Wonderland images.

Jim O'Brien was born in Philadelphia on the 4th of July. He received a BS in Chemistry from Villanova and a PhD in Chemistry from the University of Minnesota. Following a postdoc at Los Alamos, he taught Inorganic and Physical Chemistry for 35 years at Missouri State University in Springfield. While at MSU, he received three research awards and three teaching awards, including the Governor of Missouri's Award for Teaching Excellence in 2001. In 2002 he was named Distinguished Professor.

Now retired, he does volunteer work at a Springfield hospital. He continues to lecture on Sherlock Holmes as well as "Famous Mad Hatters". In 2013 his book, The *Scientific Sherlock Holmes: Cracking the Case with Science and Forensics* (Oxford University Press)[1], won an Edgar Award as the best book of the year in the critical/biographical category. One of the most popular and widely known characters in all of fiction, Sherlock Holmes has an enduring appeal based largely on his uncanny ability to make the most remarkable deductions from the most mundane facts. The very first words that Sherlock Holmes ever says to Watson are, "How are you? You have been in Afghanistan, I perceive." Watson responds, "How on earth did you know that?" And so a crime-solving legend is born. Indeed, one reason for Holmes's appeal is his frequent use of the scientific method and the vast scientific knowledge which he drew upon to solve mysteries. For instance, in the heart of the book Jim reveals that Holmes was a pioneer of forensic science who made use of fingerprinting well before Scotland Yard adopted the method. One of the more appealing aspects of the book is the description of how handwriting analysis was used to capture the New York Zodiac killer and to clinch the case against the Lindbergh baby kidnapper.

Sherlock Holmes was knowledgeable about several sciences, most notably chemistry. The book takes a close look at Holmes the chemist and discusses, for example, chemical poisons such as carbon monoxide, chloroform, and Prussic acid (the historical name for hydrogen cyanide). The author also debunks Isaac Asimov's famous assertion that Holmes was a blundering chemist. In addition, the book discusses mathematics, physics, biology, astronomy, meteorology, and geology, always in the context of Holmes's exploits.

In 2014 Jim was the Distinguished Speaker for the Baker Street Irregulars' annual Sherlock Holmes meeting in New York City. The **Elizabeth A. Wood Science Writing Award**, was named in honor of Elizabeth Wood, President of the ACA in 1957; she was the author of many science books for lay readers. It is important that the recipient should have written books or articles that bring science to the attention of a wider audience.

References

1. The Scientific Sherlock Holmes: Cracking the Case with Science and Forensics. Open a web browser; go to Barnes & Noble.com; choose Books; type in the book title.

2. J. F. O'Brien, "A Case Study of the Hatters Disease: Boston Corbett", *The Chemist*, 1997, **74,** 10-12.

3. J. F. O'Brien, "Faraday's Health Problems", *Bull. Hist. Chem.*, 1991, **11**, 47-50.

4. J. F. O'Brien, "Sherlock Holmes: The Eccentric Chemist", a chapter in Chemistry and Science Fiction, edited by J. H. Stocker, American Chemical Society, Washington, D.C., 1998, pp 105-125.

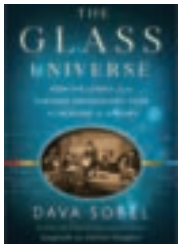
5. C. M. Teague, T. A. O'Brien, and J. F. O'Brien, "Theoretical Comparison of the Bonding in $CpCr(CO)_2NX$ [X = O, S, Se, Te]," *J. Coord. Chem.*, 2002, **55(6)**, 627-631.

6. J. F. O'Brien and D. T. Haworth, "Organometallic Computational Exercise: Semi-empirical Molecular Orbital Calculations on $(C_6H_6)Cr(CO)_3$" and $(B_3H_3N_3H_3)Cr(CO)_3$, *J. Chem. Education* 2001, **78**, 134.

7. J. F. O'Brien and J. Pranata, "Ab Initio Study of the Base-Promoted Hydrolysis of N-Methylformamide", *J. Phys. Chem.*, 1995, **99**, 12759-12763.

8. J. F. O'Brien and T. A. O'Brien, "Molecular Orbital Study of the Anionic Carbonyl Cluster, $Fe_2Co(CO)_9CCO^-$, and the Products of its Reactions With Phosphines", *Organometallics*, 1992, **11**, 3340-3343.

The Glass Universe: How the Ladies of the Harvard Observatory Took the Measure of the Stars Dava Sobel, Viking Press, ISBN 978-0-670-01695-2



When we think of the scientists and astronomers who studied the far reaches of our universe, men like Galileo Galilei and Stephen Hawking often come to mind. But Dava Sobel's latest work tells the untold story of the women who worked at the Harvard Observatory over the course of the late 19th and early 20th century, mapping the stars and paving the way for future generations of astronomers and astrophysicists to study the mysteries of our universe.

Sobel begins her narrative with the recently widowed Manhattan socialite and benefactor of the National Academy of Sciences, Anna Palmer Draper, who came to Harvard following the death of her husband to pursue her true love of the stars. She worked with Dr. Edward Pickering of the Harvard College Observatory.

Anna Draper established the Henry Draper Memorial, a means by which she could funnel her considerable funds into the observatory's coffers, fueling Pickering's research. Draper's deceased husband had desired to photograph the spectra of the stars, and it became her pet project to see his unfulfilled dream realized. She donated numerous pieces of equipment to the observatory that would be used by future generations of female researchers.

One of these researchers started out as Pickering's maid. Williamina Paton Stevens Fleming went from dusting bookshelves to establishing a system for classifying stars by their spectra. She worked as a female computer for the Harvard Observatory (even in the 1800s, men still preferred to have a woman do the math—not much had changed 70 years later when women were doing most of the calculations for the Apollo missions at NASA). Fleming was also a curator of astronomical photographs at Harvard—a highly coveted position.

But Draper and Fleming are only two of the incredible women who contributed to the Harvard Observatory successful ventures into studying the stars, and it would do these women, and Ms. Sobel a disservice if I were to futher discuss them here. If you want more (and you should), read *The Glass Universe*.

The Greatest Story Ever Told – So Far: Why Are We Here? Lawrence M. Krauss, Simon and Schuster, Inc., New York, 2017, 336 pages, ISBN-13: 978-1476777610

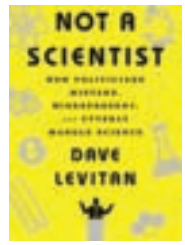
I first learned of Professor Krauss when he published *The Physics of Star Trek* in 1996. I have read most of the books he has published since then. When Krauss was interviewed on Science Friday in March, I immediately pre-ordered my copy of this title.

This book is thought provoking. The three divisions of the book share titles with divisions of another book often referred to as "The Greatest Story Ever Told": Genesis, Exodus and Revelation. The prologue describes why Krauss has chosen this particular title and then uses the rest of the book to provide evidence for the secular version of The Greatest Story Ever Told.

The book is actually a history of modern physics. Krauss follows the timeline through the discovery of the forces of nature: gravity, electromagnetism, the weak nuclear and strong nuclear forces, and the theories that unify the forces, and the tools to validate the theories. The history ends with the experiments at the Large Hadron Collider and Laser Interferometer Gravitational-Wave Observatory. The last chapter attempts to answer the title question from the secular and non-secular point of view. You will have to decide which you choose.

The author artfully chooses a quotation to open each chapter. I particularly liked the opening for the Chapter titled "More Questions than Answers": "A fool takes no pleasure in understanding, but only in expressing his opinion" – Proverbs 18:2.

Not a Scientist: How Politicians Mistake, Misrepresent, and Utterly Mangle Science, David Levitan, W. W. Norton & Company, New York, 2017, ISBN-13: 978-0393353327



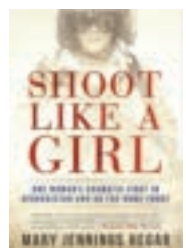
This is another book I learned about on Science Friday. The author is a science journalist whose credentials include a Master's in journalism from NYU program and published articles in periodicals like *Scientific American* and *Time*.

The author walks the reader through 13 different methods politicians use to debunk science. Most of the book was written before 11/9/16 but the forward does cover more recent events. The author goes through each of the methods, which you will likely recognize, and provides real-life examples of how politician used those methods. Here are the tricks of the trade:

The Oversimplification, The Cherry-Pick, The Butter-up and Undercut, The Demonizer, Blame the Blogger, Ridicule and Dismiss, The Literal Nitpick, The Credit Snatch, The Certain Uncertainty, The Blind Eye to Followup, Lost in Translation, The Straight-up Fabrication and last but not least Conspicuous Silence.

The author attempts to alert us to politicians who use these tricks and what to do to combat them. Some are so ludicrous you will laugh, but then you will either get mad or sad because these lies live on. The book is a quick and easy read, and while numbers are discussed, it is done only to illustrate how data is easily manipulated to "prove" a desired point.

Shoot Like a Girl: One Woman's Dramatic Fight in Afghanistan and on the Home Front, Mary Jennings Hegar, New American Library, New York, ISBN 978-1-101-98843-5



Mary Jennings Hegar's memoir about her time in the US Air Force and California National Guard is a must-read. In it, she shares her experience as a woman in the US armed forces.

Her story isn't about what she was able to achieve in spite of being a woman, but rather what she was able to achieve in spite of being subjected to the abuse and prejudice aimed toward women like herself in the military.

She eloquently mixes the good with the bad with the ugly, giving enough personal detail to make her narrative compelling, but not so much that is belies the point at hand. She covers her abuses, both at the hands of a military doctor and those of her

first husband. But she also covers her triumphs--moments shaped by trust and comradery, including the circumstances by which she earned a Purple Heart.

It is partly thanks to Mary Jennings Hegar that women are now allowed to fight in active combat. After her retirement from the military, Hegar joined the ACLU lawsuit to further gender equality in the military, which resulted in the removal of the sexist and outdated policy.

Part of what makes the book feel so authentic is the occasional blackout text, where the Department of Defense deemed certain details not fit for public consumption.

Shoot Like A Girl was a quick, cleverly written and honest read. I enjoyed it immensely, and I would recommend it to anyone with an interest in dogs, guns, the military, or strong female role models.

Skills for a Scientific Life by John R. Helliwell, CRC Press, Boca Raton, 2017, 215 pp., ISBN-13: 978-1498768757

When I agreed to review this book I had no idea that Helliwell would reference me as a reviewer in his chapter on how to review a book. Nevertheless, I kept this review unbiased just like the previous review I wrote for a book by the same author.

Helliwell has been a scientist of renown for both his contributions to the crystallography community as well society in general for over three decades. In recognition of his contributions to the crystallographic community, Helliwell was named winner of the American Crystallographic Association's 2014 Patterson Award and the European Crystallographic Association's 2015 Max Perutz Prize, just to name two of his many honors.

In this book the author sets out describe how to be a good scientist and a good citizen. While the book is directed towards academic scientists and scientists-to-be, industrial scientists will benefit from reading it. For example, the chapter on promoting gender equality is relevant to all aspects of human endeavor given the recent steps backward we have been reading about lately. This book is half memoir and half how-to-manual. In other words, Helliwell provides guidance on being a well-balanced scientist through numerous examples from his own scientific career.

The book is broken down into eight sections consisting of 34 chapters. Each chapter is a short essay covering a particular topic, so the book is an easy read. The sections broadly cover how to know if you really are cut out to be a scientist, how to be a better researcher, how to be a good citizen scientist, how to be a good teacher, how reach larger audiences, how to be a leader in the community and guidance on dealing with the outside world.

There is one error, in which Eisenhower is wrongfully given credit for starting the Manhattan Project. This will be rectified in subsequent printings. I do have one complaint—the typeface is rather small. This is typically done to make the reader pay attention, but it is not necessary and makes it difficult for older readers like myself.

Further Recommendations: Another book I recommend is *Thank You for Being Late* by Thomas Friedman. This is *The New York Times* op-ed columnist's latest work. It could not have come at a better time. Friedman does a great job of analyzing an issue, in this case how the latest technology is changing the world and how to have a healthy respect for that change. Perhaps the most important lesson is that life is a learning process and that in order to thrive we have to keep learning.

The final book of The Dark Forest Trilogy, *Death's End*, by Cixin Liu and translated by Ken Liu has come out. This is first class science fiction and when I have some time I will go back and reread *The Three-Body Problem* and *The Dark Forest* to catch any of the nuances I may have missed the first time around.

March is TRYPOD month. Apparently, only 1 in 5 Americans listen to podcasts and podcast publishers are trying to raise the awareness of podcasts to the general public by asking people who listen to podcasts to let others know about them. Here is my contribution. I listen to a wide variety. KCRW's *Left, Right and Center* and KAMU's *1A* are balanced (really) political podcasts. WHYY's *FreshAir* is always a great listen with interviews and reviews for modern living. To balance things out, I listen to PRI's *ScienceFriday* podcast, the *Nature Podcast* and *This Week in Technology* from TWIT.tv. Finally, humor is the best medicine and I really look forward NPR's *Wait, Wait Don't Tell Me* every Saturday.

All reviews by Joseph Ferrara

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Frank C. Hawthorne Selected to Receive the 2018 Martin J. Buerger Award

Frank C. Hawthorne, Distinguished Professor of Geological Sciences at the University of Manitoba, has been selected to receive the 2018 ACA Buerger Award which recognizes mature scientists who have made contributions of exceptional distinction in areas of interest to the ACA. Frank has revolutionized our fundamental understanding of minerals and their behavior in Earth's processes and is seen by many as the world's foremost mineralogist.

Hawthorne has spent his career at the University of Manitoba, from his time as a post-doctoral fellow to the present. His graduate work was done at McMaster University studying amphiboles, the most complex group of rock-forming minerals. His continuing interest in these minerals led to a 1983 journal article (of 308 pages!) for which he was awarded one of his three Hawley Medals.

During his career, Hawthorne has studied an extremely wide range of crystalline materials and with a range of techniques. Using crystallographic techniques to probe long-range order and various spectroscopic methods to evaluate short-range order, Hawthorne has developed an unparalleled intuitive feel for the behavior of atomic arrangements in general. His work has gone beyond the typical bounds of mineralogy and has provided insight into the wider field of solid-state chemistry.

Hawthorne is well-known for his systematic studies of the crystal chemistry of major mineral groups, including amphiboles, tourmalines, staurolites, borosilicates, sulfates, and diverse transition element oxysalts. It has been said that "He has left few stones unturned in the mineralogical world."

Over the past decade, using chemistry, physics and mathematics, Hawthorne has focused on developing a mathematically rigorous understanding of what controls many aspects of the chemical compositions and arrangements of atoms in minerals. The approach he has taken also provides a link between the bond topology of a structure and its thermodynamic properties.

He has received many awards that honor the breadth and depth of his work. Among them, he has received the principal medals from the Royal Society of Canada (1993), the Mineralogical Society of Great Britain (1995), the Geological Association of Canada (1996), the Mineralogical Association of Canada (1999), the International Mineralogical Association (2010) and the Mineralogical Society of America (2013). He is one of few Foreign Members of the Russian Academy of Science (2012). He was appointed a Canadian Research Chair in Crystallography and Mineralogy (2001), was made an Officer of the Order of Canada (2005), and awarded the Killam Prize in Natural Sciences (2008). His prominence is truly international; in 2016 he was elected Honorary Fellow of the Società Italiana di Mineralogia e Petrologia and, in 2017, he was awarded the Fersman Prize from the Russian Academy of Sciences.

Simon Billinge Selected to Receive the 2018 Bertram Warren Award

Simon J. L. Billinge, Professor of Applied Physics, Applied Mathematics and Materials Science at Columbia University and Scientist at Brookhaven National Laboratory, is the recipient of the 2018 B. Warren Award. This award "recognizes an important recent contribution to the physics of solids or liquids using x-ray, neutron, or electron diffraction techniques."

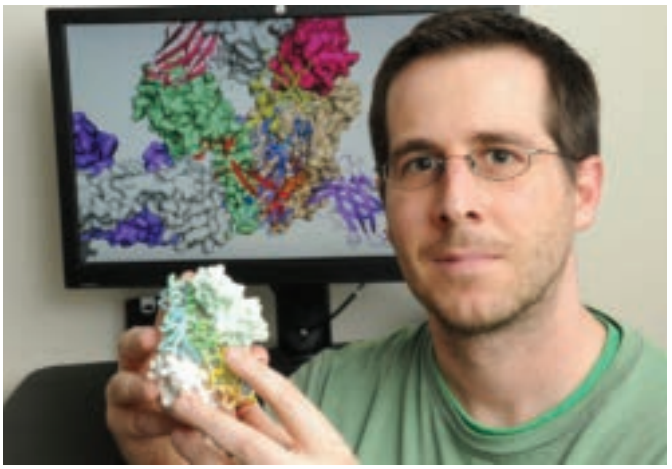
Billinge's career started in the United Kingdom where he earned a BA in Materials Science at Oxford. He moved to the United States, earned a PhD at the University of Pennsylvania in Materials Science and moved to Los Alamos where he was a post-doctoral fellow. He joined the faculty of the Department of Physics and Astronomy at Michigan State University and rose through the academic ranks. In 2008 he moved to his current position at Columbia University.

Materials research seeks to design novel materials where the atomic arrangements on the nanometer scale can be controlled to obtain some desired functionality. One impediment to this is the so-called "Nanostructure Problem." Billinge is being honored for his role in both highlighting this problem and providing seminal contributions to solving it for a bulk sample of nanoparticles. The nanostructure problem is a statement of the fact that when materials get very small (below about 10 nm), traditional x-ray crystallography breaks down because it is based on Bragg scattering which presumes periodic structures. Billinge's work is built around the use of atomic pair distribution function (PDF) methods. He has championed a generic approach which combines diverse experimental results and theory in a coherent computational framework. He is considered the world leader in characterizing structures of nanomaterials. His most significant contributions have come in the application of sophisticated x-ray and neutron diffraction techniques to study local structure property relationships in complex solid state materials.

Billinge is a committed teacher and mentor. Not only has he made highly significant scientific discoveries, he has further developed the theory underpinning the use of PDF approaches to structure analysis and the software tools needed to exploit this approach. These widely used tools have contributed to the explosive growth in the use of PDF analysis for a wide variety of different structure problems. He has taught numerous workshops and has mentored high school students, undergraduate and graduate students, postdoctoral fellows and visiting professors.

Billinge is a Fellow of the American Physical Society, a Fellow of the Neutron Scattering Society of America, and received, with his collaborator Takeshi Egami, the J.D. Hanawalt Award from the International Centre for Diffraction Data.

2018 Etter Early Career Award to Jason McLellan



Jason McLellan, Assistant Professor of Biochemistry at the Geisel School of Medicine at Dartmouth College, is the recipient of the 2018 Margaret C. Etter Early Career Award. This award "recognizes outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career."

Jason earned his Bachelor of Science degree in Chemistry from Wayne State University in 2003 and his doctoral studies were carried out at the Johns Hopkins University School of Medicine under the guidance of Daniel Leahy. Here he learned x-ray crystallography and applied this technique to Hedgehog proteins interacting with a new family of co-receptors. He had started on his path of using structural information to provide insight into the function and evolution of a disease pathway in humans.

From 2008-2013 he was a postdoctoral fellow in the laboratory of Peter Kwong at the Vaccine Research Center (VRC) at the National Institutes of Health. At this time he also met and started collaborating with Barney Graham, the VRC's head of clinical trials and Chief of Viral Pathogenesis. His time at NIH proved very productive, resulting in more than 24 publications, with Jason as first author on eight of them including two papers in *Science*, one in *Nature* and one in *Nature Structural and Molecular Biology*. The structure of the postfusion form of the respiratory syncytial virus (RSV) F glycoprotein formed the basis for a clinical development program at Novartis Vaccines (now owned by GSK). This is significant since there is currently no vaccine available to prevent RSV infection, a major pathogen, and only one drug for its treatment.

Next he was interested in the determination of the structure of the RSV F glycoprotein in its prefusion state. In order to get a crystal he developed a co-transfection and purification procedure to obtain stabilizing complexes of antibodies bound to RSV F. The information from this structure allowed him to engineer a prefusion-stabilized variant of RSV F which elicited high titers of neutralizing antibodies in mice and rhesus macaques. A paper on this work provided proof-of-principle for *structure-based vaccine design* and was declared the runner-up for *Science's* 2013 "Breakthrough of the Year."

In that same year, Jason accepted a position as assistant professor at the Geisel School of Medicine where he continues to pursue his passion for "applying structural information to the rational design of interventions for viruses." He is being very successful. One of his recent projects was highlighted on the cover of *Science Translational Medicine* (May 2017). He and his collaborators have been seeking "to develop a highly potent monoclonal antibody with an extended half-life … that could act as a vaccine surrogate to prevent severe RSV disease in infants" and this paper describes the binding of variants of a potent human monoclonal antibody to RSV F protein. Jason's lab provided structural characterization of the binding of the most potent antibody and provided an explanation as to why certain RSV isolates were not neutralized as well as others.

Jason is a productive scientist who has continued to carry out ground-breaking work as an independent researcher. As one of his colleagues said "I don't know what he will be doing in 10 years, but I am sure it will be interesting – and involve solving important biological and medical problems at the molecular level."

2017 ACA Fellows

The ACA Fellows program recognizes a high level of excellence in scientific research, teaching, and professional duties, but also service, leadership, and personal engagement in the ACA and the broader world of crystallography and science. The program celebrates the excellence of ACA members, and promotes their recognition worldwide to constituencies outside of the ACA. ACA Fellows serve as scientific ambassadors to the broader scientific community and the general public to advance science education, research, knowledge, interaction, and collaboration. This program allows the ACA to significantly recognize and honor a broader cross-section of the membership than was previously possible with other, more specific awards. ***Nominations are collected year-round with the deadline being April 1 of each year.***

Marilyn Olmstead: Early on, it was clear that Marilyn was going to make her mark. In 1965, upon graduating from Reed College, she was named a Woodrow Wilson Fellow. In that era, some called this fellowship the "domestic version of the Rhodes Scholarship." She earned a PhD in inorganic chemistry at the University of Wisconsin, Madison with Dick Fenske and it was during this time that her interest in crystallography was piqued by a thesis committee member, Larry Dahl.

Marilyn spent her career in the Department of Chemistry at the University of California, Davis, starting out as a postdoctoral fellow and lecturer. She worked with several faculty members and learned x-ray crystallography from Hakon Höpe. Because of her knowledge and training, she was hired as the staff crystallographer and the staff research associate responsible for the

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crystallographic facility. She took this as an opportunity to train and mentor generations of students and post-docs in crystallography. Marilyn's expertise led to her being asked to serve on dissertation committees even when she was a staff member. Ultimately, she was appointed to the academic faculty as Professor of Chemistry.

Marilyn's record of publication is impressive. She has more than 820 refereed publications and has deposited over 1600 structures in the Cambridge Structural Database. She is a world leader in the crystallography of fullerenes. These molecules are crystallographically challenging since, being spherical, they tend toward disorder. In a collaboration with Alan L. Balch, she pioneered a technique that revolutionized fullerene crystallography. They co-crystallized the fullerene with a metal-containing porphyrin which enhanced crystallization and reduced inherent rotational disorder. Since that time they have published hundreds of journal articles, often in collaboration with other scholars, featuring new fullerene molecules. In recent years, as she has been pursuing structures of ever more challenging molecules, Marilyn has become a regular user of the ALS synchrotron. Her work has been significant; of 125 papers that ALS considers "highlights," 24 were co-authored by Marilyn.

Service to the scientific community has been an important hallmark throughout Marilyn's career. Her breadth of knowledge led to her serving on the board of editors for *Inorganic Chemistry* and *Journal of Coordination Chemistry*; as an expert analyst for *ChemTracts-Inorganic Chemistry,* and as a co-editor for *Acta Crystallographica, Section E* (the latter for 10 years, beginning at its inception). Throughout her career, Marilyn has reached out to scientists in under-served countries. She has numerous international collaborators, often scholars who have no access to crystallographic equipment, and has also traveled to train crystallographers in their own countries. She has no doubt advanced the careers of individual researchers from countries in eastern Europe, the Middle East and Asia. In 2014 she was named an American Chemical Society (ACS) Fellow based on the strength and productivity of her research work and her service to the ACS community.

Marilyn's volunteerism for the betterment of the American Crystallographic Association has included serving as Chair of the General Interest SIG and as a member of the Continuing Education Committee. She has also served on the United States National Committee for Crystallography.

Marilyn has actively sought to change the face of science. She was the only woman in her PhD class of about 40 students and, over the years, she has worked with and mentored more than 50 women in her lab. The combination of her scientific productivity and her service to the crystallographic community provide a strong basis for her selection as an ACA Fellow.

Brian Toby: Throughout his career, Brian has intertwined his work to advance the state of the art of powder diffraction with an eye toward providing service to the larger scientific community and there are few who have had more impact on the development of both hardware and software in this field.

Early on he, with David Cox, was instrumental in getting the first real high resolution synchrotron effort going at Brookhaven National Laboratory. When he moved to the National Institute of Standards and Technology (NIST) he pioneered the use of web-based proposal submissions, user outreach and data monitoring for the BT-1 neutron powder diffractometer. This established a rapid review cycle and expanded the operation range of the instrument to include more rapid data collection. The combination of these factors resulted in BT-1 achieving the highest publication record of any thermal neutron instrument at NIST.

Brian then moved to the Advanced Photon Source (APS) at Argonne National Laboratory where he was the scientific lead for the construction and commissioning of 11-BM, the first robotically-controlled high-resolution powder diffractometer in the US and the second highest resolution powder diffractometer in the world. He was also responsible for designing and implementing sample management and instrument control systems. Brian's strong belief that synchrotron powder diffraction must serve a wide community resulted in the development of a mail-in service for crystallographers. The system robotically identifies samples and queries a database into which users have entered data collection information and then automates the instrument. The workflow goes beyond data collection to data reduction, transfer of data to users, disposing of the sample and even tracking users' success in completion of their work. This automation allows a single staff member to manage the entire workflow. Because of the integration and automation of these processes, 11-BM has become the highest-publishing beamline in the APS by more than a factor of two.

The contribution Brian has made to the development of data analysis programs for powder data rivals – some might say surpasses - the significance of his contribution to the development of accessible and beneficial powder instruments. He developed a user-friendly General User Interface (EXGUI) for the GSAS crystallographic package. Once again, he was seeking to make Rietveld analysis more accessible to non-experts in the field. To understand the impact of this interface, one needs only to see that his initial paper on this interface has been cited more than 3500 times and that 90^{+} % of GSAS users also use the EXPGUI.

Brian shares his expertise by teaching at instructional powder diffraction workshops and was the force behind the addition of a crystallographic education section within the journal *Powder Diffraction*. He does not just offer ideas, he offers his time – he co-edits this section with James Kaduk.

Besides the significant impact that Brian's hardware and software contributions have had on the crystallographic community, this community has also benefited from his considerable volunteer service. He has served the ACA by, over time, chairing the Neutron SIG, the Material Science SIG and the Synchrotron SIG. Among his other service commitments, he has served on the US National Committee for Crystallography, at one time as its chair, and been a member of the IUCr Commission on Powder Diffraction, the Commission on Neutron Diffraction, and the Committee on the Crystallographic Information File. He has served on the editorial board of the *Journal of Physical and Chemical Reference Data* and as an associate editor for *International Tables for Crystallography, Volume G*.

Over his career, Brian has truly advanced the state of the art in powder diffraction and also served the scientific community by making the technology more accessible to more people. He is a very well-respected scientist with a strong publication record and a deep dedication to the betterment of the crystallographic community.

ACA Members Honored

Nadrian (Ned) Seeman: Ned is one of two ACA members that were among the 228 scholars, artists, philanthropists and business leaders elected in April 2017 as members of the ***American Academy of Arts and Sciences.*** The new members were elected, according to Don Randel, Chair of the Academy's Board of Directors "… to strengthen our capacity to spread knowledge and understanding in service to the nation."

Ned (Margaret and Herman Sokol Professor of Chemistry at New York University) is best known for his pioneering work in the founding and development of the field of DNA nanotechnology. Structural DNA nanotechnology is now studied in scores of laboratories. His recent work includes the creation of self-assembled, three-dimensional crystalline DNA structures and the creation, with colleagues at China's Nanjing University, of a DNA assembly line with the potential to build novel materials on the nanoscale. Among his many other honors Ned was selected as an ACA Fellow in 2014

Leemor Joshua-Tor (Professor and Howard Hughes Medical Institute Investigator at Cold Spring Harbor Laboratory (CSHL)), is the second ACA member who has been elected to the ***American Academy of Arts and Sciences.*** She is also one of 84 new members elected to the ***National Academy of Sciences*** (NAS) in May. The NAS recognizes scholars for "their distinguished and continuing achievements in original research." Joshua-Tor is a structural biologist who studies the molecular basis of nucleic acid regulatory processes. She is well-known for her work in revealing structures involved in the gene-silencing mechanisms of RNAi and also for her work on the E1 helicase enzyme which acts to unwind DNA strands during the DNA replication process. CSHL President Bruce Stillman was quoted as saying "Leemor Joshua-Tor has used structural biology to provide valuable insight into some of the most fundamental aspects of how our cells work, including how the genome is copied and how gene expression is controlled."

Jane Shelby Richardson (James B. Duke Professor of Medicine, Biochemistry and Professor of Biochemistry at Duke University), was one of seven researchers who received the ***2017 Fellow of the Biophysical Society Award***. This award honors the Society's distinguished members who have demonstrated sustained scientific excellence. Richardson is recognized for "her tremendous contributions to advancing our knowledge of the beauty and complexity of protein structure." Richardson has worked in crystallography since the time when only 2 protein structures had been solved. Since then she has solved many important protein structures but, since the "beauty … of protein structure" was one reason for this award, it is valuable to remember that it was she who realized that a generalized scheme could be developed to describe the recurring patterns of structural motifs in folded proteins. Before Richardson we did not have those beautiful ribbon drawings that have graced the covers of so many scientific journals. Jane was elected as an ACA Fellow in 2012.

Shaul Mukamel, is one of three distinguished scholars that were granted ***honorary degrees by the University of Chicago*** on June 10, 2017. Mukamel (Department of Chemistry, University of California Irvine) is a theoretician whose groundbreaking work has changed and advanced the field of spectroscopy, will receive the honorary degree of doctor of science.

Mukamel has played a seminal role in research on molecule-light interactions and their consequences, with contributions to understanding complex electron and nuclear dynamics in molecules. His research has a great impact on the field of ultrafast nonlinear spectroscopy, with applications in physics, chemistry and biology.

His work has additionally created new subfields of ultrafast nonlinear spectroscopy, and provided ways to interpret essentially all experimental research in this field. Over a 40-year career, he has led the introduction of new concepts that illuminate the complexities associated with molecular electronic processes.

His research provided, for the first time, a framework and predictive theory that allowed for the unified description of many nonlinear experiments. His theory was also the first step in developing multidimensional optical and infrared spectroscopy, which revolutionized the way in which molecular spectroscopy has been performed in the 21st century.

Among his many honors, Mukamel has been elected to the National Academy of Sciences and the American Academy of Arts and Sciences, and is fellow of the American Physical Society and the Optical Society of America. He is also one of the Associate Editors for the ACA journal *Structural Dynamics*.

General News

Crystals in Space: No crystals, no crystallography. For this reason researchers continue to search for better ways to grow crystals. ACA member **Edward Snell** (HWI and SUNY Buffalo) has taken his research out of this world. He developed a crystal growing investigation called LMM Biophysics 3 for which crew members aboard the International Space Station started conducting research in April. The investigation looks at why microgravity-grown crystals often are of higher quality than Earth-grown crystals and which crystals may benefit from being grown in space.

Kaitlyn Twesme, a seventh grader from Lake Mills Middle School, Lake Mills, Wisconsin, won the ***Best Quality Crystal Prize for the Middle School Level of the 4th Wisconsin Crystal Growing Competition***. She will work on a program to grow her crystals aboard the International Space Station. Besides the technical aspects of preparing growth conditions for the flight hardware, Kaitlyn will be required to communicate her experiences through a blog. She is hopeful that she will be at the pre-launch press conference at Kennedy Space Center in Florida.

***Cryo-Electron Microscopy: An NIH Initiative*:** The "Method of the Year 2015," according to *Nature Methods* (*Nature Methods*, Vol.13, No. 1, January 2016) was cryo-electron microscopy (cryo-EM). While x-ray crystallography remains a robust technique for solving structures that will crystallize, cryo-EM is especially useful for obtaining structural information from large protein complexes and for systems that exhibit multiple conformational states. Development of direct electron detectors allowed the resolution barrier of 3 Å to be broken in 2015. This, coupled with the development of new data analysis methods, has led to much larger demand for access to this technique. However, the high cost of cryo-EM has limited the method's availability to researchers who are new to the technique.

The NIH Common Fund is seeking to address this by offering a Transformative High Resolution Cryo-Electron Microscopy program that seeks to create national cryo-EM service centers, improve technology and develop on-line instructional materials. This initiative should provide more access to better instrumentation and should "develop an expert workforce of cryo-EM practitioners."

Alexander Tulinsky (1928-2017)

Alexander Tulinsky, a protein x-ray crystallographer at Michigan State University who made seminal contributions to structural biology studies of proteins involved in blood coagulation and fibrinolysis, passed away in early March, 2017 in East Lansing, Michigan. His laboratory determined important early structures of factor Xa, prothrombin fragment 1, human alpha-thrombin and fragments of plasminogen. In addition to providing insights into their mechanism of action, many of these structures were highly sought after for drug discovery in the pharmaceutical industry. Prior to his work on blood coagulation proteins, "Doc", as he was affectionately known to all of us in his laboratory, had characterized transition-state mimics of alpha-chymotrypsin, another serine protease in the trypsin family.

Doc's beginnings were humble ones. He was born in 1928, the

son of Russian immigrants and raised in a small row house in south Philadelphia. Although later in life he would distinguish himself in the growing field of structural biology, his first nationwide recognition came not in science, but in sports. In 1945, Al quarterbacked his South Philadelphia high school football team to win the city title, in a game judged by a panel from the Daily News in 1986 to be "the greatest high school sporting event in city history" ***(www.tedsilary.com/archive/bestgames.htm)***. Coming back from a 13-0 deficit, Southern won that game in the final seconds in a trick play out of field goal formation, with Al (the quarterback and would-be holder) catching the winning touchdown pass on a fake field goal. In WWII-era America, when high school football was a big draw, the game was witnessed by an estimated 54,000 spectators and was shown in movie house newsreels across the country. The penchant for taking risks that Al demonstrated on the football field that day would continue throughout his career.

Choosing an academic scholarship over an athletic one, Al earned an undergraduate degree in chemistry at Temple University. He went on to get a doctoral degree at Princeton under the direction of John White, where he was introduced to crystallography in a research project involving benzene derivatives and was inspired by White's work on vitamin B_{12} to pursue larger structures. That opportunity came in 1955 when he took a post-doctoral research position with the Protein Structure Project at the Polytechnic Institute of Brooklyn. The PSP, formed in 1950 by David Harker, was committed to determine a protein x-ray crystal structure, targeting ribonuclease, within ten years - essentially a crystallographic "moon shot" at a time when the first structure of myoglobin was still years in the future. Doc's firsthand account of that period, "The Protein Structure Project, 1950-1959: First Concerted Effort of a Protein Structure Determination in the US" (Annual Reports in *Medicinal Chemistry*, vol. 31, 1996) underscores the tremendous technical hurdles they had to overcome and the advances in methods and instrumentation in those early years that helped pave the way for the success of this nascent field. The structure of ribonuclease was eventually solved in 1967, a bit later than the original 10-year goal. It was also during this time that Al married his wife Marjorie and started a family that would grow to include four sons: Tom, Bill, Alex, and John.

In 1959, as the PSP prepared to relocate to the Roswell Memorial Park Institute in Buffalo, Al took a faculty position at Yale; there he focused on smaller, more tractable structures as he worked to establish his own laboratory. In 1965 he moved to the Chemistry Department at Michigan State University, where

he remained for the rest of his career. The first publications on alpha-chymotrypsin and aldolase came out of his lab in the early 70's, marking the beginning of a productive program in protein crystallography. A 1971 paper (Vandlen & Tulinsky, Acta Cryst. B27, 437) describing a computer program for the new automated diffractometers, "currently prominently in vogue", which was developed to realign crystals slipping in the capillary mount over the course of a multi-day data collection, is a reminder of the problems still being addressed at that time. Doc was always very proud of the careful attention that he paid in measuring x-ray diffraction data from the in-house diffractometer and area detector, and he instilled this spirit in his students and post-docs. He enjoyed working on the instruments himself, and although he was initially a skeptic of synchrotron x-ray data, he soon realized its value. Al was an excellent writer with several high-impact and well-cited publications, often choosing to give last authorship to a lab member or collaborator, even in cases when he had done most of the writing. Over the years, Al and his students and post-docs published more than 150 research publications in top scientific journals, bringing worldwide recognition to his program at Michigan State University.

Al's enthusiasm for science was matched by a passion for his hobbies. In Michigan, he became an avid fisherman and duck hunter. Jim Gaier (MSU, 1983) recalls, "We didn't see a lot of him during duck season! But he always stopped in at the beginning or end of the day to check in with us." Doc also was a loyal and knowledgeable fan of Spartan football and basketball programs and Detroit sports. He had season tickets to MSU's basketball games and sometimes a lucky lab member or two was given an extra Spartan basketball ticket. Those were special moments to be cherished, one-on-one time with Doc, when he would analyze each minute of the exciting Spartan game.

For those in his lab, Doc was a mentor and role model in life as well as science. Usually arriving early to the lab in his signature jacket and bow tie, his manner was sometimes a bit gruff, but he was a good-hearted man who offered small unexpected kindnesses and many words of fatherly advice. Life in the lab reflected his example of integrity and honesty, a willingness to help others and gratitude for help received. Ewa Skrzypczak-Jankun, a researcher in the lab for many years, remembers how he always made a special effort to learn the correct way to pronounce a person's name, so that whoever came to his laboratory, from whatever part of the world, was always addressed properly. Despite his success and the high regard he had earned in the field, Doc remained as humble and unassuming as his upbringing. As Tom Pinnavaia, Al's long-time MSU Chemistry department colleague, friend, and duck-hunting partner, remarked while delivering a eulogy at his funeral "I always got a kick out of the bemused expression on people's faces when they came to realize that the man in bib overalls was Princeton-educated and a University Distinguished Professor at Michigan State University."

Although Al's physical health had been failing lately, Tim Rydel (MSU, 1990), who visited recently, noted that he seemed happy and at peace and was still "sharp as a tack." In Al's own words from his 1996 paper, reflecting on the the past achievements and future promises of crystallography, "I would still not trade the experiences of my marvelous past for all the wonders that most certainly lie ahead." Those of us who had the privilege to know him as teacher, mentor, colleague, and friend, remember Al Tulinsky with fondness and gratitude for the difference he made in our lives.

Anne Mulichak and Ravi G. Kurumbail

Robert Rosenstein (1922 - 2017)

Art Olson remembers: Robert Rosenstein, career crystallographer and teacher passed away on February 19, 2017, he was 94 years old. Bob got his BS and MS degrees from the Polytechnic Institute of Brooklyn, and after serving in the U.S. Army during WWII, received his PhD from Cornell University. Bob was a crystallographer's crystallographer, teaching the science and art

of the subject for many years in the Crystallography Department at the University of Pittsburgh.

I first met Bob during his occasional visits to Berkeley in the 1970's, when I was a graduate student with David Templeton. He was always keen to discuss the latest results in the expanding scope of crystallography during that time. After Bob retired, he moved to San Diego, and we reconnected. Since he wanted to have a "scientific home" he became a visiting scientist in my laboratory from that time until he passed away. Up until his last month, he would still attend my group meetings. He had many interests aside from crystallography, including linguistics. He was in the process of learning Japanese in the last year of his life.

Bob always kept a strong affinity for crystallography, and wanted to aid the study of crystallography into the future. Thus he made a generous bequest to the ACA to support student travel to ACA events – the details of which will be announced once his estate is settled. Bob had an endearing personality and a sharp wit, and will be missed by his friends and colleagues. Below are remembrances of Bob by Helen Berman and Ned Seeman.

Helen Berman remembers: I first met Bob Rosenstein when I was a graduate student at the University of Pittsburgh in the 60's. I shared an office with Bryan Craven across the hall from Bob's office. Bob would come into my office and with no preamble or introduction, launch into a description of some aspect of crystallography that he thought was important for me to know at that moment. It could be about how to determine unit cell dimensions, or how best to analyze a Patterson map or how to do direct methods. He always wrote on the chalk board and was very patient in his descriptions. This happened almost every day. In addition to his teaching skills, Bob was incredibly talented at growing crystals although in this case he never really revealed his methods. He had a little cabinet in his office in which he stashed his experiments and he checked on the samples at random parts of the day. If he got good crystals he would be sure to call me over to look at the results of his labors. He was justifiably proud of his crystallization successes. And I was lucky in that I was often the recipient of some of these crystals whose structures became part of my thesis work.

Bob loved to tell stories often about crystallographers he knew. When I eventually met these individuals, I felt as if I knew them already because of Bob's sometimes hilarious descriptions. Bob was a kind and generous person with whom I kept in touch for many years after I left Pitt. We eventually did lose touch and so I was surprised when he called me a few years ago to ask how he might help the ACA. I was thus very pleased to learn that in his will, he provided for student travel support to ACA meetings.

***Ned Seeman remembers*:** I first showed up in G.A. Jeffrey's crystallography laboratory at Pitt in early September, 1967, nearly 50 years ago. Within my first week there, I met Bob. I asked him his name, and he said, "Bob, just Bob." I started off somewhat befuddled, as most new grad students are, and I took the crystallography course mostly given by Bryan Craven, but with lectures by other faculty, including Bob. He certainly gave the clearest lectures on symmetry elements, and their matrix representations that I ever heard. He also spent an entire class period on how to use Volume I of the International Tables for Crystallography, something that was of immense value to me and my classmates.

Bob was arguably the best teacher I ever encountered. In my era, he had no students himself, but he kibitzed on just about every project that any student was pursuing. He was the one who patiently taught me how to solve structures and how to run all the programs that were necessary to obtain those solutions. In contrast to one of his less effective colleagues, he told us correctly that structures were not solved by least squares. Nothing was too simple or trivial for Bob. I wrote a Patterson Superposition program, and the first thing I had to do was put the data on disk. I just finished doing that when we all went to the Buffalo ACA meeting and he would tell people there that I had just completed doing this very easy task, as though it were a major accomplishment.

I moved on from Pittsburgh to two institutions well up the academic food chain from Pitt. It was a remarkable testament to Bob's excellence as a teacher that I found myself working with students who were far advanced over me in years of experience, but who knew much less about crystallography than I did. They knew many other things from their courses and from their exposure to superb colleagues and instructors, but they hadn't been *taught* how to do crystallography, in the way that I was fortunate to have Bob teach me.

Bob had his own way of thinking about the world, and it was often incompatible with the way American science worked. He was never comfortable writing grants, and he was interested in what he was interested in and not in the goals of the grants funding the laboratory. This attitude resulted in his moving around a lot, and certainly did not generate an easy life, either for him or for some those with whom he interacted. Nevertheless, those who knew him will never forget the brilliance and insightfulness of his mind and his phenomenal skill at imparting his knowledge to students.

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Bryan Maxwell Craven (1932-2017)

We are saddened by the death of our colleague and friend Bryan Maxwell Craven on May 2, 2017. He leaves behind his wife Pat, four children and six grandchildren.

Bryan was born in Wellington, New Zealand and received his PhD in Chemistry from the University of Auckland. He came to the United States to work with George Allen Jeffrey in the University of Pittsburgh. He was on the faculty as a professor and later as the chair of the Crystallography Department from 1987-1995. He also had a long standing collaborative appointment at Brookhaven National Laboratory. After his retirement, he continued to teach crystallography at Indiana University Pennsylvania. He was an active member of the crystallographic community and served as president of the Pittsburgh Diffraction Society and the American Crystallographic Association. He also taught in the ACA Crystallographic Summer School. His principle scientific interest was understanding the crystal structures of small biologically important molecules at the highest possible resolution using both x-ray and neutron diffraction.

Bryan was brilliant, insightful and fun to be with. The three of us were in Pittsburgh in the 60's and offer our remembrances of this very special person.

Helen Berman remembers: I first met Bryan in 1965 when he came back to Pittsburgh after a sabbatical in Australia. We shared an office in Thaw Hall and I got to see first-hand how he approached every problem using experimental, computational and manual analyses. Our office was actually a small lab with a long bench that Bryan used to make models and analyze the hydrogen bonding patterns. I was also lucky enough to take his crystallography course and have kept his notes that I have used in my own teaching.

ACA 1988 in Philadelphia: left to right - Charlie Bugg, Helen Berman, Catherine Foris, fox chase secrety, Bryan Craven, Vivian Cody and Bill Duax.

Bryan loved his cigars and beer and we all used to love to go out for "grub" in Oakland. We had informal parties in one another's homes with the many visiting scientists from around the world joining in these get togethers. Pat who was my friend from college met Bryan at one of these dos and the rest is history.

Bryan, Pat and I kept in touch after I left Pittsburgh in 1969. We saw one another at ACA meetings especially during the years that both Bryan and I were on the ACA Council. We also visited one another socially in Pittsburgh, Indiana and New Jersey. Their house in Pittsburgh was beautifully and imaginatively decorated. In Indiana, there was a separate little guesthouse adjoining their log cabin. A memorable visit was in 1999 when they came to New Jersey to see their alpaca that was in "confinement" in Stockton. I had no idea that there were alpaca farms in New Jersey. At the farm, I found a barn kitten that lived with me for many years and was a constant reminder of my friends.

The last time I saw Bryan was when he and Pat came to NY to our 50th Barnard reunion in 2014. Bryan had slowed down physically but still had that sharp intelligence and humor.

I feel very lucky to have known Bryan and will miss his intellect, good humor and warm friendship.

Ned Seeman remembers: Like all of us writing about Bryan, we all knew him for about a half-century. I met Bryan on my first full day as a graduate student in Pittsburgh in 1967. He was teaching the introductory crystallography course for a relatively large class, and Jeff told him that I would be taking my comprehensive exam at the end of the semester (Jeff didn't say this was because I was a probationary student). It was the first time I heard his trademark chortle, and he said, while puffing on one of his Marsh-Wheeling cigars, that I should take the class problem set right away, and he gave it to me. I had only a moderate idea what a crystallographer was, but there was something about Bryan that made me say to myself right then, "Ecce Crystallographer". Turned out I was right. Bryan was arguably the most talented and skilled crystallographer I ever met, and one of the most effective. He knew (and taught) the physics superbly, and he used the chemistry to bring up new aspects of electron density distributions. When I was supposed to teach crystallography myself, I got out Bryan's notes and found that I had actually learned nothing new, just repeated what he had taught me.

Left to right: Ned Seeman, Muttaiya Sundaralingam, and Bryan Craven

Bryan was not above doing anything that he felt it was necessary to do. I was in the 'shop' punching cards one night (I said it was 50 years ago), and Bryan came in wearing his ankle-length charcoal-colored lab coat. He was struggling to open a sealed glass bottle of heavy water with a file so that he could deuterate one of his barbiturate structures, and was cursing the glass that was behaving recalcitrantly. He eventually got it opened (not along the file marks he'd made), and proceeded to do the chemistry he needed to do. He was the only person I ever saw in the Pittsburgh crystallography lab actually making and breaking chemical bonds; he looked at what he wanted to do, and then proceeded to do it. Many years later, he drove me up to my grandmother's grave in a cemetery overlooking Route 51, to check out its condition. The grave was loaded with weeds, and I was kind of baffled about what to do; Bryan just solved the problem

US National Committee (1989): Front row - left to right: Bryan Craven, Charlie Bugg, Lyle Jensen, Robert Bryan. Back row - left to right: Art Bienenstock, Hugo Steinfink, Helen Berman, Judy Flippen-Anderson, Peggy from NAS, Cam Hubbard, Carol Brock, Debby Savage, Catherine Foris.

by getting down on his knees and yanking the weeds out of the ground. None who knew him will be surprised that while we were up there, he enthusiastically took a bunch of pictures of me lying on various graves, with a beer can in my hand.

At my first ACA meeting (Buffalo, 1968), I joined him and some of his friends for an afternoon picnic that had a relatively small proportion of food, but a lot of beer. I learned then that there are other things to do at meetings besides attending sessions, one of the most valuable lessons of my life. In 1971, I went to the Cold Spring Harbor meeting, whose topic was macromolecular crystallography. The bulk of the meeting was populated by very elitist-behaving macromolecular crystallographers. I was disdained as a 'small molecule' person, and was feeling kind of lonely. Suddenly, I heard Bryan laughing, and knew it would be a fun conference. Bryan discovered a small room where we could view the sessions on closed circuit TV and a fridge containing 25-cent cans of Piels beer on the honor system. We spent the whole meeting in there, rarely going to the main assembly hall. I had a pretty good time, and I think he did too.

Bryan was always the person whose personality lit up any room he was in. He had a great sense of comic timing, and it was always fun to go to the Pittsburgh Diffraction Conference and watch him direct the proceedings with his subtle humor, whether it was introducing banquet speakers or just moving the conference along. At this point in my life, I'm starting to lose a lot of friends, but I can't imagine anyone whose loss will leave as big a hole in the fun part of my life. I think everyone who knew him will feel the same.

George DeTitta remembers: I met Bryan in the first few days of my first year in the PhD Program at the Crystallography Laboratory at University of Pittsburgh. My first impressions were of his accent – not Jersey City – and of his laugh. Classes began almost immediately and from the first few lectures I thought there could be no better thesis advisor. Bryan took me on, not because I was a stellar student (far from it) but because I enjoyed the science so much. I was willing to make up my intellectual deficit with hard work and enthusiasm.

Our studies together confirmed what a wise choice I had made in an advisor. Bryan proved to match and exceed my enthusiasm and was willing to give me plenty of rope to play out in my research with him. He knew when to play out line and when to reel me in. We continued his studies of fatty acids with the first studies of cholesterol esters and choleic acids. He never took the straightest road to a crystallographic solution but explored new ways, and new wrinkles on old ways, to solve the crystallographic phase problem. I followed him some time after graduation into his experimental charge density studies and it took me quite some time to forge an independent research direction.

In the meantime, we had really become friends. Our humors were at least roughly congruent and our interests in music and arts were similar. Adele and I fell in love with his wife and children. We gave him a kitten from one of the litters we seemed to come upon regularly. Our friendship endured from that day in September 1969 to now, and he is going to be forever a part of me.

Philip Coppens (1930-2017)

As we were going to press we learned that Philip Coppens (Distinguished Professor Emeritus and Distinguished Research Professor in the University at Buffalo Department of Chemistry), passed away on June 21. He was 86.

Coppens was one of the pioneers in crystallography that was still virtually in its infancy when he joined the faculty of University of Buffalo in 1968. He officially retired last fall, but maintained a lab at UB, a postdoctoral researcher and grant funding from the U.S. Department of Energy. His most recent paper was published in May 2017 in *Structural Dynamics* (*Exploring the structural changes on excitation of a luminescent organic bromine-substituted complex by in-house time-resolved pump-probe diffraction,* Krishnayan Basuroy, Yang Chen, Sounak Sarkar, Jason Benedict, and Philip Coppens, *Structural Dynamics* 4, 024501 (2017); http://doi.org/10.1063/1.4978240)

For five decades, he had been a fixture of the chemistry department and a champion for science, whether he was publishing groundbreaking research or judging a crystal-growing contest for kids. A symposium celebrating his 48 years at UB, organized by Jason Benedict and Yu-Sheng Chen, was held at UB in 2016 (***www.buffalo.edu/ubnow/stories/2016/10/coppens-symposium.html***).

A full remembrance of Philip's extraordinary life and career in crystallography will be published in the fall issue of *RefleXions*.

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Budget Tracker – the current status of budget negotiations for research-focused agencies and budget tables that detail the proposed and final funding amounts for science programs.

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Bill Tracker (coming soon) – current status of major science-related legislation being considered by Congress.

FYI This Week - June 12, 2107

***National Academies Releases ARPA–E Assessment*:** The National Academies released a new report that aims to provide a detailed programmatic examination of the Advanced Research Projects Agency–Energy at a pivotal moment in the agency's short history. President Trump is *proposing* to eliminate the $306 million agency, which Congress created in 2007 via the America COMPETES Act. The report will appraise the appropriateness and effectiveness of ARPA-E's processes and operations with respect to its mission and goals, and also present a retrospective and technical assessment.

NSF Advisory Committees: Multiple National Science Foundation directorate-level advisory committees including those for the Mathematical and Physical Sciences, Education and Human Resources, and the Computer and Information Science and Engineering Directorates convened to disucss items such as investments in the STEM and skilled technical workforce as well as increasing public ownership of scientific research.

Trump Keeps Collins as NIH Director, Appoints Cancer Institute Head: On June 6, President Trump announced that Francis Collins, who has been director of the National Institutes of Health since 2009, will continue to serve in that capacity. Trump had already asked Collins to stay on temporarily but this arrangement appears more permanent. In addition, on June 9, Trump announced that he will appoint Ned Sharpless, a physician at the University of North Carolina at Chapel Hill, to be the next director of the National Cancer Institute. Among the challenges the two will grapple with, the administration is proposing to slash the NIH budget by 22 percent in fiscal year 2018.

***NIH Drops Controversial Grant Cap Proposal, Establishes New Fund for Early Career Scientists*:** After receiving considerable pushback, the NIH has backed off from a proposal to cap the total grant support that individual principal investigators can receive from the agency. Instead, NIH is creating a new fund to support early and mid-career scientists as part of the Next Generation of Researchers Initiative created by the recently enacted 21st Century Cures Act. In a presentation at a June 8 advisory committee meeting, NIH Principal Deputy Director Lawrence Tabak announced that *"beginning immediately,"* NIH will allocate about $210 million for the fund and will grow it over the next five years to provide an annual funding level of about $1.1 billion.

***High Energy Physics Confronting Budget Uncertainty*:** The High Energy Physics Advisory Panel (HEPAP), which advises the Department of Energy and the National Science Foundation, met on June 5 and 6 in the shadow of President Trump's proposal to cut DOE's High Energy Physics program, currently funded at almost $800 million, by 18 percent. Jim Siegrist, head of the DOE HEP office, reported the request is significantly below even the more conservative of the two funding scenarios laid out in the P5 roadmap. He said the office plans to privilege P5 priorities and seeding of long-term projects, including accelerator stewardship, particle detector R&D, and quantum information science.

House Democrats Seek Count of Scientific Jobs at Risk Under Trump Budget: In a June 9th letter led by Rep. Bill Foster (D-IL), 55 House Democrats called on the leaders of seven federal science agencies to provide projections on how many federal, laboratory, and university employees would lose their jobs if the proposed fiscal year 2018 budget were enacted. The letter argues the funding levels requested *"would cause permanent damage to our research infrastructure and workforce"* and would require the labs to lay off *"critical scientific staff."* An estimate released by the office of Rep. Randy Hultgren (R-IL), co-chair of the House Science & National Labs Caucus, projects a loss of 150 to 200 jobs out of roughly 1,700 positions at Fermilab. Science reports that DOE contractors estimate a loss of 6,700 of the roughly 29,000 jobs at 12 of 17 DOE national laboratories.

Spotlight on Stamps - The Martyr of X Rays

Wilhelm Röntgen first announced the discovery of X Rays in a brief communication submitted to the Würzburg Physical Medical Society on 28 December 1895. The seminal manuscript went to print right away, even before it was read to the society, as was traditionally done at the time. Fully aware of the potential impact of his work and without wasting any time, on New Year's Day 1896, Röntgen mailed reprints of the paper and copies of selected radiographs to dozens of colleagues and friends all over Europe. Within days, several newspapers reported the breakthrough discovery while medical doctors, physicists, and other scientists started verifying Röntgen's initial observations and began seeking practical applications for the newly discovered form of electromagnetic radiation. In Braunschweig, the German dentist Otto Walkhoff (1860-1934) successfully obtained a radiograph of his own teeth after a 25-min exposure to a beam of x rays, an experiment that he later described as "torture". In addition to obtaining the first dental radiograph, Walkhoff became the first person to realize the inherent danger of prolonged exposure to x rays. Fortunately, he survived the incident unscathed and went on to have an illustrious career as a leader in the development of dental x-ray diagnostics.

Other individuals pursuing medical applications of x rays, or the subjects of their studies, were not that fortunate. Among them was Álvaro Alvim, a physician and pioneer of radiology and radiotherapy in Brazil. Born in the municipality of Vassouras in the state of Rio de Janeiro, Alvim graduated in 1887 from the Bahia School of Medicine and in 1896 traveled to France to study medical physics with Marie and Pierre Curie. Upon his return to Brazil a few months later, he founded several clinics and took the first radiographs in the country, most notably those of a pair of conjoined twin sisters whose lives were saved by a subsequent surgical operation. His research with radioactive materials and x rays slowly started to affect his health and, despite losing several fingers in the years that followed, he continued his research and medical practice, based on which he also wrote several books. By the time he received the Humanitarian Medal from Brazilian President Arthur Bernardes, one of his hands had already been amputated, and he died of leukemia in 1928. The stamp illustrated in this note was issued in 1963 to honor Álvaro Alvim on the occasion of the centennial of his birth. Poignantly, the stamp's design includes, in a very small font size, the inscription ***Martyr of Science***. In addition, several streets, hospitals, and schools in Brazil today bear his name, a fitting tribute for such a scientific hero.

Daniel Rabinovich

Contributors to this issue: Gerald Audette, Helen Berman, Craig Bridges, Majed Chergui, Joseph Ferrara, Barry Finzel, Marie Fraser, Tomislav Friščić, Frank Fronczek, A. Michael Glazer, Jessica Hoy, Tiffany Kinniburgh, Ravi G. Kurumbail, Hong Li, Krystle McLaughlin, Anne Mulichak, James O'Brien, Art Olson, Kay Onan, Virginia Pett, Daniel Rabinovich, Connie Rajnak, Narasinga Rao, David Sanders, Paul Sanschagrin, Amy Sarjeant, Ned Seeman, Diana Tomchick, Peter Wood

Cover: Images provided by James O'Brien; production by Connie Rajnak.

Puzzle Corner

For Summer, we have a baseball-themed ***DISORDERED*** puzzle, a new ***Crystal Connections***, solutions to the previous ones, and mention of those who provided solutions.

Crystal Connections #11

What do the answers to these clues have in common?

1) Banjo player or gleaner

2) Polar rhombohedral space group lacking glides

3) To abstain from food; very sensitive film

4) Second most common Sohncke space group

5) Acronym for engineering software, followed by space group number for 4)

6) _____ Museum of Art, at the University of Chicago

7) Major source of elements heavier than oxygen

8) Lies on the ecliptic. *Castor*, *Pollux* and *Alhena* are its brightest stars

9) The Italian *tarantella* dance is thought to have origins in the bite of this animal

Solution to Crystal Connections #10 - Surnames of ACA Fellows

1) ___springs eternal in the human breast. *Pope* – Håkon Hope, 2015

2) That which we call a ___by any other name would smell as sweet. - *Romeo and Juliet*, Act II, Scene II – David Rose, 2015

3) Crater near the moon's southeastern limb; type of screw-driver – George Phillips, 2014

4) City in Kansas; county in South Dakota – Alex McPherson, 2013

5) Verb (t) - to correct a space group, particularly one of unnecessarily low symmetry – Dick Marsh, 2012

6) Originally Karfunkle – Jerome and Isabella Karle, 2011

7) Name of his widely-used software is based on his own name – George Sheldrick, 2011

8) Acronym for Institute of Biological, Environmental and Rural Sciences, Wales – Jim Ibers, 2013

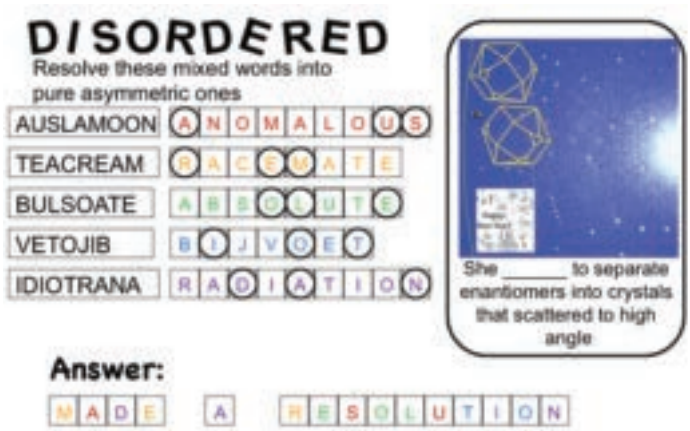
9) Das ___- First opera of *Der Ring des Nibelungen*, Richard Wagner – Arnie Rheingold, 2016

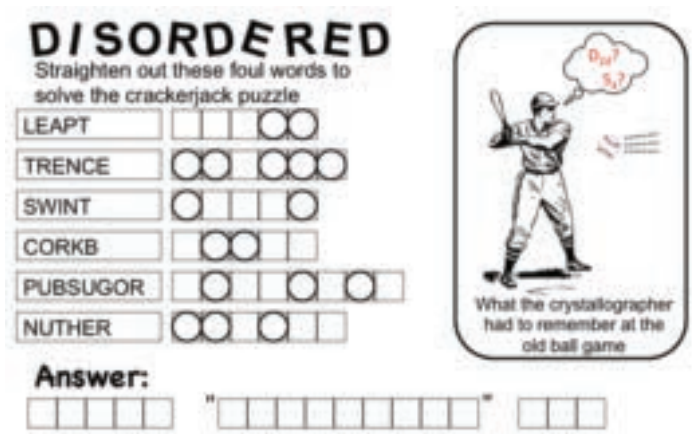
10) Color most commonly used by Rembrandt van Rijn, particularly in his later years – I. David Brown, 2016

Tim Royappa (Dept. of Chemistry, Univ. of West Florida), ***Diane Dickie*** (Dept. of Chemistry, Brandeis) and ***Marian Szebenyi*** (Cornell) each provided the solution to the DISORDERED puzzle. Tim discovered that "**M**AC**ER**ATE" also works instead of "**R**AC**EM**ATE" and yields the same letters. A number of people correctly reported the names of the crystallographers in Crystal Connections #10, of whom ***Virginia Pett*** was first, but *nobody made the connection* that all are ACA Fellows. Virginia points out that Ron Hamlin is also a possible answer for clue 4, since South Dakota has Hamlin County north of Sioux Falls, and Kansas has a town called Hamlin, near the Nebraska border between Kansas City and Omaha. However, Hamlin KS had a population of 46 in the 2010 census, so doesn't quite qualify as a **city**.

As always, I will be pleased to see your solutions and also your ideas for future puzzles. Guest Puzzlers are especially welcome!

Frank Fronczek – ffronc@lsu.edu





Structural Dynamics

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Special Topic:
Transactions of the 66th Annual Meeting of the American Crystallographic Association

JULY 22-26, 2016 | DENVER, CO

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Guest Editors
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Arwen Pearson - The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

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A short history of structure based research on the photocycle of photoactive yellow protein Marius Schmidt Structural Dynamics 4, 032201 (2017); http://doi.org/10.1063/1.4974172

Combining multi-mutant and modular thermodynamic cycles to measure energetic coupling networks in enzyme catalysis Charles W. Carter, Jr., Srinivas Niranj Chandrasekaran, Violetta Weinreb, Li Li, and Tishan Williams *Structural Dynamics 4, 032101 (2017); http://doi.org/10.1063/1.4974218*

Augmenting the anisotropic network model with torsional potentials improves the performance of PATH Srinivas Niranj Chandrasekaran and Charles W. Carter, Jr *Structural Dynamics 4, 032102 (2017); http://doi.org/10.1063/1.496142*

Insights into the mechansim of membrane pyrophosphatases by combining experiment and computer simulation Nita R. Shah, Craig Wilkinson, Steven P. D. Harborne, Ainoleena Turki, Kun-Mou Li, Yuh-Ju Sun, Sarah Harris, and Adrian Goldman *Structural Dynamics* 4, 032105 (2017); http://doi.org/10.1063/1.4978038

Partial-occupancy binders identified by the Pan-Dataset Density Analysis method offer new chemical opportunities and reveal crypticbinding sites Nicholas M. Pearce, Anthony R. Bradley, Tobias Krojet, Brian D. Marsden, Charlotte M. Deane, and Frank von Delft *Structural Dynamics 4, 032104 (2017); http://doi.org/10.1063/1.4974176*

Microfluidic addressing the challenges of serial time-resolved crystallography Shuo Sui, and Sarah L. Perry *Structural Dynamics* 4, 032202 (2017); http://doi.org/10.1063/1.4979640

The dramatic development of x-ray photocrystallography over the past six decades. Philip Coppens *Structural Dynamics* 4,032102 (2017); http://doi.org/10.1063/1.4975301

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Majed Chergui, Editor-in-Chief of Structural Dynamics, at ACA New Orleans

Structural Dynamics, which is co-published with the ACA and AIP Publishing, has had a strong start since it was launched in 2014. At the 2017 ACA meeting, we had a meet-the-editor event for ACA attendees to come meet and speak to Majed Chergui, the editor-in-chief of the journal. Many of the conversations and questions that arose involved the nature and scope of papers accepted in the journal. Most specifically, questions were asked about how much dynamical information is required and attendees were pleased to learn that there is a place for some static data. Explicitly, static information that helps the understanding of the full dynamical picture is extremely crucial and would be an excellent fit in *Structural Dynamics*. In addition, the funder mandates around Open Access have made *Structural Dynamics* a practical publication option for many authors especially when they can take advantage of the $700 (30%) ACA member discount.

In his talked entitled "Ultrafast structural dynamics of (bio) molecular systems", Majed Chergui focussed on his group's recent studies of hemoproteins. After introducing the technique of ultrafast x-ray absorption spectroscopy that retrieves element-selective electronic and structural dynamical information, he showed his group's results on Myoglobin-NO (*PNAS* 2015), which he linked to recent work at XFELs using scattering and crystallography. Dwelling on the information about large scale motion in the latter studies, he introduced novel multidimensional (MD) spectroscopies that are the optical domain analogues of two-dimensional (2D) NMR, with the advantage of reaching a much higher time resolution in the order of femtoseconds. His group was the first to extend the method into the deep-UV below <300 nm (*Science* 2013), where amino acid residues and nucleotides have their absorption bands. He thus showed how deep-UV 2D spectroscopy allowed the observation of hitherto unknown Tryptophan-mediated electron transfer processes in hemoproteins. The ability of 2D spectroscopies to monitor the cross-talk between different chromophores in the course of a biological function make them a very promising complement to time-resolved scattering and crystallography.

Left to right: AIPP SD journal managers Jessica Hoy and Anthony Solis, Editor-in-Chief Majed Chergui and Associate Editor George Philips.

Tom Koetlze and Majed Chergui at the journal booth.

Speakers in Session 3.2.1. at ACA New Orleans from left to right: George Phillips, Masaki Yamamoto, Jason Stagno, Louise LaSalle,Alan Orville, Jessica Thomaston , Nick Sauter, Majed Chergui, Alke Meents.

Featured

Defect-mediated phonon dynamics in TaS_2 and WSe_2

Molecular couplings and energy exchange between DNA and water mapped by femtosecond infrared spectroscopy of backbone vibrations

Cooperative protein structural dynamics of homodimeric hemoglobin linked to water cluster at subunit interface revealed by time-resolved X-ray solution scattering

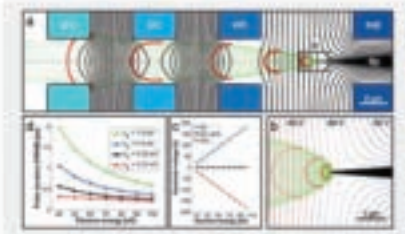
Free-electron laser-driven ultrafast rearrangement of the electronic structure in Ti

Terahertz radiation induces non-thermal structural changes associated with Fröhlich condensation in a protein crystal

Editor's Picks

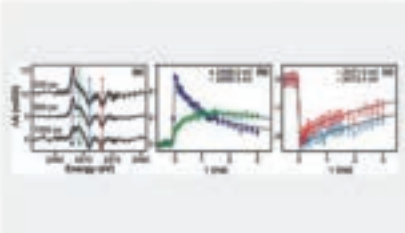
MAY 16 2017

Nanotip-based photoelectron microgun for ultrafast LEED



MAY 08 2017

Picosecond sulfur K-edge X-ray absorption spectroscopy with applications to excited state proton transfer



MAY 03 2017

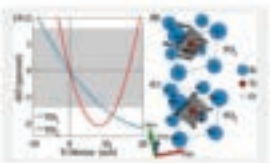
Stacking order dynamics in the quasi-two-dimensional dichalcogenide 1T-TaS_2 probed with MeV ultrafast electron diffraction

MAY 03 2017

Ultrafast X-ray diffraction probe of terahertz field-driven soft mode dynamics in $SrTiO_3$

APR 14 2017

Perspective: A toolbox for protein structure determination in physiological environment through oriented, 2D ordered, site specific immobilization



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JUN 14 2017

Preface to Special Topic: Transactions from the 66th Annual Meeting of the American Crystallographic Association

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JUN 06 2017

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RefleXions from Canada

Things are getting up to speed now, and the time for the next postcard from Canada came surprisingly quickly. While I am preparing this summer *ACA RefleXions* column on Canadian activities, a number of events have taken place but, most importantly, we are in expectation of the upcoming ***24th Congress & General Assembly of the IUCr*** in Hyderabad, India. This congress should provide strong contributions from Canadian crystallographers and researchers in general. Notably, David Bryce from the University of Ottawa will be giving a keynote lecture on *Structure and properties of materials by solid-state nuclear magnetic resonance (SSNMR) observables*. Also, Patrick Mercier from the National Research Council Canada will be co-chairing the microsymposium ***"Minerals/gems in Industrial Applications,"*** while Natalie Strynadka from the University of British Columbia will be co-chairing the microsymposium ***"Mechanisms of Bacterial Resistance"***. The chair of the Canadian Delegation in Hyderabad is Louise Dawe from Wilfrid Laurier University, and she will be co-chairing the microsymposium ***"New Approaches in Crystallographic Teaching.*** She would also like to hear any updates and news from all Canadians who are planning to attend the Congress, and can be contacted at ***ldawe@wlu.ca.***

In this postcard from Canada I would like to highlight an outstanding researcher from Canada who has provided remarkable contributions to solid-state chemistry and chemical crystallography. The group of **James D. Wuest** (Université de Montréal) operates at the interface of crystal engineering and synthetic organic chemistry and has gained international acclaim by developing elegant organic and main group synthetic chemistry, and placing it in the service of materials science of crystalline solids. The Wuest Research Group (Figure 1) are professionals in recognizing challenges of solid-state materials science and then figuring out how to make molecular targets that can meet those challenges and push the boundaries of what molecular solids can do.

Figure 1. The Wuest group, researchers that combine synthetic skills and crystal engineering. The PI, Jim Wuest, shown wearing a hat.

Some of the fascinating early work of the Wuest group has addressed mechanical properties of organic solids. For example, in 2003 they took crystal engineering by surprise by demonstrating how carefully engineered molecules, called tectons, can enable access to materials with unprecedented mechanical robustness (*J. Am. Chem. Soc.* **2003**, *125*, 14956). By using flexible silicon-carbon bonds as places of structural flexibility within each tecton, it was possible to generate materials that could undergo a change of 30% or more in their dimensions without a loss of crystallinity. Today, the Wuest group is pursuing a range of directions, creating links to surface science, pharmaceuticals, photovoltaic solids and more. A representative example of such work is the elucidation of correlations between molecular organization in three dimensions and in two dimensions, combining the power of X-ray diffraction and electron microscopy to develop more effective thin-film devices (*e.g.* see *J. Phys. Chem. C* **2012**, *116*, 13052). A very recent contribution has addressed fabrication of new molecular materials in which multiple optoelectronically active components are positioned so as to optimize performance (see *J. Org. Chem.* **2017**, *82*, 5034).

My personal favorite is the ingenious development of molecular building blocks for the synthesis of complex self-assembled covalent structures. For example, covalent organic frameworks (COFs) are among the hottest areas of materials science, but their syntheses are strongly tied to harsh conditions – often at the expense of crystallinity and crystal size, making them inaccessible to methods of single crystal X-ray diffraction. Asking the very fundamental question ***"How to synthesize diffraction-quality large crystals of COFs?"***, the Wuest group utilized the well-known nitroso dimerization reaction to synthesize the first large crystals of three-dimensional COFs, enabling the first single crystal X-ray structural characterization of this class of materials (*Nature Chem.* **2013**, *5*, 830) (Figure 2a,b). In a related development, they have carefully designed an organic building block capable of reversible assembly of carbon-carbon bonds, leading to large hexameric and tetrameric ring structures composed exclusively of carbon and hydrogen: the cyclic hexamer $C_{306}H_{180}$ is currently the largest hydrocarbon structure ever to be investigated by single crystal X-ray diffraction (*Angew. Chem. Int. Ed.* **2016**, *55*, 894) (Figure 2c).

Jim Wuest was born in Cincinnati, Ohio in 1948, and studied chemistry and mathematics at Cornell University, where he received an A. B. *summa cum laude* in 1969. His graduate studies in organic chemistry took place with the late Nobel Laureate Robert B. Woodward at Harvard University, where he was a National Science Foundation Fellow. After receiving his Ph. D. in 1973, he joined the faculty at Harvard as an Assistant Professor of chemistry, where he remained until 1981 when he accepted a tenured position at the Université de Montréal in Canada. There he has been a full professor since 1986, and now holds the Canada Research Chair in Molecular Materials. He and his group are broadly interested in the design, synthesis, structure, and properties of molecular materials. His awards include the Merck Sharp & Dohme Award in 1988 (given by the Canadian Society for Chemistry for outstanding work in organic chemistry carried out in Canada by a scientist under 40 years old), the Rutherford Memorial Medal in 1992 (given by the Royal Society of Canada for exceptional research in any area of chemistry done in Canada by a scientist under 40 years old), the Alfred Bader Award in Organic Chemistry in 2001 (given by the Canadian Society for Chemistry to recognize excellence in research in organic chemistry carried out in Canada by a scientist under 60 years old), an Arthur C. Cope Scholar Award in 2005 (given by the American Chemical Society), and the Prix Urgel-Archambault in 2008 (given by the Association francophone pour le savoir). He has also been a Killam Research Fellow (1992) and a Guggenheim Fellow (1999), and he was elected Fellow of the Royal Society of Canada in 1996.

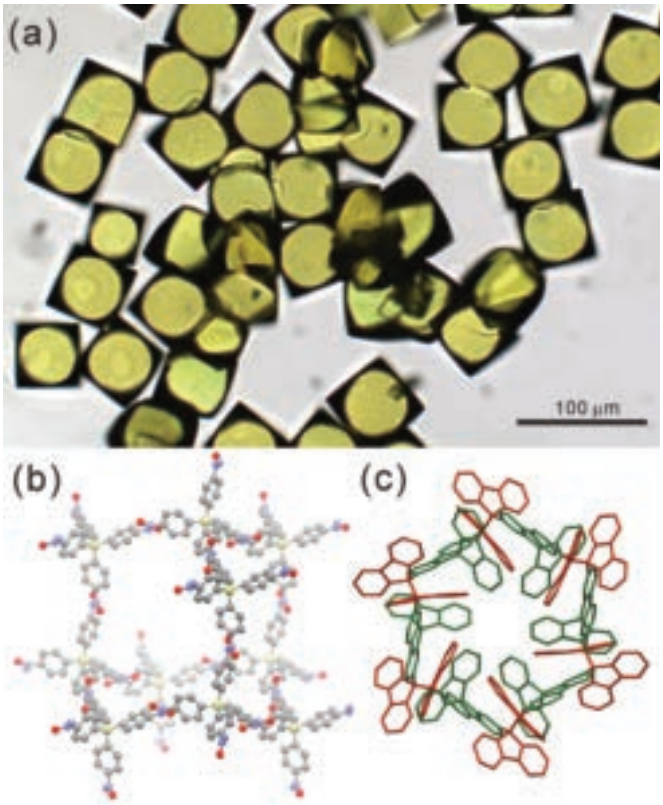


Figure 2. (a) The first large single crystals of a covalent organic framework (COF) and (b) a fragment of its multiply-interpenetrated diamondoid framework structure, designed and created by the Wuest group through utilizing reversible nitroso group dimerization as a design element (Nature Chem. 2013, 5, 830). (c) Single crystal structure of the cyclic hexamer $C_{306}H_{180}$, the so far largest hydrocarbon investigated by single crystal X-ray diffraction, synthesized by the Wuest group through reversible carbon-carbon bond formation (Angew. Chem. Int. Ed. 2016, 55, 894).

Recent events

This year's annual ***ACA Meeting*** is just behind us and it seems that the Team Canada had a pretty good and productive time in New Orleans (Figure 3a). ***Michael James*** co-organized a fantastic symposium in New Orleans on ***"Conformational Dynamics of Ligand Binding"***, while I had the chance to co-chair, along with ***Manish Mehta*** from Oberlin College, the very first ***"NMR Crystallography"*** Symposium at an ACA meeting. We were particularly pleased that this new symposium ended up being really well attended, with audience hovering around 50 for most of the time. This was certainly due to our highly dynamic speakers, of which two are from Canada: ***Mihails Arhangelskis*** (McGill University) and ***Darren Brouwer*** (Redeemer University College) (Figures 3b,c). It looks like NMR Crystallography has a bright future at the ACA, having in mind the already mentioned plenary lecture at the IUCr meeting in Hyderabad, as well as the rumours that the second NMR Crystallography Symposium is being planned for next year's annual ACA meeting in Toronto.

In almost perfect overlap with the annual ACA meeting, **Louise Dawe** and ***Kenneth Maly*** (Wilfrid Laurier University) have orga-

Figure 3. (a) ACA President Amy Sarjeant (CCDC) flanked by young Canadian crystallographers Raul Castaneda (University of Ottawa) and Mihails Arhangelskis (McGill University) at the annual ACA meeting in New Orleans. (b) Darren Brouwer (Redeemer University College, Hamilton, ON) presents at the first NMR Crystallography symposium at the ACA annual meeting, and (c) some of the presenters of the symposium (left to right): Tomislav Friščić (McGill University), Manish Mehta (Oberlin College), Mihails Arhangelskis (McGill University), Darren Brouwer (Redeemer University College), Kenneth D. M. Harris (Cardiff University) and Jim Harper (University of Central Florida).

nized the fourth consecutive ***Crystal Engineering and Emerging Materials Workshop of Ontario and Quebec (CEMWOQ-4)*** at their home institution in Waterloo, Ontario. I was told by Louise that the meeting was a massive success - bringing together over 60 participants from Canada, USA, France, Russia, United Kingdom and South Africa (Figure 4)! Excellent plenary lectures were delivered by ***Christer B. Aakeröy*** (Kansas State University) on "***Crystal engineering from molecules to materials"***, ***Vladimir P. Fedin*** (Nikolaev Institute of Inorganic Chemistry) on ***"Porous coordination polymers: from synthesis and structure to functional properties"***, and ***Marc Fourmigué*** (Institut des Sciences Chimiques de Rennes) on "***Halogen-bonded co-crystals: implications in crystal engineering and molecular conductors"***. As always, the CEMWOQ meeting was very student-focused, and this time included a hands-on OLEX2 tutorial, and a poster session with over 30 presenters. Five Student Awards have been given at CEMWOQ, sponsored by *CrystEngComm* (RSC), *Springer*, and *IUCr Journals*. The winners were ***Austin Peach*** (University of Windsor) for "***Applications of ^{35}Cl SSNMR for the study of HCl Pharmaceutical Cocrystals"***, ***Junghoon Ko*** for ***"Discotic Liquid Crystals with Internal Side Chains as Potential Organic Semi-Conductors"***, ***Mitchell Nascimento*** for ***"Expanding the Family of Palladium-DTDA Metal Complexes"***, ***David Hirsh*** for ***"Structural Effects of Ln^{3+}-ions in Nanoparticles: a Solid-State NMR Study"*** and ***Nadia Stephaniuk*** for ***"Inclusion chemistry of thiazyl and selenazyl radicals in MIL-53(Al)"***, all from the University of Windsor.

Information on this most recent CEMWOQ meeting, and links

Figure 4. Group picture from this year's CEMWOQ-4 with organizers Kenneth Maly and Louise Dawe in front row, center

to previous meetings, can be viewed at the following website: ***daweresearch.ca/cemwoq-4/***

Jim Britten has organized the ***8th Canadian Chemical Crystallography Workshop (CCCW17)*** in Hamilton, Ontario: ***xtallography.ca/index.php/xtal/meetings/cccw17/***

I hear from Jim (Figure 5a) and Louise Dawe that all the attendees (Figure 5b), students as well as the instructors, had a really good time and learned immensely. The workshop was strongly marked by the enthusiasm of the students, who all participated fully in tutorials and lectures. Besides gaining proficiency with Olex2 refinements, the attending students also participated in a valuable database mini-workshop provided by Shyam Vyas from CCDC. Indeed, there were immediate benefits of attending this workshop, as some students went from never having refined a structure before, to having a structure ready for inclusion in a talk at the 100th CSC in Toronto the following week! Jim also tells me that the next workshop, **CCCW18**, will be taking place at the University of Alberta in Edmonton in 2018.

Finally, I was very glad to have the opportunity to attend the two-day symposium on ***"Crystalline and Semi-crystalline Molecule-based Materials",*** that was organized by ***Dmitriy Soldatov*** and ***Kathryn Preuss*** (both from the University of Guelph, Ontario) at the ***100th CSC*** meeting in Toronto. It was a major success as the talks, given by 24 speakers from 13 Canadian universities and 12 international speakers, have been very well attended. In the particular session that I attended, I managed to count over 80 people in the audience.

In early June, ***Patrick Mercier*** had organized the ***10th Canadian Powder Diffraction Workshop*** in Edmonton, Alberta: ***www.cms2017.com/10thcpdw/***

According to the comments I received, it was excellent and offered a great opportunity to learn. As Jim Britten put it: "One Eureka moment after another!". So I am rather sorry to have missed it but I hear that this is now turning into an annual event that should move back and forth across the country.

Finally, let me remind you that, if you wish to know more about our ***Canadian National Committee for Crystallography,*** we have a brand new and exciting webpage that has been put up and is being continuously improved by ***Louise Dawe***: ***http://xtallography.ca/***

Let me conclude this column with the observation that there is a growing number of annual meetings and workshops in Canada focused on solid-state chemistry and crystallography. Indeed, after co-organizing the ***Crystalline and Semi-crystalline Molecule-based Materials*** symposium at the ***CSC100***, ***Kathryn Preuss*** (University of Guelph) noted that this year might have seen the largest concentration of workshops and symposia dedicated to molecular crystalline and quasi-crystalline materials. I completely agree with her assessment that this is a good time for crystallographic research in Canada.

I am sure that there is more that can be included in this brief postcard from Canada and so, if you would like me to address or highlight any special topics or events, or if there are Canadian activities that I have missed to write about, please share them with me by e-mail ***(tomislav.friscic@mcgill.ca)*** and I will make sure they get included in the next columns.

So long for now – cheers from Zagreb, Croatia on a really hot summer's day!

Tomislav Friščić

Figure 5. (a) Jim Britten in action at this year's Canadian Chemical Crystallography Workshop (CCCW17) held in Hamilton, Ontario and (b) attendees and organizers of CCCW17.

Candidates for ACA Offices in 2018

The Nominating Committee (Louise Dawe, Chris Cahill and David Rose) proposes the following candidates for 2018.

Officers:

Vice-President: **Joseph Ferrara & Barry Finzel**

Secretary: **Marie Fraser & Diana Tomchick**

Committees:

Communicatons: **Hong Li & Krystle McLaughlin**

Continuing Education: **David Sanders & Peter Wood**

Data, Standards & Computing: **Craig Bridges & Paul Sanschagrin**

To nominate write-in candidates for any office, write to the ACA Secretary: Diana Tomchick, Dept. of Biophysics, University of Texas, Southwestern Medical Center, Irving, TX 75061 (diana.tomchick@utsouthwestern.edu). Letters must be received by September 15, 2017 and must be signed by five ACA members and include a signed statement by the candidate describing his or her qualifications. Voting will be by electronic ballot. Statements from all candidates will be available on the election site. The voting window will be open in October 2017.

Joseph Ferrara - Vice-President

Chief Science Officer, Rigaku Americas Corp., The Woodlands, TX; Deputy Director, X-ray Research Laboratory, Rigaku Corporation, Tokyo, Japan.

Education: BS Chemistry, Case Institute of Technology, 1983; PhD, Case Western Reserve University, 1988, Advisor: Wiley J. Youngs.

Professional Activities: Scientific Advisory Board Lone Star College Biotechnology Program, 2005-date (Chairperson 2008-2010); Books Editor, ACA Reflexions, 2011-date; Visiting Instructor, University of Tokyo, 2012; Chairperson, ACA Data, Standards and Computing Committee (2016-date); Chairperson, ACA 2019 Annual Meeting Site Selection Committee (2016-2017); Member ACA 2.0 Transition Committee (2016); Member ACA ad hoc Committee on Meeting Reorganization (2017); Chairperson, ACA 2020 Annual Meeting Site Selection Committee (2017-2018).

Research Interests: All aspects of x-ray science: x-ray sources, optics, detectors and techniques; single crystal x-ray diffraction, small angle x-ray scattering, powder diffraction, x-ray microscopy and phase contrast imaging.

Statement: I have been a member of the ACA since I began my career as a professional crystallographer with Molecular Structure Corp. in 1988. As a member I have been active in the ACA by voting regularly and attending, exhibiting at and presenting at ACA conferences over the years. I did not become active beyond being a member in good standing until 2011. At that time Judith Flippen-Anderson, editor of *Reflexions,* asked if I would provide some book reviews. With that I became the *Reflexions* Books Editor. However, I did not become truly active until 2014 when the annual meeting attendance dropped to a level we had not seen in decades. At that point in time I decided that I needed to become part of the solution; it was time to take action to improve the annual meeting and the ACA itself. Since then, I have been an active member in the Data Standards and Computing Committee, the 2019 Site Selection Committee, and the ACA 2.0 Transition Committee.

The ACA is undergoing profound changes. In the early 2000s we had over 2200 members; we now have just over 1000 members.

Past-presidents Chris Cahill and Tom Terwilliger began, and current president Amy Sargent is overseeing, a transition in the management of the organization that was precipitated by the retirement of Marcia Colquhoun and Bill Duax's preparatons to retire. As part of this transition we need to carefully align the business aspects of the ACA with the needs of the membership. To me, this means having the appropriate number of staff running the ACA on a day-to-day basis and ensuring the organization fulfills the needs of the membership.

The ACA's investments have been growing under the management of CFO S.N. Rao. These investments provide the funds that endow our awards and are important to the standing of the ACA as a scientific society. The ACA needs to take over management of the investments in preparation for Rao's retirement. Rather than leave the investments in the hands of a single person I would organize a committee, answerable to the Council, to manage the investments through a low-cost investment firm, such as Vanguard.

The big question that needs to be answered: what can we do about increasing our membership? Every year, I see a lot of the same faces at the annual meeting. This indicates to me that we are not bringing enough young people into the ACA. We need to have a membership drive to increase the rolls. Here, I think we can learn some lessons from our sister society, the BCA, which nearly doubled their membership when Elpseth Garman became their president. Her method was very simple; provide a chance for an annual meeting registration for every 10 new members brought in. The difficult task will be keeping the new members, and there are a lot of smart people in the ACA that can help. Once we bring in more members, we will have more resources to improve the membership experience.

I am uniquely qualified for the position of vice president and eventually president of the ACA. I began studying crystallography as a graduate student at Case Western Reserve University in 1984. Thirty-three years later I am still practic-

ing crystallography and still learning. In 1988 I joined a small company called Molecular Structure Corporation (MSC). MSC was bought by Rigaku in 1996 and I have been with Rigaku since that time. I have been part of, or led, the team that brought many tools for crystallography to the market. This required me to stay in touch with the community and foster many long-term relationships. As a manager in a large company I am required to consider the fiscal consequences of any technical decision I make.

In my spare time I train as a firefighter, for which I am certified at the basic level in Texas. I have been a member of the same all-volunteer department, a 501(c)(4) organization, for almost 25 years. In addition to meeting the training requirements, I have served on the department's Executive Committee for all but 4 years. For the last 15 years I have been Treasurer. My responsibilities as Treasurer include creating budgets, managing the disbursement of all the taxpayer and non-taxpayer funds within prescribed budgets, and interacting with Emergency Services District commissioners, auditors, Texas Workforce Commission and the IRS.

These experiences have taught me how to work with people and achieve difficult goals. I believe I can effectively lead the effort to restore the ACA to the organization it once was: a family of scientists who love their chosen field and enjoy the camaraderie of like-minded professionals.

Barry Finzel - Vice-President

Professor and Director of Graduates Studies, Dept of Medicinal Chemistry, College of Pharmacy, University of Minnesota

Education: BS in Chemistry, Eastern Michigan University (1979); PhD Chemistry University of California, San Diego (1983); NIH Postdoctoral Trainee, University of California, San Diego (1983).

Professional Activities: Member, American Chemical Society (1977-1983; 2008-present), ACS Medicinal Chemistry Division (2008-present); Member, American Crystallographic Association (1983-present); Canadian Macromolecular Crystallography Facility Peer Review Committee (2009-2015); ACA BioMacSIG Chair (2016)

Research Interests: Protein crystallography, biophysical characterization of protein:ligand interactions (DSF, SPR, DLS, ITC); structure-aided drug design; exploiting macromolecular structural likeness in modeling to advance understanding structure-function relationships.

The overall goal of our research is to advance the iterative process of small molecule inhibitor design by providing timely crystallographic structural data on protein-ligand complexes. Through collaborations with synthetic organic chemists, enzymologists, cell biologists and computational scientists, we seek to generate and exploit structural information to create and understand the mechanism of action of small molecules that attenuate the biological macromolecule function and thereby, human health. The collaborative and interdisciplinary nature of our research was fostered during twenty years in the Pharmaceutical Industry (Upjohn, Pharmacia, Pfizer), where an interdisciplinary team approach to drug discovery is both the rule and a necessity. With a move to academia nearly ten years ago, we have tried to continue that tradition by cultivating collaborations with like-minded academic scientists with complementary expertise in biomedical sciences. Currently, we are actively engaged in research in antibacterial development, cancer chemotherapy and inflammation.

Statement: In conversations with both scientists and non-scientists, I always identify myself first as a "Crystallographer", then as a "Structural Biologist", then as a "Medicinal Chemist". (The last is quite a stretch for me, but more people seem to know what a "Chemist" is, and the "Professor of Medicinal Chemistry" in my title gives that identity some cred). When that also fails (as it often does when I'm talking with non-scientists), I tell people I make drugs. *That* they can connect with, because they've seen *Breaking Bad*.

For me, membership in the American Crystallographic Association has always gone hand-in-hand with my identity as a scientist. We identify with the people with whom we share life experiences. The ACA has been my scientific home since the first meeting I attended as a graduate student in San Diego in 1982. While I have not attended every annual meeting since then, I have always valued the opportunity to hook up with old friends, and to hear about the latest best practices and evolving trends in crystallographic methods, and the latest new structures. Always, when I return from a ACA meeting I feel a) energized with new ideas; b) small in the context of so many people doing good work; and c) exhausted – exactly as I would hope to feel after a successful meeting with my peers. I have participated in many Medicinal Chemistry and Biophysics meetings where structure has been presented as a component of a larger scientific or development enterprise, but it is only at ACA meetings that I really feel the camaraderie of like-minded individuals curious to learn more about the structure. It is refreshing to be able to talk with peers and complain that my crystals are twinned, or that they are too mosaic, or that the skin on the drop is a pain without needing to explain myself. I really value this community of genuine peers, and I have never found a similar community elsewhere.

One of my personal objectives over the past couple years has been to try to re-involve macromolecular crystallographers from Pharma in the ACA. Two decades ago, when the idea of structure-based design was still quite fresh and people were actively working to demonstrate the feasibility of crystallography as a timely drug design tool, participation by industry macromolecular crystallographers in the ACA, and in the Industrial SIG and the BioMacSIG was very high. Every meeting included a couple of sessions in structure-aided drug design, and there was a dynamic interchange of best practices among participants. Several ACA presidents were elected from this group (e.g., Dave Duchamps, 1990; Keith Watenpaugh, 1992; Connie Chidester, 2000; Bill Stallings, 2001). Oddly (or, perhaps

predictably), as the methodology matured and structure-based design became successfully and routinely integrated into drug discovery, this community has largely left the ACA. Sadly (in my view), these crystallographers are now mostly presenting their work to medicinal chemists or biologists that have a limited appreciation for either the structures or the effort put into them. This trend is not limited to macromolecular crystallographers from Pharma. It is a creeping problem with the ACA in general. Application scientists that formerly identified as crystallographers are taking their expertise to other scientific forums with broader impact and less specialized focus.

We all know that the vast majority of known structures have been characterized crystallographically, but as the molecular questions in material science and biology become more complex, other experimental tools need to be brought to bear. We need to embrace and welcome our colleagues in electron diffraction, low angle scattering, NMR and Cryo-EM and encourage them to also call the ACA home. The ACA needs to rebrand itself as the premier professional society representing the sciences of molecular structure. We should encourage the formation of special interest groups and organize scientific sessions at annual meetings focused on the methods and results obtained using these alternate methods, either with or without crystallography. As each of these groups creates its own little camaraderie of peers, we all become enriched with the more diverse expertise for determining and understanding molecular structure across all scientific pursuits. I imagine an ACA meeting with more concurrent micro-sessions covering methodology, and larger forums focused on the presentation of results that appeal simultaneously to large subsections of our membership.

The educational and outreach missions of the ACA are as important now as they ever have been. As many of us are working hard to make crystallography a largely automated process that can be accomplished by anyone with an index finger and a keyboard, it becomes more and more important to provide both the opportunity for people to learn more about the science and methodologies underpinning the computations, but also to generally help to promote the value of understanding molecular structures to both fellow scientists and the general public. But even beyond crystallographic workshops, we need to also apply our expertise to help others explain, interpret, visualize and understand molecular structures. The ACA has a rich history, but our future is to be defined in the present. The one tie that binds us all is our appreciation of the wonder of molecular structure - no matter what the scale, or experimental approach that reveals it.

Marie Fraser - Secretary

Associate Professor, Department of Biological Sciences, Faculty of Science, University of Calgary

Education: BSc (Honors, Chemistry), Queen's University (1983); PhD with S. Fortier, Department of Chemistry, Queen's University (1987); Alberta Heritage Foundation for Medical Research Postdoctoral Fellow with M.N.G. James, Department of Biochemistry, University of Alberta (1987-90).

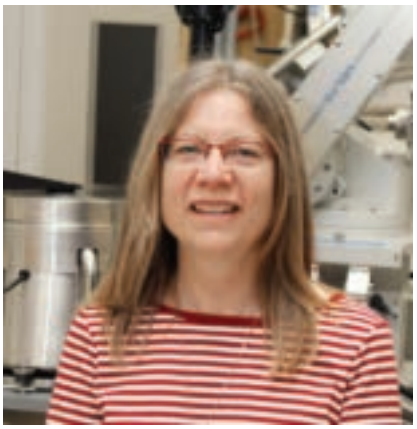
Professional Activities: Member, Accreditation Committee, Chemical Society of Canada (2012-2018); Member, Canadian National Committee (2015-2018), Treasurer (2005-2015); Member, Canadian Macromolecular Crystallography Facility Beamline Team (2013-present); Chair, Biochemistry Program (2013-16); Member, Review and Search Committee for Dean of Science (2014-15); Faculty Representative, Faculty of Science Executive (2010-2012) and Academic Appointment Review Committee (2011); Chair, Biochemistry Cluster (2009-11).

Research Interests and Responsibilities: Structural biology; macromolecular crystallography; enzyme mechanism; protein ligand-binding; protein-protein interactions. Teaching introductory biochemistry to chemists and kinesiologists; macromolecular crystallography in a structural biology course for senior undergraduate biochemists; crystallography at the graduate level.

Statement: I appreciate the opportunity to express my support for the ACA by running as a candidate for the position of Secretary. As an undergraduate student, I first thought that the bond lengths we learned in our chemistry courses came from spectroscopic measurements. In third year, I realized that most of what we know about the structures of molecules comes from the solid state, from crystals. As a graduate student and a postdoctoral fellow, I received an excellent education in crystallography. Now I consider myself a crystallographer and I rely on the meetings of the ACA and the IUCr - in addition to the literature - to keep current in the field. Serving on the executive of the ACA would give me the opportunity to give back to the crystallographic community in our region.

As a graduate student, I saw the view that crystallography is "only a tool" sweep through chemistry and I now see that view sweeping through the macromolecular field. Many faculty believe that their graduate students do not need to learn crystallography. There is a lot for our students to learn: molecular biology, protein purification, structural biology on top of the soft skills of writing and presenting. However, I think my students who are using crystallography in their research should learn more than what I teach at the undergraduate level, which is how to be an informed user of macromolecular models. My students are to be generators of those models, not just users. In my view, a major role of the ACA and the IUCr is education. We need to help both the users and generators of models from crystallography become informed.

Diana R. Tomchick - Secretary



Professor, Departments of Biophysics & Biochemistry, University of Texas Southwestern Medical Center

Education: BS, Chemistry, Washington State University (1983); PhD, Chemistry, University of Wisconsin-Madison (1990); American Heart Association Postdoctoral Fellow, Department of Biochemistry, University of Wisconsin-Madison (1990-1993); postdoc, Department of Biology, Purdue University with Janet Smith (1993-1997).

Professional Activities: Director of The Structural Biology Laboratory at the University of Texas Southwestern Medical Center; member of the ACA since 1986, and ACA Secretary since 2015; synchrotron beam time proposal reviewer for the Advanced Photon Source (2011-present).

Research Interests: The use of structural biology and especially the techniques of x-ray crystallography and cryo-electron microscopy in the study of molecular mechanisms of neurotransmitter release, bacterial pathogenicity, cell signaling and division, and enzymology; improved methods of protein crystallization, data collection and phasing of data from poorly diffracting crystals.

Statement: It has been an eye-opening and fascinating opportunity to serve as your ACA Secretary for the last 2.5 years. In addition to the typical duties of preparing meeting minutes, the ACA Secretary is a voting member of the ACA Council. In consultation with the *ad-hoc* Long-Range Planning Committee, the ACA Council has approved a 3-year plan for succession as long-serving Director of Administrative Services Marcia Colquhoun and Chief Executive Officer William Duax step down from their duties with the ACA. While this plan will help with the financial bottom line for the organization, more work needs to be done, including developing strategies for cost reduction (to the ACA and to members) at meetings and methods to attract and retain members. Targeting practitioners and students interested in novel structural techniques such as electron diffraction, cryo-electron microscopy, tomography and other methods while not ignoring the interests of our current members will be a goal that I will work towards if re-elected as Secretary.

Professionally, I work at a graduate-level biomedical institution as the Director of a campus-wide core facility that provides expertise in determining macromolecular structures. This position requires significant organizational skills as well as scientific expertise, and for many campus research groups I am the professional "face" of structural biology. Perhaps my most important role is as an educator, as I provide expertise in current methods to members of the campus community through the classroom and individual consultation on structural projects, and ensure best practices in the publication of results. The ACA provides a critical resource for members to network and keep abreast of scientific and technical advancements, and to educate the next generation of scientists as well as the general public. As Secretary I would work diligently to support the efforts of the organization as well as the other officers and various committee chairs in furthering these goals.

Hong Li - Communications

Dept. of Chemistry and Biochemistry, Institute of Molecular Biophysics, Florida State University, Tallahassee, FL

Education: BS in Physics (1983) Sichuan University, China; PhD in Biophysics University of Rochester (1994); Postdoctoral fellow (1994-1996) Brookhaven National Laboratory; Postdoctoral fellow (1996-1999), Caltech

Professional activities: ACA member 1990-; Board Member 200, SER-CAT 2007; Director 2011-, Molecular Biophysics Graduate Program at FSU; Panel member 2010-2014, NIH MSFC study section.

Research Interests / responsibilities: Understanding RNA-protein interactions in ribosome biogenesis and CRISPR-Cas immunity through x-crystallography and cryoEM

Statement: I am pleased to be nominated for the Communication Committee of the American Crystallographic Association (ACA), an organization that I have been associated with since I was a graduate student. There are several reasons I would like to contribute to ACA by taking on the responsibility as a committee member.

The first is to give back what ACA has given me throughout my own career. I learned the theory of crystallography when studying solid state physics as a graduate student and became fascinated by the power of x-ray crystallography when I obtained the electron density for several NAD analogs using heavy atom methods. ACA is the organization that has given me the opportunity to present my results and discuss my findings at the annual meetings. ACA provided the expertise, the support, and the means for me to transition from small molecule to macromolecular crystallography and from a graduate student to a faculty member. ACA continues to provide the same kind of nurture to my own students, one of whom, Rumana Rashid, was awarded the Margaret C. Etter Student Lecturer Award. Both my students and I have benefited greatly from the ACA. The second reason for me to work as a committee member is to provide a better connection between ACA and the southeast region of the United States. I can do so through my role as a board member of the Southeast Regional Collaborative Access Team (SER-CAT). SER-CAT includes 21 members, mostly from institutions in the southeast. The board oversees the operations of the SER-CAT organization and x-ray crystallography operations including communication of science to the general

public and policy makers. The third reason for me to work for ACA is to explore communications between ACA and the cryo-EM community that has taken over many of the structure determinations of large complexes. There are shared methodology and research goals between the two communities and we need to be able to learn from each other. Lastly, I have read several previous reports from the Communication Committee and found many good ideas that I can help to execute. These include organizing new symposiums with outreach goals and recruiting expertise to work on representing ACA on social media. In summary, I would love to work for the organization that has helped to shape the structural biology community.

Krystle McLaughlin - Communications

Assistant Professor, Chemistry Department, Vassar College

Education: BA Physics, Colgate University (2006); PhD Biophysics, University of Rochester (2011), SPIRE Postdoctoral Scholar, UNC Chapel Hill (2011-2013)

Professional activities: ACA Delegate to the AIP Liaison Committee on Underrepresented Minorities (2013-), ACA BioMac SIG Secretary (2016-2018), Steering Committee for the African Synchrotron Light Source (2014-), Society of Physics Students Awards Committee Chair (2015 -), Pennsylvania DNA Day Director (2015-)

Research Interests: Structural basis of protein-nucleic acid interactions during conjugation in *Staphylococcus aureus* and *Salmonella typhimuirum*; undergraduate crystallography education.

Statement: It is an honor to be nominated, and I thank the nominating committee, as I am enthusiastic about the opportunity to serve on the Communications Committee. This Committee plays a vital role in showing ACA members, others in the scientific community, and the public all of the excellent work and events coming out of the ACA, and I would be excited to be a part of that. As an educator, I am very passionate about communicating and generating interest in science as well as discussing issues in science and society.

Since attending my first ACA meeting as a graduate student, I have been pleased to be a part of such a vibrant community of scholars. For the past several years I have enjoyed working to support and grow the ACA. For example, through a partnership with the Society of Physics Students I helped start a student symposium and a new undergraduate poster prize to encourage and excite undergraduates to attend the ACA annual meeting. I also worked to introduce the Diversity and Inclusion Session at the ACA meeting, where we highlight research and strategies on diversity issues from crystallographers in our community. Additionally, through online platforms such as blogs, newsletters and social media platforms like Twitter, I actively engage with the wider scientific community on a regular basis and would enjoy helping ACA expand its reach in these areas. I enthusiastically want to continue to support the ACA, and as a part of the ACA Communications committee I believe I can continue to help ACA grow, adapt and expand.

David Sanders - Continuing Education

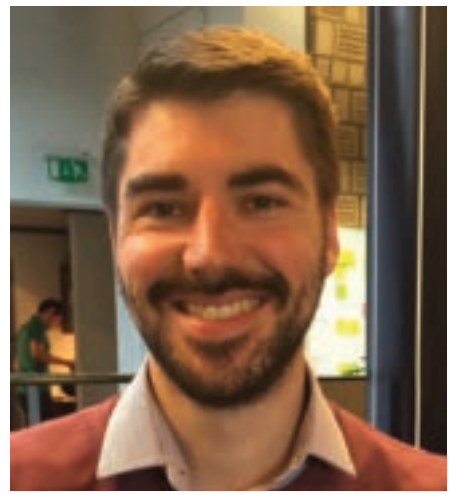
Professor, Department of Chemistry, University of Saskatchewan, Canada

Education: BSc Honors Biochemistry (Co-Op), University of Guelph (1991); PhD Biochemistry, University of Arizona (1998); post-doctoral work in the lab of J. Naismith, St. Andrews University, UK. Member of ACA since 2001; Chair of Organizing Committee PSFaM (2013-14); CIHR Thrust Mentor (2012-2015).

Research Interests: Protein structure-function relationships, enzymology, x-ray crystallography, protein-protein interactions, inhibition/inhibitor design.

Statement: . I feel very privileged to be nominated for a position on the Continuing Education Committee. It should be clear to everyone following the news over the last few years that science communication is becoming increasingly important to connect scientific experts with the public and with those who make public policy. I believe that it is essential for scientists to develop better ways to engage with the public. I have had the privilege to speak with elementary, high school and university students on crystallography and science in general and have seen the positive effects that a proper understanding of science can make. Both the Continuing Education Committee and the Communications Committee will play fundamental roles in bringing attention to the ACA and what we offer as knowledge creators and to make the public aware of the importance of crystallography and the impact that it has and will continue to have in our lives. As a member of the ACA Continuing Education Committee I will work to continue improving that ways that the ACA educates the media, policy makers and general public.

Peter Wood - Continuing Education



Senior Research & Applications Scientist, Cambridge Crystallographic Data Centre, Cambridge, UK

Education: MChemPhys, University of Edinburgh (2004); PhD in x-ray crystallography with Simon Parsons, University of Edinburgh (2008).

Professional activities: ACA Industrial Group committee (2013-2015, Chair 2014-2015). BCA Chemical Crystallography Group (2010-2017, Chair 2015-2017). ECA Young Crystallographers General Interest Group (2010-2013, Founding Committee Member). Lecturer & tutor on the biannual BCA/CCG Advanced Crystallography School in Durham, UK every iteration from 2009 to 2017. Lecturer & tutor at the 4th CNRS Crystallography School in Nancy, France (2009). Lecturer at the Erice International Crystallography School in Erice, Italy (2016). Lecturer & tutor at the 3rd European Crystallography School in Bol, Croatia (2016). Organizer of >12 CSD workshops at academic crystallography meetings in the last 10 years.

Research Interests: My particular focus for research is in the areas of intermolecular interactions and crystal engineering. Current research areas cover a range of topics including polymorphism, co-crystal design, metal-organic frameworks and the fundamentals of intermolecular interactions. The interplay between experimental, knowledge-based and computational methods to understand interactions in the solid state underpins all of this research.

Statement: I am really pleased to be nominated to serve on the Continuing Education Committee and would very much welcome the opportunity to be involved with this committee. Education has always been a strong interest of mine right from the beginning of my postdoctoral career. I've been involved with a number of crystallography schools targeted at postgraduates over the last 8 years, but particularly the biannual advanced crystallography school held in Durham, UK. The experience of tutoring PhD students in the nitty-gritty details of the math, physics, chemistry and symmetry underpinning crystallography all day for 7 days straight is hard work, but incredibly fulfilling! It's always exciting to talk through the concepts with a fresh new batch of students, to hear different perspectives/backgrounds and to refresh my own knowledge of the field.

I've also been involved in organizing and running educational workshops at a wide range of academic crystallography meetings over the last decade (including the ACA). These kinds of workshops are extremely helpful for both academic and industrial scientists - to be able to expand one's knowledge and skills in a particular area at a conference you are already going to be attending. When you are tight for time and travel budget, making the most out of the one or two conferences you can attend is even more important. This of course means that it should be a strong focus for the Continuing Education Committee to keep abreast of developing and emerging techniques to ensure that the workshops being planned are appropriate, current and of strong interest to the community.

In recent years I've also become more interested in the presence and impact of crystallography in undergraduate education, in schools and in public outreach. I think we, as a community, have a responsibility to continue to communicate the benefits of crystallography and, in particular to help to connect crystal structures into undergraduate chemistry courses. Compared to other experimental techniques, crystallography and crystal structures are strangely underrepresented in undergraduate chemistry.

I've been coming along to ACA annual meetings since 2007, organizing workshops at three meetings, speaking at four and chairing sessions at five, but always enjoying the experience, the science and the atmosphere. Despite not being based in the USA myself, I've always felt warmly welcomed into the ACA community and it would be an honor to serve that community as a part of this committee.

Craig Bridges - Data Standards and Computing

Materials Chemistry Group, Chemical Sciences Division at Oak Ridge National Laboratory.

Education: BS (1995) University of Alberta, PhD (2002) McMaster University, postdoc (2002-2006) University of Liverpool,

Professional Activities: 2015-present Reviewer for the APS structural sciences proposal committee, 2009-2016. Reviewer of neutron proposals for the C2 neutron diffractometer at Chalk River Laboratories, 2011-2017 - Session organizer for ACA meetings, 2009-2010 - ACA Neutron Scattering SIG (Chair: 2010)

Research Interests: My interest lies in areas including electrochemical energy storage, electronic properties, neutron detection, neutron scattering, diffraction, crystal structure solution, and nanoscale effects in materials design. My current main focus is on the development of novel inorganic materials in the areas of electrode and solid electrolytes for battery and solid oxide fuel cell (SOFC), and the reactions that occur at interfaces in electrochemical energy storage systems, as well as quantum materials.

Paul Sanschagrin - Data, Standards & Computing

User Application Scientist, Cambridge Crystallographic Data Centre, Piscataway, NJ

Education: BS Biochemistry, Michigan State University (1996), PhD Biochemistry, Michigan State University (2001), Postdoc, Philipps University, Marburg, Germany (2002-2004)

Professional Activities: Member of ACS (2008, 2014-), Member of ACA (2006-), Member of Structural Biology Grid (SBGrid) group (2012-2014)

Research Interests: My main research area of focus throughout my scientific career has been using structure-based computational methods for drug discovery and design. This has included large scale docking and virtual screening studies, using in-house software that I co-developed (SLIDE), and commercial packages for both methods development and improvement as well as applying to real world discovery projects. In recent years, I have also started to look at how large scale structural data and chem-informatics approaches can be applied to drug discovery problems, making extensive use of the Cambridge Structural Database, as well as expanding into ligand-based design approaches. I have also begun using cloud-based systems, such as Amazon Web Services' EC2 service to enable large scale computation at an approachable cost.

Statement: I want to thank the nominating committee for putting my name forward and would be honored to serve on the ACA Data Standards and Computing committee. As someone who has spent his career utilizing structural data as a basis for research, I am keenly aware of the importance of data standardization, both of the data itself and of the metadata that provides context to the data. This is a time when not only is the amount of chemical structural data, crystallographic data and data from other techniques, growing at a significant rate, the amount of data from other connected scientific fields is exploding. The possibility of connecting the structural data to this other data holds promise for enabling scientists to discover deep insights into biological processes, materials properties, and many more important areas. Key to this data synthesis is the ability to understand the content and context of the data, both for humans and computer systems. In the crystallographic community, we are fortunate to have a long history of uniform data formats including CIF, PDB, mmCIF, and PDBML. Therefore, it is key to continue to maintain these standard formats and to work with database organizations, software developers, and instrument manufactures to ensure the community's needs are met. It is also important to consider where future data may come from that is not be well covered under existing formats, such as x-ray free-election lasers or Cryo-EM, fields that may also be relevant to structural chemistry and biology. In addition to considering the structural data, which may be considered the results of the experiment, it is becoming more apparent that having the raw data, at least structure factors but perhaps even the x-ray images themselves, can have significant advantages as refinement and other data processing methods improve. This poses significant challenges in terms of reading the data in proprietary or obsolete instrument formats, storage sizes, and network bandwidth issues.

We must also consider the potential for the widespread use of large-scale computing through cloud services, such as Google Cloud, Amazon Web Services, and Microsoft's Azure, as well as through shared systems such as XSEDE. Having uniform standards for data, including metadata for providing context for the data itself, is especially key where users from various organizations and research groups may be utilizing the same datasets. The ACA can, and already does, play a significant role in maintaining data standards and it is key that it continues to play a role.

ACA Denver - WK.03: Serial Crystallography Data Analysis with Cheetah and CrystFEL: Concepts and Tutorials

The 2016 ACA hosted the third installment of the popular Serial Crystallography Data Analysis Workshop series sponsored by NSF BioXFEL STC. The workshop was a great success and was attended by about 20 students, postdocs, and faculty from academia, industry and government labs. The morning session included an advanced introduction to serial crystallography data reduction, with a hands-on tutorial of the Cheetah software. The tutorial included accessing and interacting with real data remotely at LCLS. The data reduction steps began with reading raw data collected at LCLS, selecting appropriate hit-finding parameters, and understanding the resulting format of the "clean" data for further processing. The afternoon session introduced processing the reduced data using the CrystFEL software. This hands-on tutorial including indexing, integration and merging, resulting in a set of reflections for structure determination that may be used with conventional crystallographic software.

Organizers: Thomas Grant and Nadia Zatsepin

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Workshop attendees - Organizer Tom Grant is in the back row - 3rd from the left and Organizer Nadia Zatsepin is in the front row - also 3rd from the left.

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AUGUST 2017

20-25 **XXVI International Materials Research Congress**. Cancun, Mexico
www.mrs.org/imrc-2017

21-28 **24th Congress and General Assembly of the IUCr**. Hyderabad, India
www.iucr2017.org

OCTOBER 2017

8-13 **Int' l School on Fundamental Crystallography and Electron Crystallography** Sofia, Bulgaria
www.crystallogra[jy.fr/mathcryst/sofia2017.php

16-31 **X-ray Methods in Structural Biology**. Cold Spring Harbor, NY
meetings.cshl.edu/courses

19-21 **75th Annual Pittsburgh Diffraction Conference** Indiana, PA
www.pittdifsoc.org/conference.htm

NOVEMBER 2017

26-Dec 1 **MRS Fall Meeting & Exhibit**. Boston, MA
www.mrs.org/fall2017

DECEMBER 2017

3-7 **The 31st Biennial Conference of the Society of Crystallographers in Australia and New Zealand**. Pullman Bunker Bay, Western Australia
crystal31.com/

7-14 **Structural and Biophysical Methods for Biological Macromolecules in Solution**. Singapore
meetings.embo.org/event/17-macromolecule

JULY 2018

20-24 **ACA 2018 Annual Meeting**. Toronto, ON, Canada
www.AmerCrystalAssn.org

JULY 2019

20-24 **ACA 2019 Annual Meeting**. Covington, KY
www.AmerCrystalAssn.org

The AIP State Department Science Fellowship

Most of the foreign policy issues faced by the US Department of State have a scientific or technical component. This fellowship is intended to enhance the S&T capacity of the Department by enabling at least one scientist annually to work at the Department's Washington, DC headquarters for a one-year term.

This is a unique opportunity for a scientist to contribute scientific and technical expertise to the Department and raise awareness of the value of scientific input. In turn, scientists broaden their experience by interacting with policymakers in the federal government and learning about the foreign policy process.

Application deadline: November 1 of the year prior to the fellowship term of the year applied for.

The AIP Congressional Science Fellowship Program

The American Institute of Physics, in partnership with the Acoustical Society of America (ASA), annually sponsors one scientist to spend a year providing analytical expertise and scientific advice to Congress. A second fellowship is sponsored by the American Physical Society. The program enables scientists to broaden their experience through direct involvement with the legislative and policy processes.

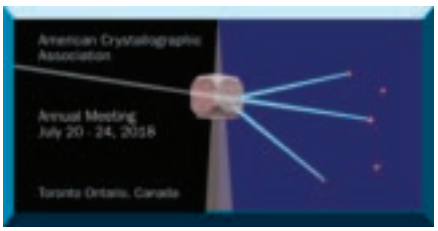
Fellows gain a perspective which, ideally, will enhance not only their own careers but also the physics community's ability to more effectively communicate with its representatives in Congress.

Benefits: Stipend of $70,000 - $72,000 per year. Relocation allowance. Allowance for in-service travel for professional development. Reimbursement for health insurance premiums up to specified maximum.

Application deadline: January 15 of the year of the fellowship term. Fellowships are for one year, usually running September through August.

Scientists at all career stages, including mid- and late-career professionals, are encouraged to apply. Although the fellowship is a full-time position, arrangements to supplement the stipend by continuing to receive a salary from a current employer while taking a sabbatical or leave of absence during the fellowship term may be worked out on a case-by-case basis.

www.aip.org/gov/fellowships/both_apply.html



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http://www.amercrystalassn.org/2018-meeting-homepage

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Etter Early Career Award in honor of Jason McLellan
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Jason McLellan
Etter Early Career Award

Simon Billinge
Warren Award

Frank Hawthorne
Buerger Award

Opening Session Keynote Speaker

John Polanyi - 1986 Nobel Laureate in Chemistry

Gerald Audette
audette@yorku.ca

Tiffany Kinniburgh
Kinnibrught@gmail.com

Program Co-Chairs

Poster Chairs

Louise Dawe
Ldawe@wiu.edu

David Rose
david.rose@
uwaterloo.edu

Photographer
Peter Müller
pmueller@mit.edu

Transactions Symposium
Shining a Light on Structure-Based Drug Design

Micro-Symposia

Remembering Dick Marsh
Organizers: Paul doyle, Louise Dawe, Alexander Filatov

Remembering Philip Coppens

Crystallization on the International Space Station
Organizers: Debbie Wells and Marc Giulianotti

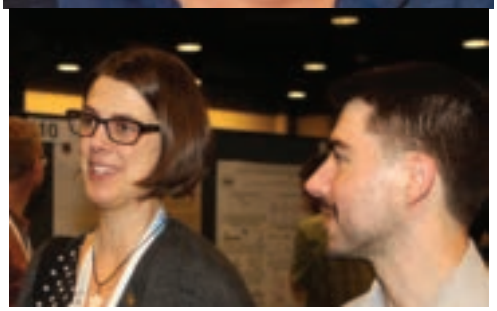
More to come - check the meeting website on a regular basis









Top row: The Brazilian contingent, Mike James and John Helliwell; Second row: Kay Onan and Connie Rajnak, Jim Fettinger and Sir Fraser Stoddart, Third row: Jeanette Krause and Allen Oliver (see the fall issue of RefleXions to find out why that cake is sitting between them); Fourth row: B.C. Wang, Anna Gardberg, Andrzej Joachimiak, Amy Sarjeant and Pete Wood.

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Travel Grants

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Miguel Torres (Calgary)

Hong Kong

Madiha Nisar (Hong Kong)

Mexico

Barbara Ramirez (Nacional Autóonoma de Mexico)

South Africa

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Alice Brink (Free State)
Gertruide Venter (Free State)

United States

Thomas Bohl, (Minnesota)
Andrea Bruck (Stony Brook)
Benjamin Frandsen (Berkeley)
Justin Kurian (Florida)
Shukun Luo (Columbia)
Suzanne Mays (Emory)
Steve Meisburger (Princeton)
Govinda Remesh Soumya (Lawrence Berkeley Natl Lab)
Kyle Stiers (Missouri - Columbia)

2017 SIG Etter Lecturers:

Powder Diffraction - Ying Zhang (Brigham Young)
Small Molecules - Korey Carter (George Washington)
Service - Niko Giordana (University of Edinburgh)
Light Sources - Seth Corey (Texas A & M)
BioMac - Avni Bhatt (U. of Florida)
YSIG - Kyle Stiers (U. of Missouri)
Neutron - Daniel Olds (Oak Ridge National Lab)
Materials - Andrea Bruck (Stony Brook U.)
Industrial - Madushani Dharmarwardana (UT Dallas)
Small Angle - Eric Manley (Northwestern U.)
Canadian - Matt McLeod (.U. of Waterloo)

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- ✓ Aliquot and normalize salt screens for LCP reactions
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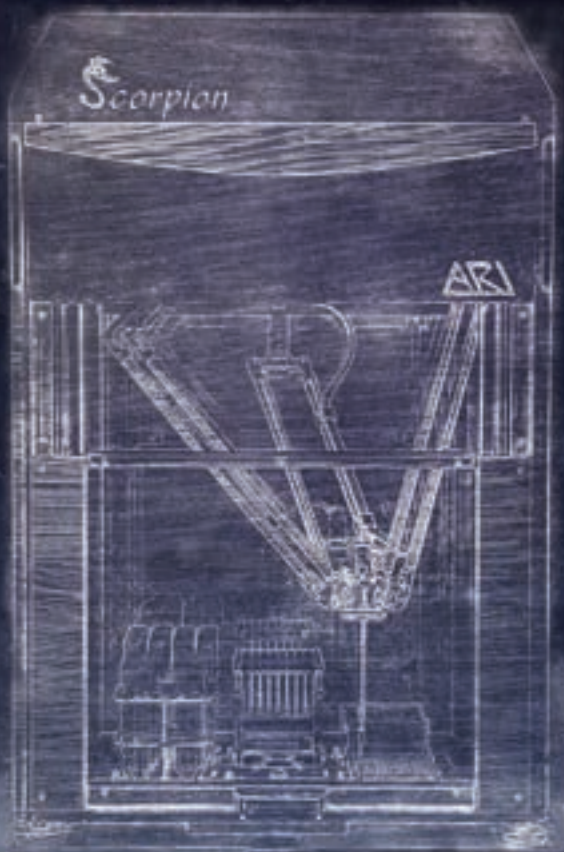
- ✓ Build multi-dimensional grids, pH, concentrations & titrate additives
- ✓ Set up 24-well plates, protein + screen
- ✓ Anything you can do with a handheld pipettor



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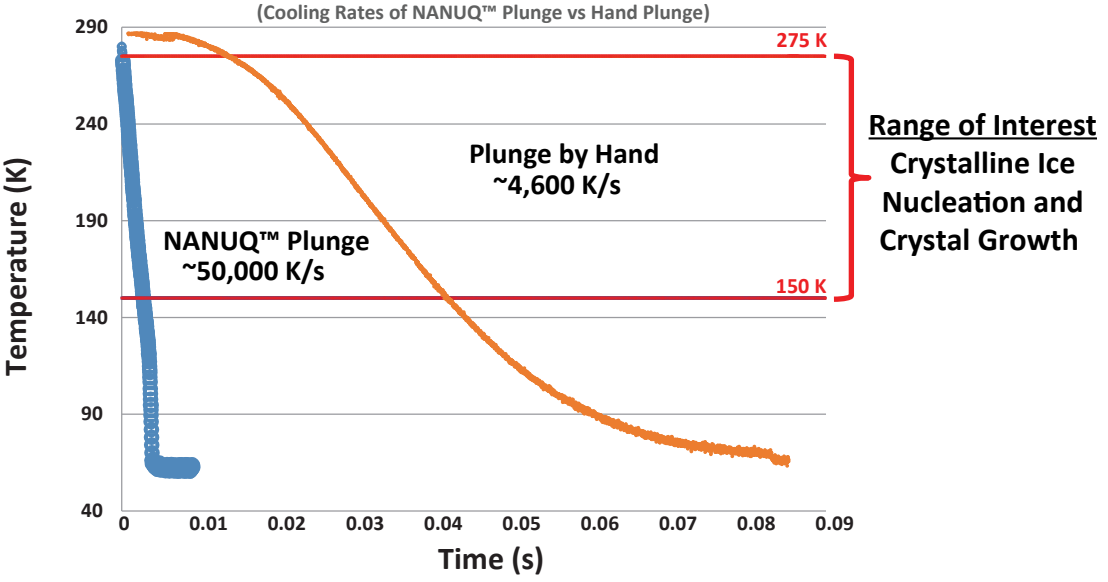

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