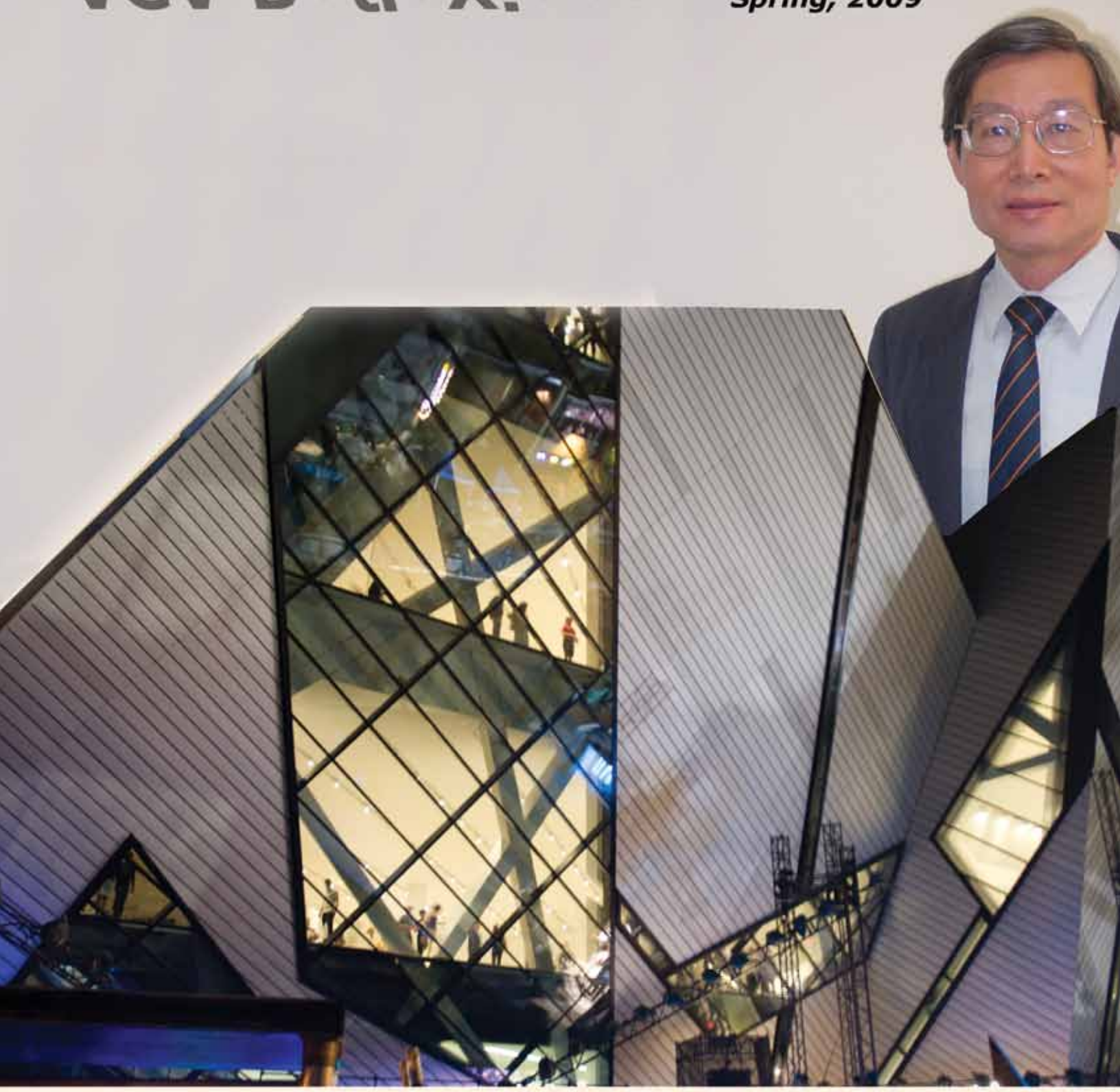
ACA RefleXions

American Crystallographic Association

Number 1
Spring, 2009



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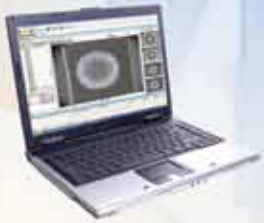

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ACA HOME PAGE: **www.AmerCrystalAssn.org**

Cover: see page 22. Shih-Lin Chang will receive the Warren Award in Diffraction Physics at the 2009 ACA meeting in Toronto. Below: the Michael Lee-Chin Crystal addition to the Royal Ontario Museum in Toronto.

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think forward

Crystallography

Happy New Year, 2009, the year of Change! We have an exciting year ahead for the ACA with our annual meeting this time hosted by our neighbor to the north; in Toronto, Canada, July 25-30.

First, I would like to extend my gratitude to the out going ACA President Marv Hackert and ACA Secretary Lisa Keefe for their excellent service and to our ACA Past President Alan Pinkerton for his timely advice in council deliberations. I know I will be grateful for Marv's continued presence on council as ACA Past President. Additionally, I thank Annie Heroux, Gloria Borgstahl and Bernard Rupp for their services on the ACA Standing Committees.

Welcome to the new ACA Vice President, Judy Kelly, and the new ACA Secretary, Carrie Wilmot; they join Bernie Santasiero, (ACA Treasurer); Jim Britten, (Canadian Representative); Marvin Hackert, (Past President); Bill Duax, (Chief Exeutive Officer); S. N. Rao, (Chief Financial Officer); Louis Delbaere, (IUCr Representative); and Marcia Colquhoun, (Director of Administrative Services). I look forward to working with all of them this year. Also congratulations to the three new ACA Standing Committee members: Thomas Proffen, Allen Hunter and John Rose, and to the new chairs and other officers of our SIGs. These groups are the real backbone of the ACA, especially as they actively formulate the program and workshops for the ACA annual meeting.

The main business of the ACA is our annual meeting, and this year it will be held in Toronto, Canada, (David Rose is the local chair), and managed by Marcia Colquhoun in the ACA's Buffalo office. My first impressions came from the meeting, held after the Knoxville ACA Meeting, that included past local and program chairs and all those who will be involved in the Toronto meeting. Toronto program chair Jim Britten organized the meeting. The layout of the sessions came together very smoothly and, thanks to the SIGs, we have a very exciting program which shows the broad scope of crystallography in a wide variety of sciences. Many of the sessions are sponsored by more than one SIG, showing the strong interrelationships within our science. After looking at the program (at the bottom of **http://www.cins.ca/aca2009/**), I'd say there should be something for everyone on every day of the meeting.

In addition to the program, we will be making a number of awards: the Warren Award in Diffraction Physics will be presented to Shih-Lin Chang (National Tsing Hua University, Taiwan), the Martin J. Buerger Award to Michael James (Univ. Alberta, Canada), and the Etter Early Career Award to Svilen Bobev (Univ. Delaware). The program also features Plenary Lectures by Phillip Coppens (SUNY, Buffalo) and Ted Baker (Univ. Auckland, New Zealand). At this meeting we are trying a new twist by starting each day with an unopposed plenary or award lecture.

Do be sure you have all the appropriate documents (e.g. passport) if you are coming to Canada from another country (especially the US). There is nothing more embarrassing than being turned away at the border especially when trying to go home. Please encourage your students and postdocs to come to the meeting and to submit abstracts; the rules this year require that 40% (e.g. 2 talks out of 5) of the sessions be taken from the submitted abstracts. There are limited funds for student travel; see the ACA web site for details and application forms.

We will be back in Chicago for the 2010 meeting (July 24-29); nominations for the 2010 awards (Isidor Fankuchen, Kenneth N. Trueblood, and Margaret C. Etter Early Achievement)) are encouraged. Go to the ACA web site **www.AmerCrystalAssn.org** for details.

In the past year there has been a vast improvement in the ACA's web site. I strongly recommend that you have a look, at least to check out your own member information. You can become a member of the ACA or renew your membership (still only $100 for regular members). One very interesting link is to Xforum; a moderated forum created in 2006 "for discussing x-ray diffraction and crystallography matters." Currently it has about 220 members and appears to have several active and interesting discussions in progress. I recommend that you check it out (you do need to join) and perhaps contribute your thoughts. We can all learn something from these contributions. Other links go to sites that feature previous ACA meetings (with photos!), various workshops, and schools of interest to crystallographers. We thank the folks in the Buffalo office for putting together this useful tool for all to use.

Finally, we note with sadness the loss of Bob Bau who passed away late last year. He had just finished his term as ACA Past President in December 2007, and I'm sure many of you will remember his Hawaiian Love Song at the Salt Lake ACA Meeting banquet. His will be a tough act for me to follow when it's my turn next year in Chicago.

All the best; see you in Toronto!

Bob von Dreele

The Editors regret that on page 24 of the Fall 2008 issue of RefleXions, (in the boat trip collage), Trixie Wagner is the person talking with Elspeth Garman, NOT Ima Dix as was published.

I was asked to pilot a new idea for ***RefleXions***, the creation of a "guest editor." I was thrilled when an article about the Margaret C. Etter Early Career Award and its recipients was suggested as my written contribution to this issue. It gave me an excuse to learn more about the remarkable career of Margaret "Peggy" Etter, as well as get to know some of the crystallographers who have received this award.

By all accounts Peggy was a remarkable woman[1]. A graduate of the University of Pennsylvania, she conducted her doctoral studies with Jack Gougoutas at my personal tenure home, the University of Minnesota, on the chemistry of topotactic reactions. In 1976 she went to work for 3M, where she established an organic solid-state chemistry group. Always an educator and champion for underrepresented groups, she helped form the 3M Visiting Women's Scientist program, and was a Director and Instructor for the Science and Technology Enrichment Program STEP, which is intended to encourage female and minority students to pursue scientific careers. Following a postdoctoral experience in solid-state NMR, she rejoined her alma mater, the chemistry department at the University of Minnesota, as a tenure-track assistant professor. In seven short years she built a world-renowned research group, publishing over eighty manuscripts. For Len MacGillivray receiving the Etter Award had special meaning: "Margaret Etter was a force early on in the field of organic solid state chemistry. As an undergraduate and graduate student, I constantly read her papers. In that way, it was a great honor to have been selected for the award." She was also extremely active in the ACA. She served as Program Chair for the 1991 meeting in Toledo, was Chair of the Small Molecule SIG and edited the 1988 *Transactions* entitled *NMR and X-ray Crystallography: Interfaces and Challenges*. Her untimely death from cancer at the age of 48 cut short a career that had touched so many. Look no further than the ACA list of awards for testimony of the high regard she was held in. There are no less than three separate annual awards in her name; the Margaret C. Etter Early Career Award, the Student Lecturer awards and the Student Travel Awards. They are all early career awards, and reflect her commitment to young scientists who are the future of crystallography. Finally, if you navigate to the web-page of the chemistry x-ray crystallography facility at the University of Minnesota, the first words that greet you are a quote from Peggy which all of us can relate to: "Crystal growth is a science and an art".

So what are on the minds of Margaret C. Etter Early Career Award recipients at this time? By email, I posed various questions to my fellow awardees about the future of crystallography, the role of the ACA and any advice they wished to pass on to President Obama regarding science policy (I am sure he is an avid reader of *RefleXions*).

Any advice for President Obama on science policy?

Wilmot (2006): "Mr. President (Obama that is, rather than Von Dreele*) I realize that you are a busy man, so we will get right down to our collective thoughts. Then you can get back to pushing through the American Recovery and Reinvestment Act that brings cheer to our hearts. We note that as it stands the Stimulus Bill will give NIH $10.4 billion, including $1 billion for construction and renovation, and $300 million for shared equipment; NSF $3.0 billion; DOE $2 billion; NOAA $280 million; NASA $550 million; NIST $580 million. We all agree that this is a very good thing for both our personal scientific futures and the economic future of the United States. We are glad that you have placed science so high on your agenda."

*Note to President Bob: We mean no disrespect in the order we list Presidents. However, unless you have a few billion $$$ tucked away in the ACA coffers, we know on which side our financial bread is buttered. Don't worry, we have some advice for you later.

MacGillivray (2004): "Obama's legacy will be determined many years from now. I believe that it is well known that

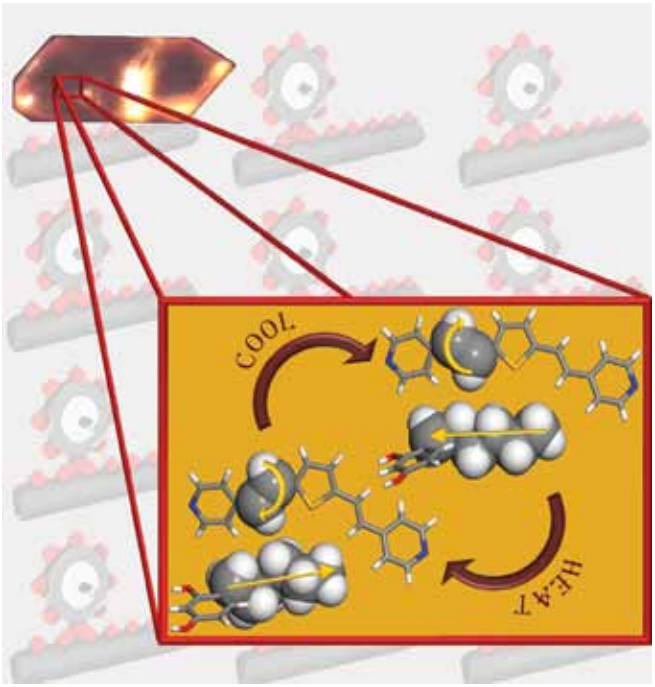

Image from Len MacGillivray

putting money into science research pays long-term dividends. Thus, I would suggest that Obama look beyond the 4 to 8 years that lie ahead and think deeply about the role of science."

Where do you think crystallography is going, both in terms of growth and decline? We all seem to agree on three things:

(1) Crystallography (including neutron, electron and powder) is always going to be an important part of the analysis of materials.

MacGillivray (2004): "Crystallography will always play a prominent role in our research. We cannot live without it. One gets a certain satisfaction when ones determines the structure of a new solid – whether it is for confirmatory reasons or in the context of a discovery. Thus, I believe that crystallography will always be an indispensable tool for small molecule and even more so for supramolecular chemists. As long as the properties of materials continue to surprise us, there will always be new avenues for research in crystallography."

Chan (2003): "Crystallography is certainly an important aspect of crystal growth and the discovery of new materials."

Lind (2007): "As solid-state chemists, we live and die by our ability to structurally characterize our materials. The exciting developments especially. in the neutron community (SNS coming online) are currently opening new avenues for our research, and we are planning to make good use of these opportunities."

Bobev (2008): "In terms of what we do now – we are continuing our efforts to put the big puzzle together – what are the relationships among the composition, structure, and electronic structure in complex intermetallic compounds and their properties. Crystallography, both powder and single-crystal (and most recently electron diffraction) is an integral part of our work(life). And it will be for the foreseeable future."

This leads to our second point:

(2) The user base is increasing rapidly.

Wilmot (2006): "In macromolecular x-ray crystallography the number of PX beam-lines at synchrotrons has grown rapidly. Robotic mounting of crystals has exponentially increased the number of crystals that can be screened within a short timeframe. Microfocus beamlines are enabling usable data to be collected from tiny crystals. Remote data collection reduces logistical concerns and cost. There are now many options for phasing, particularly SAD and MAD. Robotic crystallization trials can search a large number of conditions with small amounts of protein. The growth of integrated, automated "data to protein model" software makes straightforward structure solutions appear easy. This is encouraging researchers from non-traditional labs to try crystallographic experiments."

Bobev (2008): "I think the trends for fully automated "structure solutions" are full steam ahead, which somewhat undermines the value of what we do (or used to do before the computer that can run 100 refinement cycles in 2 sec came on board). I am a bit worried that small-molecule crystallography does not have the magic it had for me when I first started doing it – for most of my students it is just a black-box, a mouse click or hit "return" on the keyboard."

Which leads to:

(3) With the expanding user base, we need to increase teaching and training opportunities.

Lind (2007): "The number of users is certainly growing fast. To counteract any "decline" tendencies, it is our duty to find creative ways of making crystallography teaching available to the growing user base. Crystallography is not part of many universities' curricula, leaving students (and faculty) who depend on crystallography for their research with limited knowledge resources. There should be a strong effort to make schools and web based resources available to ensure growth not just in numbers, but in knowledge."

Chan (2003): "Crystallography needs to be emphasized in our curriculum as it is vital for careful correlation of materials and properties."

Wilmot (2006): "I worry about the non-traditional user groups in macromolecular crystallography. Luckily many are in close proximity to crystallographers, but this places significant training demands on the crystallographic groups to help the untrained. Macromolecular crystallography is data poor, and so care must be taken with all aspects of data handling and interpretation. Each step requires training and understanding of many metrics to make sure all is well. Even the structure of a site-directed mutant by a crystallographic neophyte is fraught with potential pitfalls. I know within my own group that helping newbies has been increasing to the point that my people are experiencing significant impact on their own research, and this reduces my lab's productivity. I have been hearing from synchrotron beam-line scientists that they also are experiencing this "sea change", and phasing data has become an increasing part of their remit. ACA could help in making this rapid shift clear to granting agencies, such as DOE, NIH and NSF, and that requests for additional support personnel focused on training new users

may be required, both at synchrotrons and large universities, to address the increase. We should do everything we can to attract new users – it is our future – but we require resources to give the necessary training that these keen, bright-eyed young researchers deserve."

Do you have any suggestions of how the ACA can better serve the crystallographic community?

Lind (2007): "With regard to the annual meeting: try to find some more affordable hotel options. I realize that this may be difficult as the ACA meeting is not as big as, for example, ACS national meetings, thus limiting the number of hotels that can be offered. Free wireless should be a must - and if the hotel doesn't offer that, the meeting website should clearly specify whether there will be an ACA wireless network available."

Note: The ACA has recently negotiated some multi-year deals with certain cities that will host the annual meeting at regular intervals, e.g. Chicago, to lower future costs.

Wilmot (2006): "I am not sure how to go about this, but I am always surprised how few PIs go regularly to the annual ACA meeting unless they are invited to speak. In contrast the annual British Crystallographic Association meeting, along with the CCP4 study weekend, is attended by just about everyone. The meetings are based at universities, and most people slum it in the student residence halls or nearby cheap accommodation, which makes it very affordable. I would always go to breakfast early and join the tables of the PIs so I could get to know them and learn about the "latest and greatest" trends / topics. It was wonderful for a young researcher to sit with such experienced people, and of course I could get their specific advice and input. I wish we could ignite that kind of community spirit in the US. Whenever I meet up with US based PIs they are as enthusiastic and excited about the science as their British counterparts. I wish we could persuade them that the ACA annual meeting is a "must" to catch up with old friends, hear about the latest innovations and to meet young crystallographers who might energize them even more with their passion, science and ideas."

So finally what did receiving the Margaret C. Etter Early Career Award mean to all of us? It was obviously a great honor, and it helped with our tenure process. I even received a hefty discretionary addition to my base salary from the Provost that year. However, perhaps the most spectacular example of its worth is how the US government, in particular the US Citizenship and Immigration Services, rates the award. Due to some misunderstandings, I ended up having to apply for Permanent Residency as an Outstanding Professor (EB-1), which is a huge amount of work. With monumental effort whilst muttering under my breath about what a waste of my time it was, I just made the deadline to avoid being slung out of the country during processing of my application. It should be noted that the USCIS web-site on Outstanding Professor eligibility contains the following text: "You must be one of "that small percentage who have risen to the very top of the field of endeavor," to be granted this classification. For example, if you receive a major internationally recognized award, such as a Nobel Prize, you will qualify for an EB-1 classification. Other awards may also qualify if you can document that the award is in the same class as a Nobel Prize. Since few workers receive this type of award, alternative evidence of EB-1 classification based on at least three of the types of evidence outlined below etc." Granted a small Amazonian rainforest had been sacrificed to provide the paper for my application and supporting documentation, but right on the top was proof of my Margaret C. Etter Early Career Award. Following its mailing to the USCIS I went on-line to check it had arrived safely, and to my astonishment it stated that my application had been approved. I thought I was misinterpreting the information, but a week later I got a letter telling me I had been deemed worthy of Permanent Residency. The University of Minnesota was shocked; I believe the quickest prior approval had been three months (and my application was during the aftermath of 9/11). So I guess that means USCIS views the ACA Margaret C. Etter Early Career Award in the same class as a Nobel Prize! Joking aside, what ultimately meant the most to me was the honor of bringing the award back to the academic home of Peggy Etter. It made me realize what a fantastic fit the University of Minnesota was for my science, and that, like Peggy, it had become my home too.

I wish to thank the following people: My fellow Margaret C. Etter Early Career Award recipients; Julia Chan (2003 recipient), Department of Chemistry, Louisiana State University; Len MacGillivray (2004 recipient), Department of Chemistry, University of Iowa; Cora Lind (2007 recipient), Department of Chemistry, University of Toledo; Svilen Bobev (2008 recipient); Bill Gleason, Department of Medicinal Chemistry, University of Minnesota.

Carrie Wilmot

1. Gleason et al. (1992) Molecular Engineering 2: 213-214.

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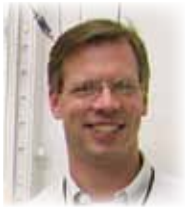

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IUCr Roster cont'd on page 16

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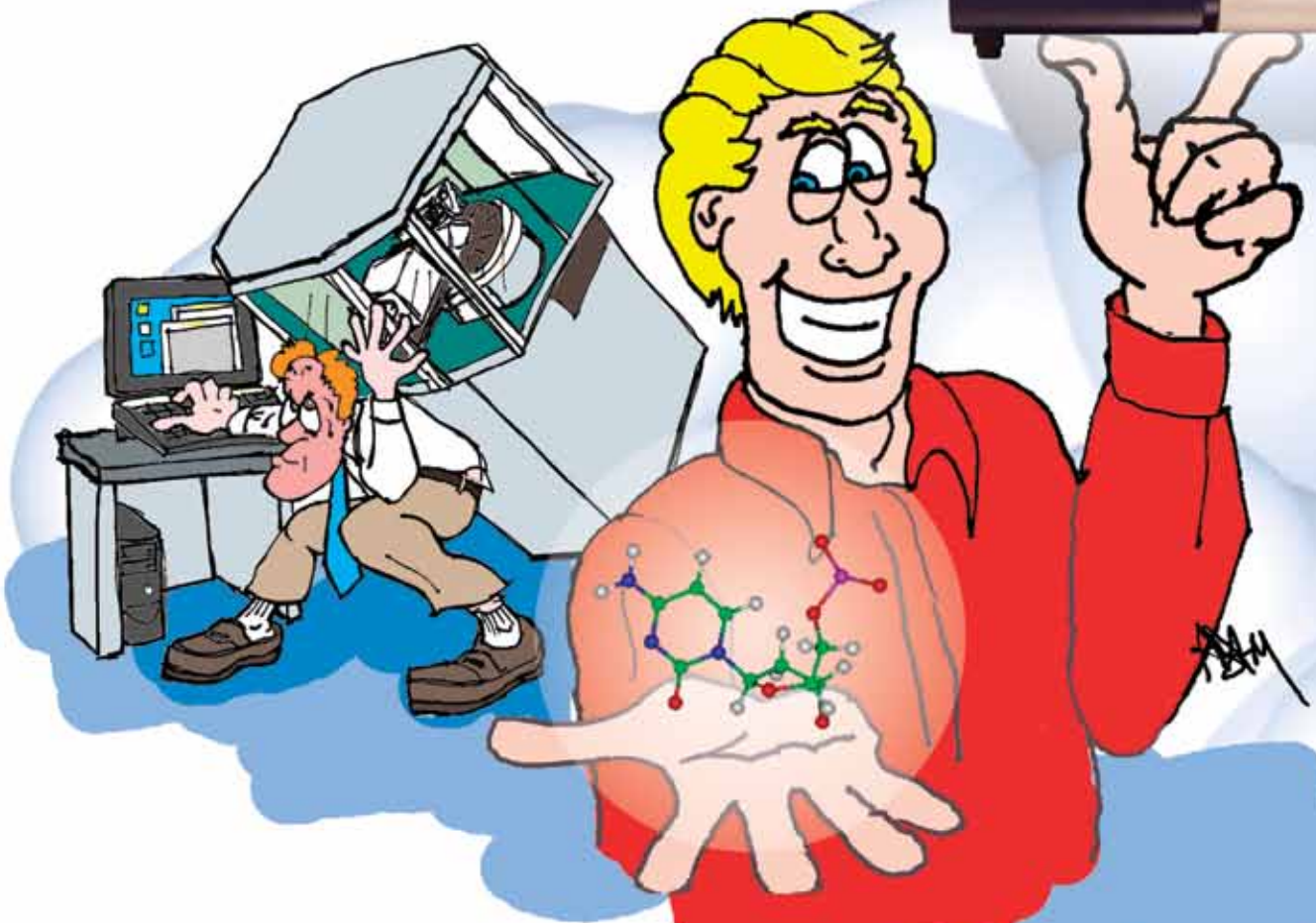

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Dorothy Hodgkin Award to Janet Thornton

The photo is from the Brunel University citation when Thornton was awarded an honorary degree.

The **Protein Society's 2009 Dorothy Crowfoot Hodgkin Award**, sponsored by Genentech, is granted in recognition of exceptional contributions in protein science. **Janet Thornton** (European Bioinformatics Institute) will receive the award in June, 2009 for her pioneering work in the field of bioinformatics. Throughout her career, Thornton has led the scientific community in the analysis of protein structures in a way that has transformed our knowledge of almost every aspect of their properties and their evolutionary history. Her most significant contributions have been to identify unexpected relationships between different proteins, considering their 3-dimensional structures and sequences. To achieve this she has developed new computational tools to store, retrieve, analyze and classify the growing body of structural data, including programs and databases that are used by the international community. The relationships derived from her analyses have proved practically useful, not only in understanding protein stability but also in prediction, modeling and design of protein structure. Often her contributions bring together disciplines, drawing attention to the links between them. She has changed the views of many crystallographers, NMR spectroscopists and theoreticians by causing them to view their work differently. She also helps those outside of structural biology - including industrialists - to understand the impact of the field for their work. In her present position as Director of the European Bioinformatics Institute, she continues to carry out research at the highest level as well as performing an increasingly important service to the community of protein scientists.

HHMI Award to Douglas Rees

The **Howard Hughes Medical Institute** (HHMI) started a $10 million/year program to fund **Collaborative Innovation Awards** which will go to 8 teams of scientists doing "transformative" research. HHMI investigator **Douglas C Rees**, Caltech, was chosen to lead one of these. Ree's four person team will use the HHMI funds to develop a more efficient and accurate method for solving the 3-dimensional structures of menbrane proteins.

Doudna Elected Fellow of AAAS

Jennifer A. Doudna, HHMI Investigator and Professor of Biochemistry and Molecular Biology at UC Berkeley, was elected a fellow of the AAAS.

Ludo Frevel Scholarship to Tobias Beck

The **International Centre for Diffraction Data** (ICDD) announced that a **2009 Ludo Frevel Scholarship** will go to **Tobias Beck**, Göttingen University, Göttingen, Germany for his crystallographic studies on biomimetics: *Learning from Metal Sites in Proteins*.

Kalamazoo is the new Biotech Hotbed

Lisa M Jarvis, writing in the February 23rd ***C&E News***, noted that a cluster of life sciences businesses sprang up in the wake of the 2003 hit when Pfizer closed down drug discovery research in Kalamazoo. Already, the medical device firm **Stryker** had been in the area for 60 years, and **MPI Research**, a contract firm, had been around for a decade.

In 2003, the City of Kalamazoo and the State of Michigan provided seed capital for potential entrepreneurs. The Southwest Michigan Innovation Center, a 58,000-sq-ft facility with lab and office space for rent, conveniently opened its doors just two months after Pfizer closed in 2003. Anticipating an upheaval in the drug industry, **Southwest Michigan First (SWMF)** began planning this incubator space for entrepreneurs in 1998. Several firms have been particularly successful: **Kalexsyn**, a chemistry-driven company, has moved from the Innovation Center to its own $5.5 million facility in Kalamazoo. It is starting to augment its staff, once dominated by older, ex-Pfizer scientists, with younger chemists who can benefit from the mentoring of their more experienced peers. **Proteos**, a firm focused on peptides, has grown from seven ex-Pfizer scientists to a staff of 17. It has become the anchor company at the Innovation Center, taking up over 10,000 sq ft of lab space.

In 2006, SWMF established a life sciences venture capital fund with two goals: to spur economic development and to sustain the science base in Kalamazoo. An early addition to the fund's portfolio is **Metabolic Solutions Development,** a diabetes drug discovery firm that can trace its roots to the Upjohn site. Cofounders Rolf Kletzien and Jerry Colca had both worked at Upjohn and survived as it changed hands, first to Pharmacia and then Pfizer. Both scientists moved to Pfizer's St. Louis site when research ended in Kalamazoo, but they still had a lot of ideas about a promising diabetes target they worked on in their Upjohn days.

Global Warming:

In a NY Times column in January, Thomas Friedman advocated giving a quick $5,000 to everyone who is academically eligible and willing to go back to school. He also said that "one of the smartest stimulus moves we could make would be to eliminate federal income taxes on all public schoolteachers, staple green cards to the diplomas of foreign students who graduate from any U.S. university in math or science (instead of subsidizing their educations and then sending them home), and offer scholarships to needy students who want to go to a public university or community college for the next four years." He suggested that the new administration and Congress should be guided by reading John Maynard Keynes (get as much money injected as quickly as possible) and by reading *Rising Above the Gathering Storm: Energizing and Employing America for a Brighter Economic Future*, published by the National Academies Press (March, 2007; ISBN-10: 0309100399; ISBN-13: 978-0309100397. (*Gathering Storm* was the report produced in 2005 by our National Academy of Science about keeping America competitive by improving math and science education, investing in long-term research, recruiting top students from abroad, and revising US laws to make them favor innovation.)

While attending the Energy and Resources Institute's Climate Conference in New Delhi, two American women, recent Yale grads (and one of their mothers), invited Thomas Friedman to go for a spin in the plug-in electric car (also powered by rooftop solar panels). They had just driven this car all over India in a "climate caravan" to highlight the solutions to global warming being developed by Indian companies, communities, campuses and innovators. In New Delhi, on one of the main streets, Panchsheel Marg, the US Embassy and the Chinese Embassy are directly across the street from each other. The US Embassy is loaded with antennae and listening gear. The Chinese Embassy is loaded with new Chinese-made solar hot water heaters.---

(The second paragraph was adapted from Thomas Friedman's column in the *NY Times*, Sunday February 15th)

The following was adapted from *Electric Cars for Everybody Soon?* in the *Washington Post National Weekly Edition* February 9-15.

On January 23, the entire Michigan congressional delegation sent a letter to President Obama urging support of renewable-energy industries, particularly electric-car batteries.

So far, Asian battery makers have a leg up. General Motors announced in early January that it had passed over US battery firms and chosen LG Chem, a Korean firm, to make the lithium-ion battery cells for the Chevy Volt. (GM plans to assemble the cells at a $30 million plant it wants to build in Michigan.) GM Vice-President Bob Lutz said that thanks to many years and massive support from Korea Incorporated, LG Chem has a head start of several years over American firms. For carmakers, the choice of battery is a matter of strategy as well as technology. Most American motorists drive 40 miles or less a day, so GM is planning on a battery pack big enough to last 40 miles, at which point a small gasoline engine would take over.

Connie Rajnak

Appeal for Volunteers

In the spring '08 issue, we announced that Carrie Wilmot agreed to be a Guest Editor --that is to be in charge of an entire section. We suggested that she do email interviews, posing questions such as *how the award has influenced your career* to all the Etter Award winners, (Carrie herself won the award in 2006). She accepted with alacrity, and the result (see pages 4-6), was terrific. In fact her success caused light bulbs to go off in our brains -- suppose we had an entire volunteer staff! Judy and Connie are volunteers, and so is our staff photographer, Peter Müeller. We can envision volunteers in charge of the *Books* section; the *Opinion* columns; the *Calendar; Meeting Reports; Future Meetings;* and articles on topics including but not limited to: crystallography education, nanoscience, PDF theory & techniques, SAS & SASX, or synchrotron facilities. Note that we don't do all of these sections in every issue. The *Books* section appears in two issues; *Opinion* columns are about twice a year and have up to now included global warming updates and threats to the scientific teaching of evolution. *Meeting Reports* and *Future Meetings* are in every issue, but the editor's work is limited to editing for style and content since reports, meeting flyers and photographs are contributed by meeting attendees. Carrie Wilmot's article is an example of a report on a special topic and such reports depend on volunteers, so they might only happen once per year. If you have an inclination to make our dream a reality, please contact either of us: Judy Flippen-Anderson <flippen@rcsb.rutgers.edu>, or Connie Rajnak, <connie-chidester@earthlink.net>.

Darwin - Evolution - Threats to Science Education

The Rev. Michael Dowd, author of *Thank God for Evolution: How the Marriage of Science and Religion Will Transform Your Life and Our World* (Viking) brought his cosmic gospel to west Michigan on January 14th. Michael and his wife Connie Barlow, a science writer, presented evolution as theology, not theory, and science as divine revelation. (!!!)

The Kalamazoo Gazette, early January, 2009

Charles Darwin was born February 12, 1809, 200 years ago. *The Economist,* in honor of his 200th birthday carried an article February 7th titled *Unfinished Business,* from which the following was adapted.

In 1859, Darwin published his radical book *On the Origin of Species,* in which natural selection was proposed to account for marvels of nature that had been by many attributed to the wisdom of God. In 1858, the previous year, both Charles Darwin and William Charles Wells, a Scottish doctor, presented the idea of natural selection to the Linnean Society in London. Wells had presented a paper on race to the Royal Society in 1813, and he had mentioned natural selection in this paper, so Darwin was not the first to conceive the idea. However Darwin became more famous because he had devoted the previous two decades to the accumulation of evidence in support of the theory. Evidence was emerging at the time that Darwin's book was published that the earth was extremely old. Darwin understood (and was troubled by his understanding) that natural selection rather than divine intervention could account for all the marvelous diversity he had observed. The trouble persists. A Gallup poll conducted in 2008 found that only 15% of people agreed with the proposition that humans developed over millions of years.

Found on the National Center for Science Education website: **ncseweb.org**

Evolution education is being battered every day in school districts across the U.S. by creationists, whether they're pushing young-earth creationism, intelligent design, or antievolutionism in the guise of "academic freedom." What's going on here? Why is the United States the only country where teaching evolution is so controversial? Why are scientists so sure that evolution is good science? Are people of faith truly unable to accept the central principle of modern biology? Is it really "fair" for creationism to be taught alongside evolution? What have the courts said? And will attacks on evolution ultimately undermine not only American education but American competitiveness? These and many other questions are answered in the 2nd edition of Eugenie Scott's *Evolution vs. Creationism*. Scott is one of the leading promoters and defenders of teaching evolution in the schools.

The October 23, 2008 *Houston Chronicle,* published a column by Alan Leshner, AAAS CEO and Executive Publisher, *Science*:

Board's Actions Could Put Students at a Disadvantage. The previous week the Texas State Board of Education appointed three anti-evolution activists, including a leader of the intelligent design religious campaign, to a six-member panel that will review proposed new science education. The new standards would shape how science education is taught in Texas for the next decade. Leshner commented that this anti-evolution push might hurt efforts to teach science in Texas.

Connie Rajnak

2008 USNCCr cont'd

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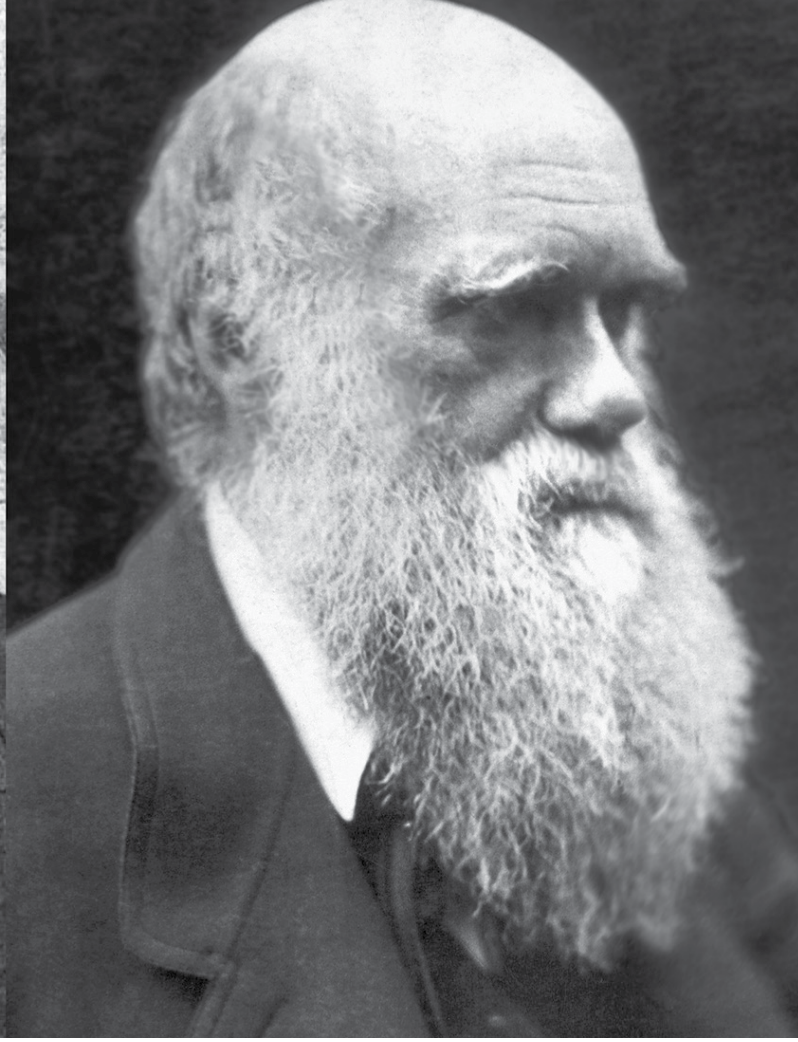

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Robert (Bob) Bau died on December 28, 2008, in Los Angeles. Bob was Professor of Chemistry at the University of Southern California, where he was a member of the faculty from 1969 until the time of his death. Bob served as ACA President in 2006, selflessly devoting countless hours to ACA affairs. In his research, Bob possessed remarkable insight and was a master at extracting the critical nuggets of information from groups of complex structures. He was a much beloved teacher and mentor, who introduced generations of first-year USC students to chemistry with his trademark sense of the broad historical sweep of chemical science, while also mentoring numerous graduate students who have gone on to their own distinguished, independent careers. His untimely passing leaves a deep void among his many friends in the scientific community.

Bob's research focused on structural chemistry, where his interests were unusually broad and deep. He was author or co-author of more than 250 research publications. Bob and his collaborators made major contributions to the development of the technique of single-crystal neutron diffraction and to its application in chemical crystallography. Indeed, they have been among the most active users of neutron facilities worldwide, carrying out their work at neutron scattering centers in Asia, Europe, and North America.

Bob's research group is perhaps best known for its work on the structures of covalent transition-metal hydrides, in which they systematically explored the principles for bonding in these systems and published several highly-cited reviews. They did pioneering work using neutrons to determine the absolute configuration of organic molecules having chiral methylene (-C(H,D)) groups. More recently they studied the structures of small proteins using neutrons as well as synchrotron radiation. Bob was intensely involved in developments at the Spallation Neutron Source (SNS) in Oak Ridge, serving as Principal Investigator of the Instrument Development Team (IDT) for the SNS Single-Crystal Diffractometer, TOPAZ, and as a member of the IDT for the Macromolecular Neutron Diffractometer, MaNDi. He was influential in the decision to hold the 2008 ACA meeting in Knoxville in order to showcase the nearby SNS facility.

Bob was born in Shanghai and grew up in Hong Kong, where he completed his undergraduate studies at the University of Hong Kong in 1964. He enjoyed telling friends about the adventure that brought him to America (he embarked literally by ship) - to do his graduate work at UCLA. His mentor there was the distinguished inorganic chemist, Herb Kaesz, but Bob was introduced to crystallography in the laboratory of Mel Churchill at Harvard, where Bob accompanied Kaesz during a sabbatical. After receiving his Ph.D. in 1968, Bob returned to Harvard for a year of postdoctoral studies with Bill Lipscomb, joining the group that was studying the enzyme aspartate carbamoyltransferase. Bob then was appointed to the USC faculty, where he served with distinction for 40 years.

Bob received many honors and awards over the course of his career. He was named a Fellow of the Alfred P. Sloan Foundation (1974-1976) and was an NIH Career Development Awardee (1975-1980). USC honored Bob with its Associates Awards for Excellence in Teaching (1974) and in Research (1979). In 1982 Bob was elected a Fellow of the AAAS. He received the prestigious US Senior Scientist Award of the Alexander von Humboldt Foundation in 1985.

Beyond his many accomplishments summarized above, important intangibles combined to make Bob an extraordinary scientist and person. Above all, through his humanity and integrity, Bob set a very high example that made him an unusually effective and sensitive mentor. Bob was, in the classical sense, a man of great taste. His broad knowledge of chemistry and his taste in scientific problems guided those who had the good fortune to know and to collaborate with him. In his understated way, Bob was a great ambassador for chemistry and for crystallography. In today's highly competitive world, Bob's modesty was the more remarkable. Many remember how genuinely flattered he was to be asked to run for President-elect of the ACA. Indeed, at the time, he was heard to remark that he'd, "Never been asked to run for anything before!"

Bob's Past President's 'speech' at the 2006 ACA meeting Award's Banquet. (He had everyone laughing with his lip-synched rendition of the "Hawaiian Love Song"

Bob is survived by his wife, Margaret Bau Churchill, his daughter and two sons, and two beloved grandchildren. He will be sorely missed by colleagues, friends, and family alike.

Tom Koetzle

Editor's note: Please contact either of the Co-Editors if you wish to contribute memories of Bob.

Professor Luis G. Roldan of Greer, South Carolina, passed away February 1st in his home, succumbing to advanced Alzheimer's disease. He is survived by his loving wife of 48 years, Carmen, their four children, José, Luis, Mary & Carlos, and three grandchildren.

He was born in Garafía, Spain on the Canary Islands in 1925 and raised in Seville, Spain, where he obtained his doctorate of science degree at the Universidad de Sevilla in 1957 in Chemistry & Crystallography.

Throughout his career he did research, first in the UK with British Rayon and then with Allied Chemical in Morristown, NJ, and finally for JP Stevens, where he worked from 1968-1986, beginning in Garfield NJ and concluding at the Greenville SC research & development facility.

After retiring from JP Stevens, he worked for NIST certifying laboratories for asbestos testing. He also was a professor and dean at the Universidad da Beira Interior in Portugal and was an adjunct professor at North Carolina State University.

He published over 40 articles in scientific journals. He was fluent in both Spanish & English and had a working knowledge of French, German & Portuguese. He belonged to various scientific organizations and was considered an expert in his field of material science using x-ray diffraction and electron microscopy.

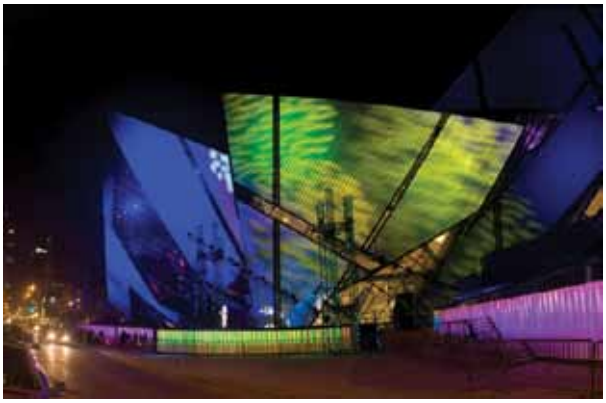
His body was donated to advance the knowledge of science and his ashes will be returned to Spain. Contributions in his memory may be sent to research Alzheimer's disease.

José Roldan

2009 Art in Crystallography Contest

We are accepting entries to the **2009Art in Crystallography Contest** in the form of images emailed to either Editor (**conniechidester@earthlink.net** or **flippen@rcsb.rutgers.edu**). Entries should be accompanied by a paragraph explaining the science and the method of producing the image. A photo of the artist would be appreciated but is not required. Prizes consist of a small monetary award and a banquet ticket at the annual meeting. Winning entries will be posted on the web and will be displayed at the ACA Meeting. (Winners are not required to attend the meeting). We will also feature images in *ACA RefleXions* from time to time. Please let us know if you are interested in being a judge.

The deadline for 2009 Contest is May 1st



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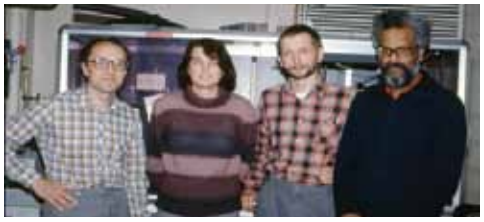
The determination of the structure of retroviral protease (PR) is a story that began 20 years ago. In fact, the 20th anniversary of retroviral PR structure almost coincides with the 50th anniversary of the first protein structure which was announced in 1958 by Kendrew.



The RSV PR team in 1988. L to r: Alex Wlodawer, Maria Miller, Mariusz Jaskolski, Mohana Rao.

In 1988, I joined the retroviral PR team at the Frederick Cancer Research Facility. The team was headed by Alex Wlodawer, and included Maria Miller and Mohana Rao. Jonathan Leis, Case Western Reserve Univ., provided the material, PR from the Rous sarcoma virus (RSV). Because proteins from HIV were very difficult to come by at that time, we decided to work on the enzyme from the closely related chicken virus. (We found out later that parallel work was being done on the authentic HIV-1 protein at Merck.) In 1988 single crystals of RSV PR were grown by Maria Miller, and x-ray diffraction data were obtained, first at 3, then 2.7 and ultimately at 2 Å resolution.

Our protein was composed of 124 residues and behaved like an aspartic PR; for example it could be inhibited by pepstatin, which also inhibits pepsin, but other details were not well known. Retrospectively, one wonders at our lack of faith in the information already at hand. But it all looked so bizarre because the virus itself was so bizarre… The amino acid sequence contained the DTG signature (or DSG in the case of RSV), so the enzyme indeed looked like an aspartic PR, but there was only one copy of the DTG motif and the enzyme had only 1/3 the number of residues found in the typical pepsin-like aspartic PR. We noted the ~1978 papers by Tang, which predicted that cell-encoded two-domain pepsin-like aspartic PRs might have evolved via gene duplication from much smaller, homodimeric ancestral enzymes. In 1987, sequences of retroviral PRs became available, allowing a hypothetical model of HIV-1 PR to be built by Pearl and Taylor. Their bold modeling exercise was done in spite of almost no sequence conservation between cell-derived and retroviral PRs. We knew of that model, but were not completely convinced because we did not think it applicable for molecular replacement, because it lacked non-crystallographic symmetry, and because molecular replacement methods were not well developed in the 1980s. But even with today's powerful algorithms and computers, it is not clear that the Pearl and Taylor model would be sufficiently accurate to solve the experimental structure.

The MIR method was the only experimental approach available to us. Maria Miller managed to produce heavy atom derivatives of RSV PR, and one of them, obtained with the application of uranyl acetate, was especially important. Mohana Rao used his programming skills to squeeze out phasing information from the scanty derivatives. Eventually, the electron density maps started to show some recognizable features. Surprisingly, among the first recognizable features were two segments of helical density and a very clear electron density at the uranium site, symmetrically flanked evidently by two carboxylates. When we realized that those carboxylates might be the aspartates of the two-fold symmetric DSG/DSG active site, everything started falling into place, and in a relatively short time the model of RSV PR was completed. It was not 100% complete but it immediately showed that the early predictions were correct: we had a dimeric aspartic PR resembling the monomeric two-domain pepsin. The active site had the same architecture, including the fireman's grip of the two DSG elements, and there was a water molecule between the aspartates. The similarity to pepsin allowed us to name the secondary structure elements as in one domain of pepsin. But there were also very significant differences with pepsin. Because of the symmetry, the two flaps were the same length and both prominent, although the tips in their elevated position over the empty active site were disordered. The subunit interface was formed by a tight four-stranded antiparallel ß-sheet woven from all the termini in the order: NA-CB-CA-NB.

Subsequently, Irene Weber built a homology model of the HIV-1 enzyme. The model looked very plausible; it had all the features of the template, and differences were limited to loop regions. The structure of RSV PR was published in *Nature* in 1989.[1] A week later, also in *Nature*, the crystal structure of HIV-1 PR was published by Manuel Navia, Paula Fitzgerald and coworkers from Merck[2]. In the same week, Irene Weber's model was published in *Science* [3]. After the first burst of joy, there was suddenly consternation because the crystal structures of the RSV and HIV-1 PRs, while similar in the basic features, also showed some perplexing differences, especially in the C-terminal part of the molecule. Where the RSV model had a clear α-helix, the HIV-1 structure had a ß-strand, and the topology of the dimer interface was completely different. Instead of the interlaced termini with three inter-subunit ß-sheet connections, the HIV-1 structure had a hairpin with only one area of intersubunit contact, and a disordered N-terminus. The latter difference was not trivial because it had profound consequences for the stability of the dimer and for the way the PR is able to liberate itself from the gag-pol fusion polyprotein. Moreover, it was not a purely academic question because an accurate HIV-1 PR model was badly needed for structure-guided design of inhibitors that might be developed into AIDS drugs.

Since the retroviral PR is translated as part of a polyprotein containing the structural and enzymatic proteins, all the proteins, including the PR, must be liberated from the precursors in order for the virion particles to mature.This maturation process is carried out by the viral PR itself, posing a puzzling topological question - how the PR can fold properly while still embedded in the polyprotein; form an active dimer; and ultimately cut itself out? (All this in the restricted confinement of the viral particle.) The disorder of the N-terminus suggested by the Merck model would allow PR excision not only in *trans* but even in *cis* conformations!

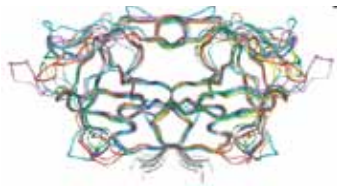
The big question in 1989 was which HIV-1 PR model should be used for design of AIDS drugs? The dilemma could only be resolved by experiment. The question was, where to get the protein? Help came from Stephen Kent at CalTech, who was pioneering the methodology of protein synthesis as a purely chemical process. He and Jens Schneider provided Maria

Miller with a minute sample (0.2 mg!) of synthetic HIV-1 PR, and she was able to grow single crystals. This was a notable accomplishment because it proved the principle that synthetic proteins can be properly folded outside of any biological context, and crystallized. From this tiny sample, Maria Miller was able not only to grow single crystals of apo HIV-1 PR but also to produce heavy atom derivatives. Phasing information had to be obtained experimentally to produce an independent model of the protein. And there it was, exactly as in the RSV enzyme, consistent with the model of Irene Weber. The dimer had fully visible, elevated flap arms, a tightly interlaced intersubunit ß-sheet, the C-terminal α-helix, and even a well defined water molecule between the catalytic aspartates. The definitive structure of HIV-1 PR was published in 1989.[4]

The next goal was the structure of retroviral PR in complex with inhibitors. The first inhibitors were the obvious choice: oligopeptides with substrate sequence, but with the scissile peptide bond replaced with a non-hydrolyzable surrogate, such as reduced peptide, or various hydroxylated ethyl groups. Also, the existing inhibitors of cell-derived aspartic PRs, such as pepstatin, could be immediately tried. However, if selective inhibitors of retroviral PRs were to be found, they should not interfere with the host enzymes, exploiting instead the unique features of retroviral PR: the perfect symmetry of the binding site: the existence of two flaps: or the presence of a structural water molecule. This water molecule, with perfect tetrahedral coordination at the inhibitor/flap interface, was first observed in the crystal structure of a complex of HIV-1 PR with MVT-101 inhibitor (Maria Miller[5]). Later, this interface water molecule was included in a novel class of inhibitors, based on a cyclic urea scaffold; some of the inhibitors have been developed into very potent drugs for treating HIV. The first PR inhibitor, Saquinavir, was approved for clinical use in 1995, only 6 years after the structure of the first inhibitor complex had been published and less than 7 years from the publication of an experimental model. Structural biology can now lead quickly to efficient therapies against a disease which only a few years ago was considered a global threat. So far, 10 PR inhibitors have gained FDA approval for the treatment of HIV. All those molecules are competitive inhibitors. The first, MVT-101, was characterized by a submicromolar dissociation constant. Picomolar inhibitors were subsequently developed through fine-tuning to the enzyme binding sites. Other options might include irreversible modification of the active site, or binding of the inhibitor molecule in a place different from the active site (hindering flap closure or distupting dimer formation). However, none of these have yielded usable pharmacological agents.

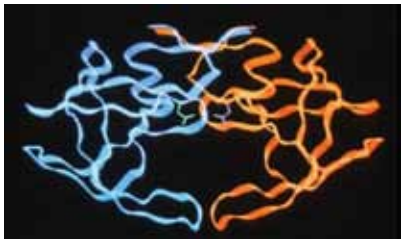
The virus reacts to a potent drug by developing resistance to PR inhibitors, either by selection of existing variants or by mutating. Understanding the mutations in order to design more clever drugs is the challenge for structural research in this arms race. The structure of PR from different retroviruses is another area of research. The enzymes corresponding to HIV-2, SIV, FIV, or EIAV have also been studied. All these proteins share the same fold and domain organization. Knowing how they differ, especially in the context of inhibitor complexes, contributes to our understanding of drug resistance through sequence alterations. Alla Gustchina has contributed an enormous volume of information on this subject. The most recent addition to the collection of retroviral PR structures is the enzyme from the HTLV-1 retrovirus that causes human leukemia. Thus, suddenly, the efforts to cure AIDS and cancer have a common structural point. When the structure of HTLV-1 PR was solved, it became obvious why the AIDS drugs tried on HTLV patients have no effect. Although HTLV was discovered before HIV, the PR from HTLV had resisted structural characterization for a long time, partly because of various crystallographic obstacles. For instance, the rms deviation between the Ca traces of HTLV-1 PR and the molecules from other retroviruses is as high as 1.93 Å (RSV PR) and average 1.72 Å, which complicates molecular replacement calculations and shows that there are indeed significant variations of the canonical retroviral PR fold. Incidentally, similar rms deviations are obtained in comparisons with pepsin, albeit for a smaller number of superposed atoms. However, when only the atoms of the active site are compared, the match is nearly perfect, with an rmsd of about 0.5 Å in superposition of retroviral and cell-derived aspartic PRs.

Structural studies of a broad range of retroviral PRs have the added advantage that they allow one to look at bottlenecks and obstacles from a different perspective. One such difficulty stems from the mixed blessing of the two-fold symmetry of retroviral PRs. With HIV-1 PR, this has led to ambiguity of space-group assignment and to two-fold disorder of the bound inhibitors. This drawback was turned into an advantage when C2 symmetric (or pseudosymmetric) inhibitors were synthesized. A serious problem, as with many other PRs, is autodigestion on prolonged incubation. This difficulty can be removed by the use of inhibitors or by mutations, usually D->N, in the active site. Mutation, in the simplest varient leads to simultaneous change of both catalytic aspartates. Now, asymmetric mutations are possible through a clever engineering trick whereby the two subunits are tethered via a CA-NB linker.



Superposition of PR molecules from several retroviruses. HIV-1, green; HIV-2, blue; SIV, olive; RSV, pink; FIV, red; EIAV, orange; HTLV-1, turquoise. Adapted from Li et al, PNAS, 102, 18332-7.

These structural studies of retroviral PRs have been an important stimulus for structural biology. HIV PR is the most studied protein on earth: there are hundreds of structure determinations. The overwhelming majority of the structures have been determined by protein crystallography, but there are also NMR structures, including a monomeric form of the protein. HIV PR has helped to advance the frontiers of structural biology in many different ways.



Synthetic HIV-1 PR determined by Alex Wlodawer's team. The two subunits of the homodimer are colored red and blue. The flap arms are lifted symmetrically over the empty active site, which is marked by the two catalytic aspartates.

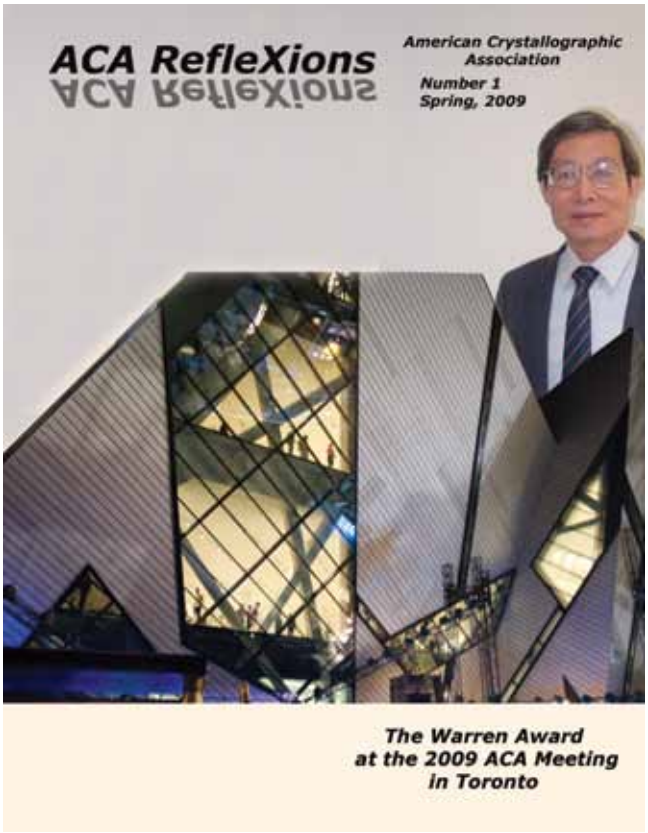
Retroviral Proteases, cont'd: The method of chemical synthesis has been used by Stephen Kent to obtain the D-enantiomer of HIV-1 PR and to demonstrate that this mirror twin of the natural enzyme behaves identically in a looking-glass world. Recently, huge single crystals of HIV-1 PR have been grown in preparation for a neutron diffraction experiment, which, by visualization of hydrogen atoms, will hopefully help to answer the persisting questions about the catalytic mechanism. HIV-1 PR has already been characterized at ultra high resolution; 0.84 Å.

Mariusz Jaskolski

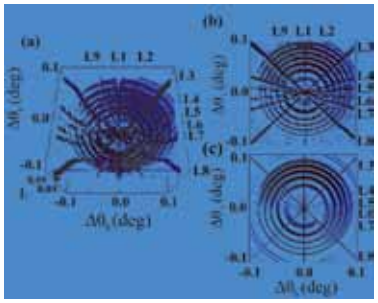
(1) M. Miller, M. Jaskolski, J.K.M. Rao, J. Leis, A. Wlodawer (1989) Nature 337, 576-579. (2) M.A. Navia et al. (1989) Nature 337, 615-620. (3) I.T. Weber, M. Miller, M. Jaskolski, J. Leis, A.M. Skalka, A. Wlodawer (1989) Science 243, 928-931. (4) A. Wlodawer et al. (1989) Science 245, 616-621. (5) M. Miller et al. (1989) Science 246, 1149-1152.

Editor's note: see Alex Wlodawer's Meeting report, page 27.

On the Cover



Above: 2009 Warren Award recipient Shih-Lin Chang. Below: Southwest view of Michael Lee-Chin Crystal addition to the Royal Ontario Museum in Toronto: the Architectural Opening, June 2007. © ROM.



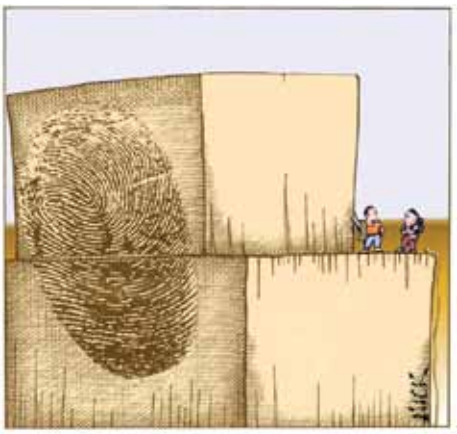
The **Bertram E. Warren Award** for 2009 will be presented to **Shih-Lin Chang** at the ACA Annual Meeting in Toronto in a special symposium organized in his honor. The award recognizes his important recent contribution to the physics of solids or liquids using x-ray diffraction techniques. The figure above shows cavity resonance interference observed in the x-ray back diffraction of (12 4 0) from a two-plate crystal cavity of silicon at 14.4388 keV; (a) shows a 3-dimensional intensity plot of the transmitted (000) beam versus the vertical $\Delta\theta_v$ and horizontal $\Delta\theta_h$ tilt angles of the crystal cavity relative to a normal incident beam; (b) is the 2-dimensional projection; (c) is the calculated intensity distribution of (b) based on the dynamical theory of x-ray diffraction. The 3-dimensional plot revealing the interference intensity distribution (a) is like a Roman amphitheater. The 2-dimensional fringes show concentric rings of alternating maxima and minima and the straight lines are due to the coplanar diffraction lines. The (000) and (12 4 0) reflections are omitted in each of the coplanar diffractions mentioned. The 24-beam diffraction occurs at the intersection of the 9 coplanar diffraction lines.

The figure was published in *Phys. Rev. Lett.* **94**, 174801-4 (2005). S.-L. Chang, Yu. P. Stetsko, M.-T. Tang, Y.-R. Lee, W.-H. Sun, M. Yabashi, and T. Ishikawa; *X-ray Resonance in Crystal Cavities: Realization of Fabry-Perot Resonator for Hard X-rays*.

Contributors to This Issue

Jane Andrew, Svilen Bobev, Jim Britten, Julia Chan, Shih-Lin Chang, Marcia Colquhoun, Lachlan Cranswick, Bryan Craven, Howard Einspahr, Ana Ferreras, Bill Gleason, Mariusz Jaskolski, Kathy Kantardjieff, Tom Koetzle, Charles Lake, Cora Lind, Len MacGillivray, Peter Müller, José Roldan, David Rose, Tim Rydel, Bob von Dreele, Carrie Wilmot, Alex Wlodawer.

Cartoon courtesy of Nick D. Kim, an analytical environmental chemist who currently works for Waikato Regional Council. He is an honorary lecturer at the University of Waikato in New Zealand



"Of course, it's still a complete mystery as to how the ancients even managed to MOVE these massive stones..."

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The ACA Summer Course in Small Molecule Crystallography, 2009

The 10-day intensive course will be offered June 22nd through July 1st, 2009 at the Indiana University of Pennsylvania. IUP is located in the town of Indiana about 80 miles east of Pittsburgh, PA. The course will cover both single crystal and powder diffraction and each day will consist of lectures in the morning, hands-on workshops in the afternoon and computer tutorials at night. While some advanced topics will be introduced (structure solution from powder data, advanced probability methods, solving difficult structures), the curriculum will mostly emphasize fundamental crystallography and no prior crystallographic experience will be assumed. Attendees are encouraged to bring their own single crystal or powder samples for x-ray data collection and are expected to have completed at least undergraduate courses in chemistry, physics and mathematics and are advised to read in advance *Crystal Structure Analysis: A Primer*, by Jenny P. Glusker and Kenneth N. Trueblood, Oxford Univ. Press (1985).

The organizers aim for a total of 24 attendees, who in past years have come from the U.S. and abroad; from academia (students and faculty), government and corporate institutions. There will be at least 12 experienced teaching faculty present. Tuition will be $300 (or $800 for applicants from corporate labs). Student apartment housing at IUP (including breakfast and lunch) is available for an additional $450 ($750 or $1,250 for corporate labs). Approximately 12 student scholarships will be offered (exceptional undergraduate students will be considered) and will consist of a waiver of tuition and living costs. The scholarships will be awarded based on the student's (1) scientific ability, (2) expected benefits from the course and (3) skills in English. We encourage applications from Latin America.

Instruments at IUP will include two Bruker-Nonius CAD4 single crystal diffractometers, a Bruker D8 Advance and a Rigaku Miniflex powder diffractometer. In the past four years, Rigaku-Americas brought a SCXmini X-ray Crystallographic System to the IUP laboratory. Students will also have access to the Duquesne University X-ray Facility which has a Bruker APEX II single crystal diffractometer and a PANalytical X'Pert Pro powder diffractometer. The IUP computer facilities are excellent and each student will have access to an individual computer during the nightly tutorials. Access will also be available to the Cambridge Structural Database and the ICDD powder diffraction database. The software used in the course will be Bruker-Nonius SHELXTL, Rigaku Americas CrystalClear, GSAS/EXPGUI, FullProf, CRYSFIRE and CRYSTMOL.

The course registration form can be obtained from the ACA web site at **www.AmerCrystalAssn.org**. Full consideration will be given to completed forms received before May 15th, 2009. The forms may be mailed to Charles H. Lake, Chemistry Department, Indiana University of Pennsylvania, Indiana, PA 15705, or sent to **lake@iup.edu**. Further information will be updated on the website or can be obtained from **lake@iup.edu** or **craven@icubed.com.**

We shall observe the basic policy of nondiscrimination and affirm the rights of scientists throughout the world to adhere or to associate with international scientific activity without restrictions based on nationality, race, color, age, religion, political philosophy, ethnic origin, citizenship, language, or sex, in accordance with the Statutes on the International Council of Scientific Unions. At this course, no barriers will exist which would prevent the participation of *bona fide* scientists. Foreign students may be accepted early to provide extra time to process VISA's

Charles H. Lake and Bryan M. Craven, Organizers.

"That's the trouble with the older generation—they're too intolerant."

Cartoon courtesy of Nick D. Kim, an analytical environmental chemist who currently works for Waikato Regional Council. He is an honorary lecturer at the University of Waikato in New Zealand

In front: Christina Hoffmann, Brenda Dougan, Maren Pink, Shengqian Ma, Katie Tietz, Jane Andrew, Lauren Borkowski, Nattamai Bhuvanesh, Sue Byram. In back: Yevheniy Horyeshnik, Cantwell Carson, Debasis Banerjee, Shengchang Xiang, Stephan Scheins, Milan Gembicky, Natalia Shustova, Daqiang Yuan, Anatoliy Volkov (back), Jim Britten (front), Christos Malliakas, Tibor Koritsanszky, Christine Beavers, Adam Stash, Travis Holman, Joe Reibenspies, Charles Campana, Houston Perry, Yu-Sheng Chen. Not pictured: Cary Bauer, Chunhua Hu, Yuzhou Liu, John Schlueter, Airon Soegiarto.

A workshop on advanced crystallography techniques was hosted December 3-5, 2008, by ChemMatCARS, which operates sector 15 of the Advanced Photon Source (APS). The 24 participants were introduced to the upgraded ChemMatCARS crystallography beamline and to the latest software and techniques for solving difficult structures. Most participants collected and analyzed data on their own samples and were able to receive on-the-spot advice from experts. In the opening talk, ChemMatCARS research beamline scientist Yu-Sheng Chen gave an overview of the crystallographic experiments possible at the sector and introduced a new setup that was commissioned in February 2008. Now, with a D8 diffractometer and Bruker APEX II detector, users can do structure determination and high-resolution charge density studies to a spatial resolution of 2.1 $Å^{-1}$, yielding complete data often in less than one hour. Charles Campana of Bruker AXS Inc. reviewed some specialized capabilities of Bruker's APEX II suite of software, including new tools to determine the q-vector for analysis of modulated structures. Attendees also learned about ways to obtain beam time on the new instrument: Susan Strasser of the APS User Office explained proposal-based access through the APS General User Program, and Maren Pink of Indiana University introduced the Service Crystallography at the Advanced Photon Source (SCrAPS) program, which provides a mail-in and screening service and beam time is collectively used by participating scientists. As an example of the kind of questions that can be answered with the high resolution available at ChemMatCARS, Christos Malliakas of Northwestern University reported on his work with incommensurate charge density waves in square nets of tellurium. Jim Britten of McMaster University concluded the lectures with a vivid demonstration of 3-D visualizations of reciprocal space data, which can point the way to new ways of conceptualizing data relationships.

The workshop was cosponsored by Bruker AXS Inc., ChemMatCARS, and the Center for Advanced Radiation Sources of the University of Chicago. Several presentations are available on the workshop web site: **http://cars.uchicago.edu/chemmat/pages/wkshopadvcryst/**. Information on the ChemMatCARS microcrystallography setup is at **http://cars9.uchicago.edu/chemmat/pages/microxtallography.html.**

About ChemMatCARS: ChemMatCARS is a high-brilliance national synchrotron x-ray facility dedicated primarily to static and dynamic condensed matter chemistry and materials science. It is supported by the National Science Foundation and the Department of Energy. The scientific focus of the facility includes the study of surface and interfacial properties of liquids and solids as well as their bulk structure at atomic, molecular, and mesoscopic length scales with high spatial and energy resolution.

Jane Andrew and Yu-Sheng Chen

Index of Advertisers

20 years of structural studies of retroviral proteases

A meeting entitled "HIV Protease and Beyond: The Past, Present, and Future of HIV Structural Biology" took place on the Frederick, MD campus of the National Cancer Institute on January 30-31, 2009. The meeting celebrated publication of the crystal structures of proteases, the first retroviral enzymes to be characterized in structural terms, almost exactly 20 years after these events first took place. Sponsored by the Center of Excellence in HIV/AIDS and Cancer Virology (headed by Stuart LeGrice) and supported financially by the Intramural AIDS Targeted Antiviral Program, the meeting was very appropriately opened by **Michael Gottesman,** Scientific Director of the NIH. The theme of his presentation was the necessity of emphasizing basic scientific research even in these days of targeted, goal-oriented science, since we can never be completely sure what new and unexpected information will contribute to providing cures for diseases such as AIDS and cancer. Ten anti-AIDS drugs targeting HIV protease that are in current clinical use are proof of the success of such an approach. The next four speakers (**Stephen Oroszlan, David R. Davies, Mariusz Jaskolski**, and **Alexander Wlodawer)** summarized the discovery of retroviral proteases, the current state of research on pepsin-like aspartic proteases, and the steps that led to the determination of the structures of the Rous sarcoma virus protease (the first retroviral enzyme for which a structure became available) and ultimately the most medically relevant target, namely HIV-1 protease itself. **Stephen Oroszlan** received a special prize for being a co-discoverer of the retroviral proteases. These historical talks were followed by **Dale Kempf** describing the process of drug design at Abbott Laboratories, **David Davis** discussing a possibility of oxidation-mediated oligomerization of retroviral proteases, and **Alla Gustchina**'s continuation of the theme introduced earlier, namely how what we have learned from pepsin-like aspartic proteases could be handy in designing drugs against the retroviral enzymes and vice versa. Speakers during the next session moved to new areas of research on retroviral proteases, with **Celia Schiffer** and **Irene Weber** discussing the structural aspects of the development of drug resistance, **Jan Konvalinka** presenting the use of metallacarboranes as inhibitors, **Ernesto Freire** discussing thermodynamic approaches to the studies of inhibition, and **Marius Clore** giving a fascinating talk on visualizing transient events in autoprocessing of HIV protease using a paramagnetic enhancement technique. In addition, more than a dozen posters dealt with various aspects of research on retroviral proteases.

Although the field of studies of retroviral proteases is very interesting by itself, the organizers of the meeting decided to enlarge its scope by including other subjects as well. The second day was devoted to structural studies of reverse transcriptase and RNase H, with **Stuart LeGrice** discussing molecular gymnastics of these complicated enzymes, **Stephen Hughes** the ever-present drug resistance, and **Wei Yang** comparing the cellular and retroviral RNase H. A session on the elusive retroviral integrase, an enzyme much less well characterized in structural terms, included interesting talks by **Robert Craigie** and **Yves Pommier** on general properties of this enzyme and the ways of drugging its active site, as well as a talk by **Daria Hazuda** showing how Merck accomplished that task in practice. The final session of the meeting dealt with the subject of assembly and entry of the retroviruses into host cells, with talks on these subjects given by **Richard Wyatt, Eric Freed,** and finally by **Hans-Georg Kräusslich**.

Although AIDS continues to ravage large parts of the world and is still a very serious disease requiring long-term treatment, it is no longer an automatic death sentence as it was when first identified close to 30 years ago. Unlike with most other diseases, discovery of a variety of drugs has been from the beginning very closely linked to the progress in structural characterization of protein targets, using the tools of structural biology in general and protein crystallography in particular. This meeting has shown us how much has been accomplished in a comparatively short time and how much more we can expect in the future.

Alexander Wlodawer

Editor's note: See Mariusz Jaskolski's "Retroviral Proteases 20 years later," pages 20-22.

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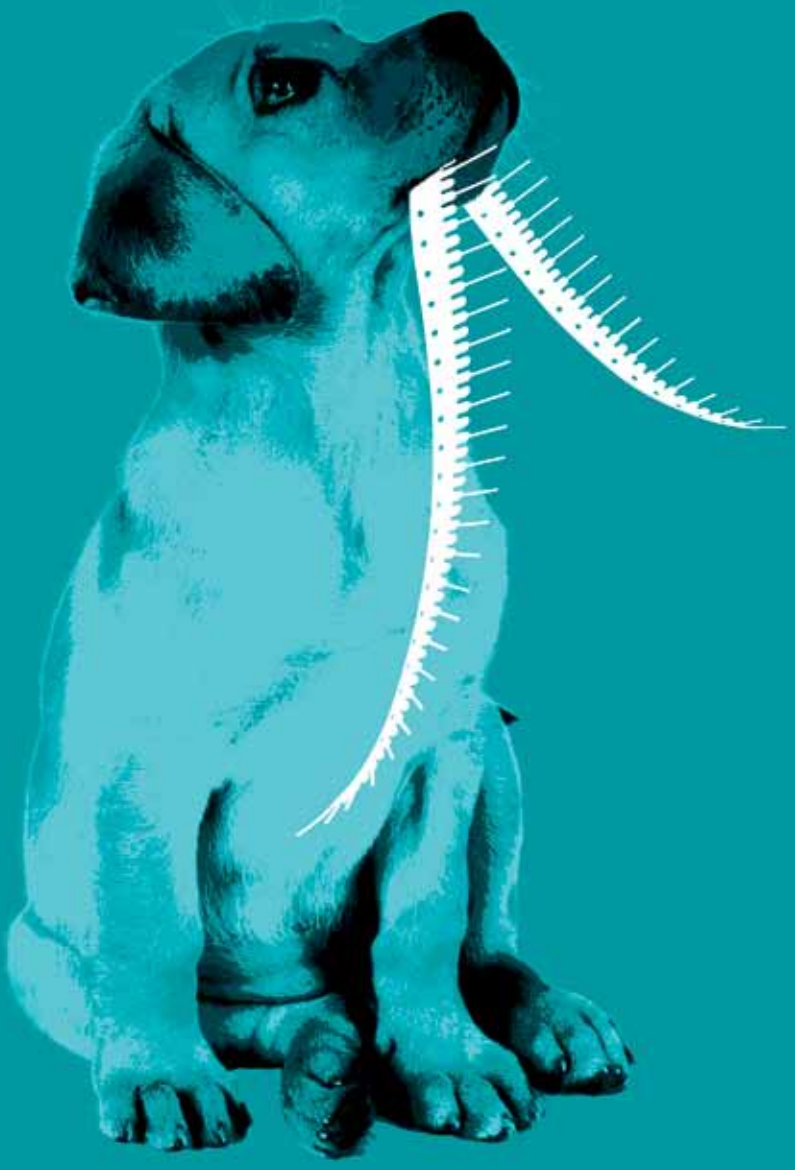

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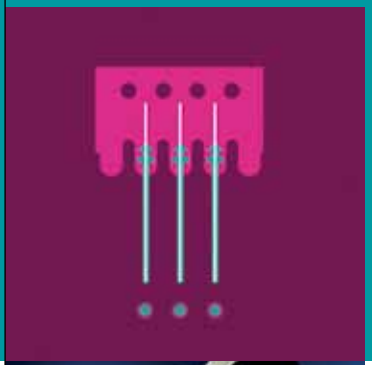

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July 25-30, 2009
Toronto Sheraton City Centre Hotel
123 Queen Street West
Toronto, Ontario, Canada

Advance Registration Deadline: May 31st
Hotel Reservations: June 24th
Register Online and see Call for Papers
at www.AmerCrystAssn.Org

Local Chair
David Rose
University of Toronto
drrose@uwaterloo.ca

Program Chair
Jim Britten
McMaster University
britten@mcmaster.ca

Workshops

JANA Incommensurate Crystal Structures
Friday - Saturday July 24-25, 2009
Chairs: Jim Kaduk and Olivier Gourdon

Handling Twinning in Macromolecular Cyrstallography
Saturday July 25, 2009
Chairs: George Sheldrick, Garib Murshudov, Peter Zwart

Award Symposia

Buerger Award
in honor of Michael James
Chair: Emil Pai

Warren Award
in Diffraction Physics
in honor of Shih-Lin Chang
Chair: Bruce Noll

Margaret C. Etter Early Career Award
in honor of Svilen Bobev
Chair: Ross Angel

Transactions Symposium

Phase Transitions - covering the whole range of phenomena from soft materials and proteins to hard materials and alloys, etc.
Sponsored by the Powder, Materials, Service, Small Molecule and General Interest SIGs

Plenary Lectures

Ted Baker (Chair: Wm Duax); Philip Coppens (Chair: Sine Larson)

Panel Discussion

Professional Directions on Academic and Industrial Careers
Sponsored by the Industrial and YYSIGs

Microsymposia - Organized by SIGS

Biological Macromolecules

Crystallization Methods - Chairs: Alex McPherson & Aled Edwards
Exciting Structures - Chairs: Zhe Yang & Ladislau Kovari
Vaccine Design - Chairs: Peter Kwong & Ian Wilson
Chromatin Remodeling - Chairs: Jinrong Min & Jan-Francois Couture
Carbohydrate Recognition - Chairs: Ken Ng & Stephen Evans
"Green" Biochemistry - Chairs: Carrie Wilmot & Bernie Santarsiero

Industrial

Application of New Technologies - Chair Matt Peterson

Small Molecule

Cool Structures -Chair: Peter Müller

Small Angle Scattering

Characterization of Surfaces & Interfaces - Chairs: D. Schaefer & B. Lee
SAS Modeling & Simulation - Chairs: G. Beaucage & J. Llavsky
Advances in Small Angle Scattering - Chairs: Ken Ng & Stephen Evans
Structure of Nanophase Materials - Chair: Tad Koga

Joint SIG Symposia

Neutron & Materials
Shape - Memory Materials - Chair: Steve Shapiro
Small Molecule & Industrial
Supramolecular Chemistry - Chairs: Christer Aäkeroy & Gary Enright
Synchrotron, Small Angle Scattering & BioMac
Complementary Methods for PX - Chairs: Hiro Tsuruta & Wah Chiu
Membranes & Associated Proteins - Chair: T. Weiss
Industrial & Powder
Accuracy & Standards in Powder Diffraction - Chair: Pam Whitfield
Energy Related Materials - Chair: Ashfia Huq
Synchrotron & BioMac
Structural Enzymology - Chairs Emil Pai & Felix Vajdos
Diagnostics During Data Collection - Chairs: Michel Fodje & Ernst Bergmann
Instrumentation: Sources, Optics - Chairs: Marc Allaire & Craig Ogata
Instrumentation: Detectors - Chairs: Marc Allaire & Craig Ogata
Powder & General Interest
Educational Outreach in Crystallography - Chair: Cora Lind
Materials & Neutron
Ferroic & Multi-ferroic Materials - Chair: Peter Gehring
Superconducting Materials - Chair: John Mitchell
Service, General Interest & Small Molecules
Tips & Tricks of the (Computing) Trade - Chair: Xiaoping Wang
Problem Structures - Chair: Richard Staples
Would you Publish This - Chairs: Carla Slebodnick & Peter Müller
Large Small Molecules - Chairs: Christine Beavers & Ilia Guzei
BioMac and Young Scientists
Refinement (Computational) - Chairs: Edward Collins & Peter Horanyi
Powder, Neutron, Materials & Synchrotron
Diffraction Studies & Mechanical Properties of Engineering Materials - Chair: Ron Rogge
BioMac & Industrial
Structure-Based Drug Design - Chairs: Duncan McRee & Eddy Arnold
Neutron & Powder
Cooperative Phenomena in Magnetic Materials - Chair: Ovidiu Garlea

Going Green:

This year we will be distributing the full set of abstracts only on CDs. A hardcopy Program Schedule will also be distributed. We will not have a new meeting bag so if you like to use a bag, please remember to bring your favorite from an earlier ACA meeting. In addition to making the meeting more **'Green'** these measures will be more cost effective allowing us to continue offering morning and afternoon coffee breaks as well as food at the opening reception and snacks at the poster sessions without a major increase in registration costs.

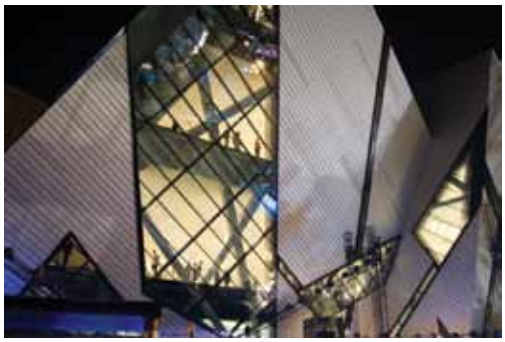
Traveling to Canda:

Porter Airlines is going to start flights from Chicago MidwayAirport to theToronto downtown (Island) airport. This would be a good option for anyone coming from Chicago or surrounding areas. Non-US nationals working in the US should be able to attend the meeting and return to the US but they are advised to fully understand the travel restrictions associated with their US Visa and to be sure to get any re-entry documents that might be needed. Please read ***"Traveling from the United States"*** on the US National Academy of Sciences website: **www7.nationalacademies.org/VISAS/Traveling_from_US.html.**

Exhibit Show 2009:

An exhibition of the latest instruments and techniques for sample isolation, purification and preparation, crystal growth and data collection, computer software for data storage, retrieval analysis, graphics systems, databases, and books, journals and other materials essential to modern crystallographery is scheduled to begin Saturday evening, July 25, in conjunction with the Opening Reception. The 2009 ExhibitShow will run through Tuesday evening July 28th. The show will be closed Wednesday July 29th, but posters will remain accessible. The Advertising and Exhibits Div. of the AIP is managing the show. For further information contact Bob Finnegan, AIP, 2 Huntington Quadrangle, Suite 1NO1, Melville, NY 11747, **rfinneg@aip.org; 516-576-2433**; fax: 516-576-2481. ACA Corporate Members will receive 10% off one booth fee. Not a member? Join now! Not-for-profits groups are eligible for a discounted booth fee of $400 for one booth. Booth rental is $1,400 for all others.

Register online at: www.AmerCrystalAssn.org



Above: © Royal Ontario Museum.

Registration fees

Fee	Advance (before May 31)	Late (after May 31)
Regular Member	$400	$600
Retired Member	$160	$240
Post doc Member	$200	$300
Student Member	$160	$240
Nonmember*	$600	$900
Post doc Nonmember*	$300	$450
Student Nonmember*	$240	$360
Guest**	$ 50	$ 50

WK.01 (fee includes lunch) $130

WK.02 (2 days - fee includes lunches) $250

* The nonmember registration fee includes a complimentary membership to the ACA for one year. Those registering as nonmember post docs or nonmember students must include documentation of this status with registration form.

***Guest registration includes Opening Reception, Exhibit Show and Get Together on Sunday morning.**

Mentor/Mentee Dinner

Mentor	**$35**
Mentee	**$25**
Banquet	**$60 ($30 students)**
YSSIG Mixer	**Free for students and post-docs; $20 for all others**

Register on-line or download forms to register by fax or mail: . **www.AmerCrystalAssn.org**

Questions: **aca@hwi.buffalo.edu**

APRIL 2009

15 **Pre-conference training course: Microwave-Assisted Organic Synthesis,** Edinburgh, Scotland

16-17 **2nd Annual Advances in Synthetic Chemistry,** Edinburgh, Scotland, topics include *Advances in Synthesis Techniques and Technologies, Flow Chemistry and Microwave-Assisted Organic Synthesis*. **www.combichem.net/r/redirect.aspx?contentid=95808&url=http://www.selectbiosciences.com/conferences/ASC2009/**

18-22 **ASBMB '09,** New Orleans, LA. **asbmb.org/meetings.aspx.**

MAY 2009

18-22 **International School on Biological Crystallization**. Special emphasis on crystallization of membrane proteins and large macromolecular complexes, on biomineralization and on challenges in protein crystallization. **www.isbcgranada.org**

25-29 **International School on Crystallization of Drugs, Food and Agrochemical Products.** Lectures on the science of crystallization technology. **lafactoria.lec.csic.es/iscgranada**

JUNE 2009

4-14 41st School of Crystallography: **High Pressure Crystallography: From Novel Experimental Approaches to Applications to Cutting Edge.** Erice, Italy. **www.crystalerice.org/2009.htm.**

JULY 2009

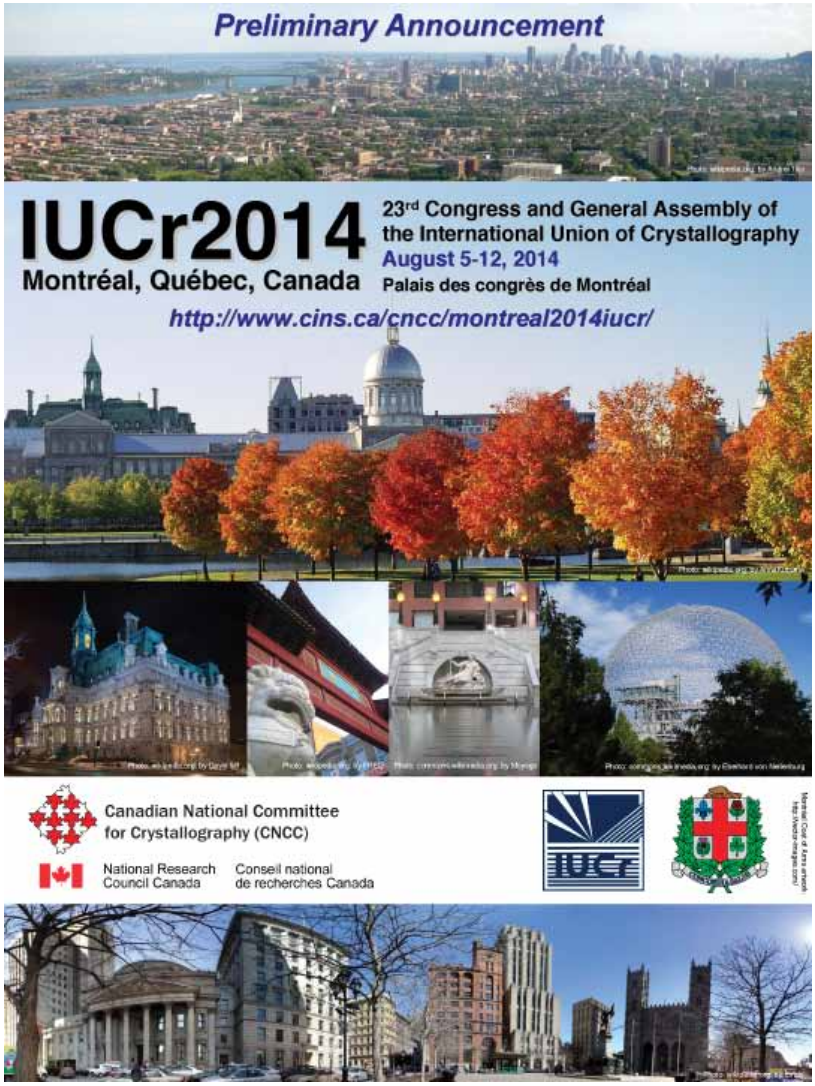
25-30 **2009 ACA Annual Meeting.** Toronto, Ontario, Canada. ***Program Chair: Jim Britten***, McMaster Univ. **britten@mcmaster.ca**); ***Local Chair David Rose,*** Univ. Toronto, ***drrose@uwaterloo.ca***

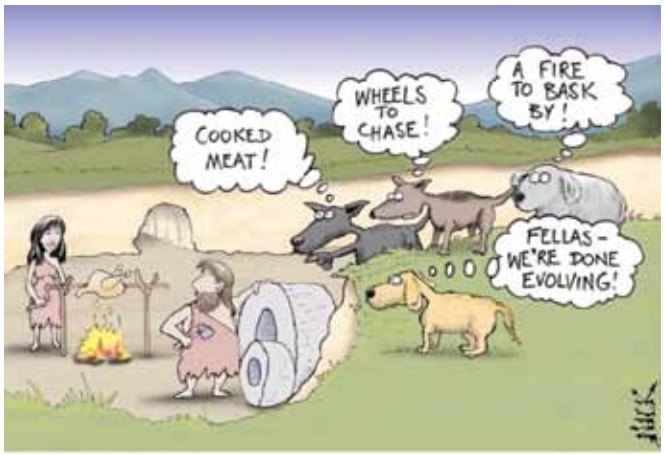
AUGUST 2009

9-14 **ECM-25** Istanbul, Turkey. **www.ecm-25.org**

AUGUST 2011

22-29 **XXII Congress and General Assembly of the IUCr.** Madrid, Spain. **www.iucr2011madrid.es.**





Forget the experts; domestication of the dog only took about 8 seconds.

Cartoon courtesy of Nick D. Kim, who is an analytical environmental chemist who currently works for Waikato Regional Council. He is an honorary lecturer at the University of Waikato in New Zealand

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