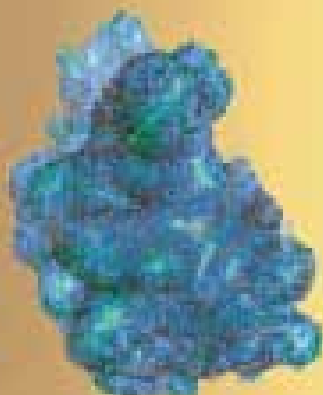


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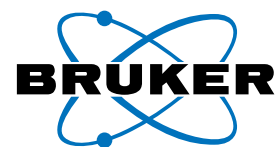
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Chicago 2010



**Plenary Lectures
by Steitz, Yonath
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Cover: Images from the Nobel-winning research on the ribosome. The historical sequence of work by Ada Yonath, Thomas Steitz, and Venkatesan Ramakrishnan is shown. See page 14 for a more complete description.



Table of Contents

- 3 President's Column
- 4-6 Awards to crystallographers
- 6 Travel Award report -2009 ACA Meeting
New History Portal, Art in Crystallography, Appeal for *Opinions* editor
- 7 2010 ACA Council Officers and Appointments
- 8 2010 ACA Standing Committee Members
- 10-12 2010 Special Interest Group Officers
- 13-14 2010 USNCCr Roster
- 14 On the Cover
- 15 Lachlan M. D. Cranswick
- 18 Corporate Members
- 19-20 Lieselotte Templeton (1918-2009)
- 20 Contributors to this issue
Index of advertisers
- 21-23 Shih-Lin Chang's 2009 Warren Award Lecture
- 24-26 Books
- 26 Joe Ferrara is our new *Books Section* Editor
- 28-30 Meeting Reports
- 32 Opinion
- 33 Crystallography Education Workshop
- 34-35 2010 ACA Meeting in Chicago
- 36 Calendar of Meetings



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During all my years as an ACA member reading *ACA Newsletters* and now *RefleXions*, I never envisioned myself writing the President's Column. But, here I am penning my first communication to you, my ACA colleagues. With global conferences on climate change and headlines almost every day on the H1N1 influenza virus, it is clear that science matters more than ever, and crystallography is right in the forefront. The importance of crystallography is underscored by the Nobel prizes in Chemistry that were awarded in 2009 to three structural scientists - Ada Yonath, Venki Ramakrishnan, and Tom Steitz - recognizing their fundamental contributions to our understanding of the structure and function of ribosomes. We are fortunate, indeed, that all three Laureates will be participating in the 2010 Chicago Annual ACA Meeting, July 25 to 29, making an already exciting meeting even better.

An essential role for the ACA is facilitating the education and training of young scientists. Examples of this outreach are the ACA travel grants that allow students to attend our annual meetings and our workshops. In Chicago this year, in addition to our classical workshops, Cora Lind (newly elected to our Data, Standards, and Computing Committee) will be running a tutorial workshop to introduce high school teachers to the fundamentals of crystallography. The aim is to provide teachers with the background to spark student interest in science in general, and structural studies in particular.

The ACA Council serves as the administrative arm of our organization, and it has a representative of the IUCr as a non-voting member to ensure good communication between these two crystallographic associations. In October 2009, we lost our dear friend and colleague Louis Delbaere, who was serving in that role. Recently, the IUCr Executive Committee appointed Marv Hackert to serve the IUCr until 2011, when Louis's elected term would have expired. While Louis will be sorely missed, we are fortunate to have someone like Marv step into this role. Marv's extensive scientific and administrative experience coupled with his knowledge and service to the ACA make him a valuable link between the ACA and the IUCr.

As we begin 2010 with a newly constituted Council, one realizes that the thing that keeps the ACA functioning smoothly is the ACA headquarters staff in Buffalo. As officers and Council members serve their short terms, it is the experience and knowledge of Marcia Colquhoun, Jen Shepard, Patti Potter, and Crystal Towns that provide the continuity to keep the ACA functioning as the professional organization that we have come to value so highly. Until one takes on a job such as Local Meeting Chair, Program Chair or serving as an ACA officer, things just seem to work automatically. But it is not automatic - it is due to the hard work and dedication of Marcia, Jen, Patti and Crystal, who support your elected representatives. So when you see one of the ACA staff in Chicago, take a moment to thank them for helping to make the ACA what it is. Two of our headquarters staff will be leaving Buffalo this spring. Jen and her husband Ben will be moving south, so the ACA is going to lose her valuable contributions as Membership Secretary at ACA Headquarters. Patti and her husband George are moving north to Alaska, where Patti will continue to prepare the *IUCr Newsletter*. We thank both Jen and Patti for their contributions over the years and wish them well as they move on to new adventures.

The mission of the ACA is to promote interactions among scientists who study the structure of matter at or near atomic resolution. Our 2010 meeting is going to be a very exciting one and a great opportunity for doing even more of just that. I hope you are all planning to attend.

Judy Kelly



*Chicago River -image from www.dreamstime.com/.
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Susan Taylor to receive both the Vanderbilt Prize & FASEB Excellence in Science Award



Both the **Vanderbilt Prize in Biomedical Science** and the **FASEB Excellence in Science Award** honor and recognize the outstanding achievement of a woman scientist of national reputation in biological science. Winners have contributed significantly to our understanding of a particular discipline by their excellence in research and are known for their mentorship of other women in science. This year, for the

first time, both the Vanderbilt Prize in Biomedical Science and the FASEB Excellence in Science Award will be awarded to the same scientist, **Susan S. Taylor**.

Taylor completed her BA in Chemistry at the University of Wisconsin in 1964, a time when men dominated the field of physical science. She was not discouraged, however, by her lack of female classmates and went on to receive her PhD in Physical Chemistry from John's Hopkins University in 1968. She then completed two short postdoctoral fellowships, first working with Brian Hartley at the Medical Research Council Laboratory of Molecular Biology in England. It was there that she shifted her studies to proteins. Her second postdoctoral position was at UC San Diego where she quickly secured a faculty position and is now Professor of Chemistry and Biochemistry, and Pharmacology. She has also been a Howard Hughes Medical Institute investigator since 1997.

In 1991, Taylor and colleagues solved the first structure of a protein kinase and her lab has since solved the structures of the protein's regulatory subunits. Her lab continues to study the structure, dynamics, and localization of cAMP-dependent protein kinase as a prototype for the protein kinase superfamily involved in signal transduction. Taylor is regarded by many as the world's leading expert in this area of research.

The Vanderbilt Prize was established by Vanderbilt University School of Medicine in 2006. It includes a \$25,000 award and a funded scholarship named after the awardee that will support a woman beginning her M.D./Ph.D. studies at Vanderbilt. The FASEB Excellence in Science Award is sponsored by Eli Lilly and Company and holds a purse of \$10,000. Taylor received the Vanderbilt Prize in February when she gave the Vanderbilt Discovery Lecture. She will give her Excellence in Science Award lecture *Dynamics of PKA Signaling* at the 2010 ASBMB Annual Meeting in Anaheim this April.



Snowcrystals from the Patricia Rasmussen Collection 2002. © Rasmussen 2002.

Doug Rees Awarded the ASBMB Lipmann Lectureship



The **Fritz Lipmann Lectureship**, established by his friends and colleagues, honors the memory of Fritz Lipmann who won the Nobel Prize in Physiology or Medicine in 1953 for his discovery of coenzyme A. The Lectureship is awarded every two years by the **American Society for Biochemistry and Molecular Biology (ASBMB)** for conceptual advances in biochemistry, bioenergetics, or molecular biology. This year the honor goes to **Douglas C. Rees**.

Rees has been a Howard Hughes Medical Institute investigator since 1997 and is currently the Roscoe Gilkey Dickinson Professor of Chemistry at the California Institute of Technology as well as an Adjunct Professor of Physiology at UCLA. His research has made pivotal contributions to understanding the structure of integral membrane proteins, membrane transport mechanisms, and metalloenzyme structure and mechanism. Rees will give his lecture: *Structural and Mechanistic Diversity of ABC Transporters* at the 2010 ASBMB Annual meeting April 24-28th in Anaheim, CA.

Ronald Breslow Award to Stephen Lippard



The ACS recognized the scientific achievements of **Stephen Lippard** by presenting him with the **2010 Ronald Breslow Award**. The Breslow Award is sponsored by The Ronald Breslow Endowment and was established in 2001 at a symposium held at Columbia University in honor of Breslow's 70th birthday. A Professor of Chemistry at Columbia University since 1956, Ronald Breslow's current research focuses on the synthesis and study of molecules that imitate enzymatic reactions, such as the development of artificial enzymes. In this vein, the award recognizes outstanding contributions to the field of biomimetic chemistry. This year's award winner is **Stephen J. Lippard**, Arthur Amos Noyes Professor of Chemistry

at MIT. He was honored at a ceremony during the 239th ACS National Meeting in San Francisco in March.

Lippard's lab studies the reactions and physicochemical properties of metal complexes in their natural systems and as synthetic models for the active sites of metalloproteins. He has extensively investigated the mechanism of soluble methane monooxygenase as well as other members of its operon. He is also widely known for his work on the mechanism of cisplatin, an anti-cancer drug primarily used to treat testicular and ovarian cancers. Cisplatin-DNA adducts inhibit the processive nature of RNA polymerase, leading to phosphorylation and ubiquitination of the large subunit of the enzyme. His lab has also developed novel fluorescent sensors for zinc for the investigation of neural network formation and communication within the brain and for biological nitric oxide.

John Tesmer will receive ASBMB Young Investigator Award



The **ASBMB Young Investigator Award**, formally the **Schering-Plough Research Institute Award**, recognizes outstanding research contributions to biochemistry and molecular biology by those who have no more than 15 years postdoctoral experience. This year's winner is ACA member **John Tesmer** from the University of Michigan. Tesmer finished his BA in Biochemistry and English at Rice University in 1990 and his PhD in Biological Sciences at Purdue University in 1995. After a 3 year postdoctoral fellowship at U.Texas Southwestern Medical Center he started his independent career as junior faculty member at UT Austin. In 2005 he moved to the University of Michigan where he is now Research Associate Professor at the Life Sciences Institute and Department of Pharmacology, as well as Faculty Mentor for the Chemical Biology

Doctoral Program. Tesmer is honored for his outstanding work in the structural studies of proteins and protein complexes involved in G-protein coupled receptor signaling pathways. Tesmer will present his award lecture *Structural Analysis of Heterotrimeric G Proteins and G Protein-Coupled Receptor Kinases* April 26th at the ASBMB Annual Meeting in Anaheim, CA.

ICDD Award to Lakshminarasimhan



To encourage promising graduate students to pursue crystallography-related research, the International Centre for Diffraction Data (ICDD) has established the **Ludo Frevel Crystallography Scholarship Fund**, named in honor of the founder of the fund, Dr. Ludo Frevel. Multiple recipients are selected on a competitive basis,

each receiving an award of \$2,500. All applicants should be enrolled in a graduate degree program during the calendar year for which they are applying, with a major interest in crystallography. Fifty-five commendable applications for the year 2010 awards were received by the ICDD. ACA Member **Mahadevan Lakshminarasimhan**, of Ruhr University and the Max Planck Institute in Bochum, Germany was among the ten recipients chosen for the **2010 Ludo Frevel Scholarship Program**. He was selected for his work in *Exploring the regulation of mammalian sirtuins using structural biology*.

Ferguson-Miller named Biophysical Society Fellow

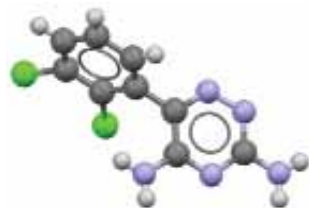


ACA member **Shelagh M. Ferguson-Miller** was one of the six scientists in the 2010 class of **Biophysical Society Fellows**. The award recognizes distinguished members who have demonstrated excellence in science and have

contributed to the expansion of the field of biophysics and support of the Biophysical Society. Ferguson-Miller, Distinguished Professor of Biochemistry and Molecular Biology at Michigan State University, was chosen for her "contributions to understanding the structure and function of integral membrane proteins involved in respiratory electron transport, as well as detergent-based methodologies for isolation, purification and crystallization of membrane proteins." She was honored at a ceremony during the 54th Annual Meeting of the Biophysical Society in San Francisco in February.

Cambridge Crystallographic Data Centre archives 500,000th crystal structure

The Cambridge Crystallographic Data Centre (CCDC) has just announced the archiving of the 500,000th small molecule crystal structure to the Cambridge Structural Database (CSD). A non-profit, charitable institution whose objectives are the general advancement and promotion of the science of chemistry and crystallography for the public benefit, the CCDC serves the scientific community through the acquisition, evaluation, dissemination and use of the world's output of small molecule crystal structures. It compiles the CSD, the world repository of small-molecule crystal structures. This unique, scientifically rigorous database, built over 45 years, is the international *de facto* standard for small-molecule chemical structures and has become an essential resource to scientists around the world. The CCDC also develops scientific products and services, such as structural knowledge bases and applications software for the life sciences and crystallography, maximizes worldwide accessibility to the CSD for scientists in academia and industry, performs and supports fundamental research using CSD information and CCDC products, and promotes and supports applications of crystal structure information in academia and industry.



The CCDC began operations in 1965 in the Department of Chemistry at the University of Cambridge, UK. Compilation of the CSD began with just a few hundred structures. Today, the CCDC archives approximately 150 new experimentally determined structures each working day. Each structure is fully checked and validated by expert chemists and crystallographers, and entries are further enriched with valuable chemical data. The CSD's 500,000th structure is the anti-convulsant drug **Lamotrigine**, published in *Acta Crystallographica*, C65, pp.460-464, 2009, by **Balasubramanian Sridhar and Krishnan Ravikumar** of the Indian Institute of Chemical Technology in Hyderabad. The CSD reference code for the structure is EFEMUX01.

2009 ACA Travel Award



It was a pleasure to attend the 2009 ACA Meeting in Toronto. I enjoyed the opportunity to share and discuss my research with others in the community, and I was honored to be one of the **2009 Margaret C. Etter Student Lecturer Award** recipients. I am grateful for the support from the ACA and Powder Diffraction SIG which helped me to attend the meeting - it signifies the encouragement the community and association extend to developing scientists.

As a first time ACA meeting attendee, I was impressed by the breadth of topics represented in the sessions and the lively discussions. The meeting certainly gave a nice cross-section of the diversity of current research in crystallography. I found it useful to gain this perspective as a student of materials physics and chemistry, even though I confess that I gravitated toward the sessions specifically involving inorganic materials. I particularly enjoyed Svilen Bobev's special lecture, which emphasized that fundamental discovery of new compounds and structures can still be made in the "simple" binary systems.

The meeting was a great opportunity to meet colleagues and collaborators, and I look forward to attending other ACA meetings in the future.

Matt Beekman

*Editor's note: comments from many other ACA Travel Award recipients are in the 2009 winter issue of *Reflexions*.*

New ACA History Archive

The ACA is planning a History Portal, to archive material on the history of crystallography. As part of this effort, we invite crystallographers to recount their own personal history. Shortened versions of these personal histories will be featured in *Reflexions*, and the full-length accounts will be deposited in the archive. If you are an author who would like to deposit your own history, please contact **Virginia B. Pett**, pett@wooster.edu, for some very flexible guidelines. If you are interested in helping with the history of crystallography project, please also contact Virginia.

2010 Art in Crystallography Contest


We are accepting entries to the **2010 Art 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 small monetary awards and banquet tickets 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; the 2009 entries were featured on the cover of the *IUCr News* in issue 17, #2. Please let us know if you are interested in being a judge. **The deadline for 2010 Contest is May 1st, 2010**

The *Reflexions* editors, Judy and Connie are hoping someone will volunteer for the position of

Opinions Column Editor

In the past our *Opinions* columns have featured two subjects: **Intelligent Design / the Evolution debates** and **Global Warming**. We can supply sources for both of these, and the column could consist of updates from these sources - or - the *Opinions* editor could choose another subject and put together something different. Please contact either editor (conniechidester@earthlink.net or flippen@rcsb.rutgers.edu).

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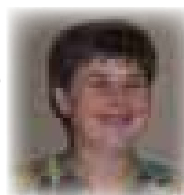


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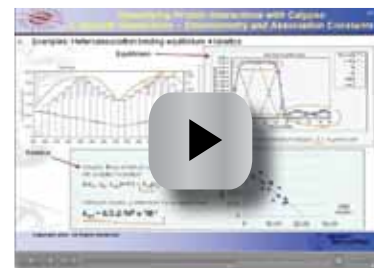
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Chicago lakefront. Courtesy of Bernie Santarsiero.

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Images from the Nobel-winning research on the ribosome



Ada Yonath, Weizmann Institute of Science, **Thomas Steitz**, Yale, and **Vekatraman Ramakrishnan**, MRC Laboratory

of Molecular Biology, shared the **2009 Nobel Prize in Chemistry** for their work that culminated in the structure, at atomic resolution, of the ribosome. They will all present **Plenary Lectures** at the **2010 ACA Annual Meeting in Chicago**.

The cover shows the historical sequence for this work. Clockwise, starting at the middle right: crystals from 70S ribosomal particles (Yonath, late 70s); rendering of low-resolution *E. coli* ribosome from electron microscopy, about 40Å resolution, (Steitz, with colleagues Peter Moore and Joachim Frank, using EM studies and diffraction maps, late 90s); higher resolution 50S ribosome structures, at roughly 20Å; and at 3Å (Steitz); at top left, a model of the 70S subunit based on the Ramakrishnan model from *Thermus thermophilus*, PDB IDs 2J00 & 2J01, (Ramakrishnan, 2000); and, at top right, the *Deinococcus radiodurans* 50S subunit (Yonath, 2001). Cover illustration courtesy of Bernie Santarsiero, Joerg M. Harms, Peter B. Moore, Max Planck Institute, Weizmann Institute of Science, and *Journal of Biology*. For additional information, see Peter. B. Moore: *The ribosome returned*, *J.Biol.*, **8:8**, 2009; and Joerg Harms' website, www.riboworld.com/.

1. Brian T. Wimberly, Ditlev E. Brodersen, William M. Clemons, Jr, Robert J. Morgan-Warren, Andrew P. Carter, Clemens Vonrhein, Thomas Hartsch & Vekatraman Ramakrishnan, *The structure of the 30s ribosomal subunit*, *Nature* **407**, 327-339 (September 21, 2000).

2. N. Ban, P. Nissen, J. Hansen, P.B. Moore, T.A. Steitz, *The complete atomic structure of the large ribosomal subunit at 2.4 Å resolution*, *Science*, **289**, (5481), 905-920 (Aug 11, 2000).

3. F. Schluenzen, A. Tocilj, R. Zarivach, J. Harms, M. Gluehmann, D. Janell, A. Bashan, H. Bartels, I. Agmon, F. Franceschi and A. Yonath, *Structure of functionally activated small ribosomal subunit at 3.3 Å resolution*, *Cell*, **102**, 615-23 (2000).

4. J. Harms, F. Schluenzen, R. Zarivach, A. Bashan, S. Gat, I. Agmon, H. Bartels, F. Franceschi and A. Yonath, *High resolution structure of the large ribosomal subunit from a mesophilic eubacterium*, *Cell*, **107**, 679-88 (2001).

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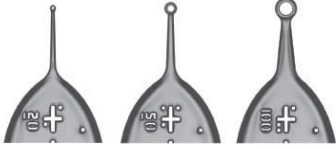
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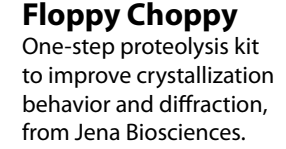
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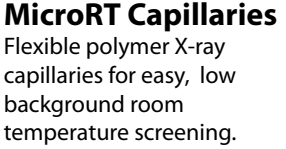
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Lachlan Cranswick has mysteriously disappeared

As we write this in February, it has been more than one month since Lachlan Cranswick was listed as a missing person by the police of Deep River, Ontario, Canada. Sadly, we have to consider the possibility that he may never come back. On February 4th the *Ottawa Citizen* carried an article about his mysterious disappearance. See <http://www.ottawacitizen.com/news/Scientist+disappearance+baffles+investigators/2520106/story.html>.

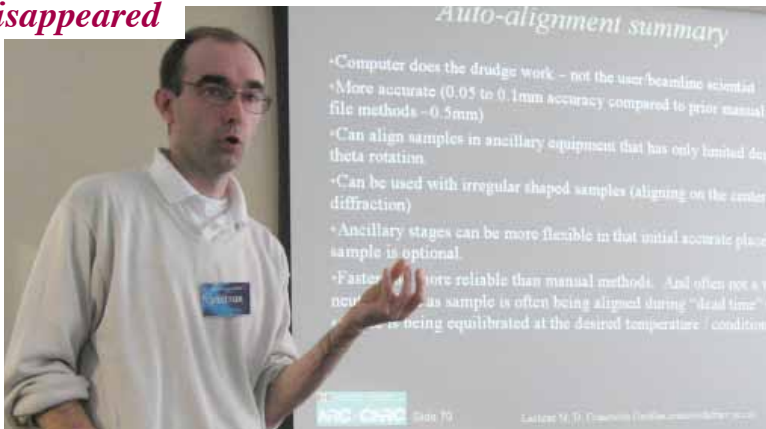
Lachlan M.D. Cranswick has been extraordinarily active in distributing both powder and single crystal computer programs as well as in crystallographic methods. He organized all kinds of events including satellite workshops at international congresses and several round robins about the Rietveld method, Structure Determination by Powder Diffraction (SDPD), and Search/Match. He was one of the original founders of the SDPD and Rietveld mailing lists and of various newsgroups on the internet such as sci.techniques.xtallography. He chaired the Commission on Crystallographic Computing for the IUCr and is a member and webmaster for the Canadian National Committee for Crystallography. He edited many *Newsletters* produced by IUCr Commissions (crystallographic computing; powder diffraction; teaching commissions, etc). The CCP14 (from 1998 to 2003; see www.ccp14.ac.uk/) gave him an opportunity to apply his talents by cataloguing the most efficient computer programs. Although not himself a developer of programs, he constantly cajoled developers to make improvements in their algorithms, and to write better explanations of their software in newsletters. It is no exaggeration to say that thousands of Lachlan emails about these topics are out there in e-space. His concern about the difficulties of doing science in developing countries prompted him to distribute his *NEXUS* CD to countries such as Cuba where internet access is difficult or impossible. That regularly updated CD contains a huge list of open



Lachlan at the top of the Eiffel Tower in 1998 from <http://sdpd.univ-lemans.fr/Lachlan/Lachlan-1998-1.jpg>

software and documentation about crystallography.

Two excerpts from his publications reveal Lachlan's professional concerns. The first is from a paper about the future of crystallography, *Z. Kristallogr.* **217**, 2002, pp 293-4: "Research institutes and departments that are not willing to reinvest in expert staff, as well as invest in the time and effort it takes to develop scientific leadership in supporting fields such as crystallography, may suffer a precipitous decline in their abilities to perform leading-edge research." The second is from *Acta Cryst.* **A64**, 2008, pp 65-87: "Unless a sufficient body of people continues to dismantle and re-build programs, the knowledge encoded in the old programs



A recent photo of Lachlan supplied by Ian Swainson.

will become as inaccessible as the knowledge of how to build the Great Pyramid at Giza." Lachlan has co-authored or authored at least 53 papers listed in the Web of Science. One in particular: *Superconductivity in LaFe_{(1-x)Co_xAsO}*, *Phys. Rev.* **B78**, 2008, 104505, has already attracted a large number of citations. He has written chapters in several recent books about powder diffraction. At the time of his disappearance he was only 41 years old - and at the beginning of a promising career.

Apart from science, many other subjects interested Lachlan: philosophy, history, literature and poetry, to name a few. His personal website, developed when he was in Melbourne: <http://lachlan.bluehaze.com.au/> is a mixture of humor and seriousness. Quality of life was always important to him; he preferred moving to Chalk River, Canada, with its spectacular natural beauty, to another job opportunity at Berkeley. The photo



Deep River Silver Spoons C trail during autumn, is from his website. It was posted in December, 2009. An avid dinghy sailor on the Ottawa River in the summer, Lachlan also enjoyed walking and cross-country skiing in the winter. He is known to locals as the Vice-President of the Deep River Curling and Squash Club. Lachlan has worked for the NRC's Canadian Neutron Beam Centre for seven years. "His collaborators from universities across Canada praise his effectiveness in supporting their research," said Daniel Banks, a spokesman for the centre. "He was a driving force in developing our scientific tools to the leading edge."

Those of us who know him well miss him as a good friend. Indeed the entire community of crystallographers, anticipating that they will find less information on the web about tools they use to solve problems, must also miss him. Please forgive us our fantasy, but rather than imagining a darker scenario we much prefer to believe that Lachlan was captured by aliens wanting to improve the level of crystallography on their planet.

Armelle Le Bail and Ian Swainson

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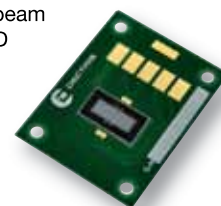
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Summer School on Exploring Structures of Molecules and Materials at U Toledo

Starting in Summer 2010, the Chemistry Department at the University of Toledo (UT) will be hosting a Research Experience for Undergraduates (REU) Site. The site will focus on “Exploring Structures of Molecules and Materials”, teaching students to utilize a variety of structural characterization methods, including many crystallographic techniques.

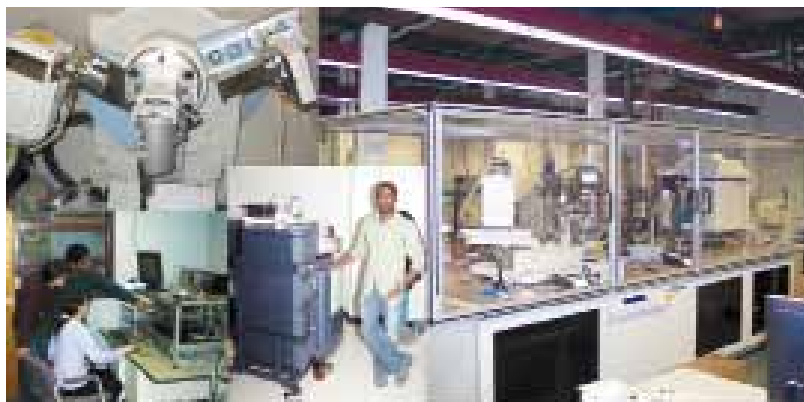
Two UT chemistry professors, **Timothy Mueser** and **Cora Lind**, developed this proposal to the National Science Foundation for an REU site at UT to contribute to training goals outlined in a 2006 National Academy of Sciences report by the USNC/Cr. This document outlines crystallography-related topics that should be incorporated into K-12, undergraduate, and graduate curricula to stimulate interest in structure determination.

Formal crystallography education is on the decline, and has often been limited to graduate level classes in the past. This REU opportunity is designed to stand in the gap, and undergraduate research activities will emphasize hands-on experience with many of the techniques used to determine and analyze structures of molecules and solid-state materials.

The summer program will start with three days of introductory coursework covering the basics of scattering and diffraction methods, NMR, mass spectrometry, and electron microscopy. Hands-on training using state-of-the-art instruments available in the Arts & Sciences Instrumentation Center at UT will be an integral part of the coursework, allowing the undergraduate researchers to get an appreciation for the applicability of the techniques covered in the theory sessions. The remainder of the first week will be spent on a two day trip to Argonne National Laboratory, where students will have the opportunity to visit the Advanced Photon Source and participate in experiments on several beamlines. This will expose the students to cutting-edge research facilities, and will hopefully instill excitement about crystallography related research. A number of students will gain additional exposure to national facilities through participation in their group’s research projects during their internships.

Participating mentors include: **Amanda Bryant-Friedrich** (analysis of oxidative damage in DNA using NMR, mass spectrometry and crystallography); **Connie Schall**, in collaboration with **Paul Langan** at LANL (fiber diffraction studies of cellulose); **Cora Lind** in collaboration with **Zhongwu Wang** at CHESS (powder diffraction studies of negative thermal expansion materials under non-ambient conditions); **Don Ronning** (study of tuberculosis infection by protein crystallography); **John Belizzi** (crystallographic analysis of circadian proteins); **Leif Hanson** (neutron and x-ray scattering techniques to study protein complexes); **Max Funk** (crystallographic and scattering methods to study lipoxygenases); **Terry Bigioni** (colloidal nanoparticles); **Timothy Mueser**, in collaboration with **Kandace Williams** at the UT School of Medicine (neutron and x-ray scattering and diffraction methods to analyze DNA replication and repair complexes); and **Wendell Griffith** (analysis of protein conformation through a combination of x-ray diffraction and mass spectrometry).

Please communicate this opportunity to your undergraduates, and have them apply through the REU website at www.utoledo.edu/as/chemistry/REU.html. The fellowship includes a stipend, housing, and the visit to Argonne National Laboratory.



Top photo: U.Toledo Instruments; under that: Jennifer Hinerman, ORNL; next down, Stacy Gates, CHESS; just above, Connie Schall and Paul Langan at BioCat. Photos courtesy of Cora Lind.

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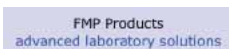
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Lieselotte in the late 1940's. Photo courtesy of David Templeton.

Lieselotte (Lilo) Templeton (née Kamm) was born in August 1918, in Breslau, Silesia, then part of Germany. She died October 10, 2009 in Berkeley, California, at the age of 91.

Until Lilo was 14 years old, she lived with her parents and her younger brother Dieter (Max Dietrich Kamm) in a large flat in Breslau. Her father Walter was a lawyer who had all sorts of cases; he once, on behalf of a fisherman, sued the civic authorities for placing a bridge support in the Oder river in a spot that was prone to causing accidents because of the prevailing currents. He won the case, and the happy fisherman paid in installments of fish. Theirs was an affluent, well-educated family. They were modern, secular and Jewish. Part of each summer was spent at the Baltic Seacoast, together with other relatives, including an aunt, Tante Munda from

Berlin, a talented painter, her husband Bruno, and their daughters, Illu and Eva. Other notable relatives included an uncle, the physicist Otto Stern, who was to win a Nobel Prize, and his sister, Tante Li, who among other things designed very modern furniture, some of which is still in use in David Templeton's house.

In 1933, her parents fortunately foresaw the political changes that were coming and decided that they needed to leave Germany immediately. (Otto Stern emigrated to the United States in the same year, resigning his post at Hamburg University in protest when ordered to fire a Jewish lab assistant.) The family lived in the town of Versailles for three years, 1933-36, and it was here that Lilo became fluent in French and completed high school. In 1936 the family emigrated to the United States, first to New York, then, in 1937, to Berkeley where Dieter had enrolled at U.C. Berkeley. Lilo also enrolled at U.C. Berkeley, achieving first her B.S. in 1946, then her PhD in 1950. In the spring term of 1947, Lilo Kamm and David Templeton were both enrolled in Professor Giauque's thermodynamics class. They met on the first day of class. A short time later, Lilo, ever resourceful, asked David for help making and repairing some needed equipment in a basement lab of Le Conte Hall. They were married in 1948.

During her graduate work in physical chemistry at Berkeley, she also worked for her thesis advisor, chemistry professor Leo Brewer, as an employee of the plutonium project of the Manhattan District. After receiving her PhD, Lilo did significant work in solid state chemistry and ceramics, and in detection of explosive materials. For some time she was not able to work in the same department as David, due to anti-nepotism rules.

Once those were relaxed, Lilo and David entered the most active period of their lives together. In Lilo's words¹ "It was really my interest in computer programming and the subsequent reworking of the analytical absorption program (AGNOST) now called ABSOR that got me seriously involved in crystallography. ABSOR was useful in helping me solve several crystal structures of heavy-element compounds, but it was particularly important in recent work with my husband on



Lieselotte and David at a Berkeley College of Chemistry event.

Photo courtesy of Dorothy Read (Berkeley) studying anomalous dispersion at absorption edges with synchrotron radiation. Our measurements with compounds of cesium and several rare earth elements demonstrated the exceptionally large effects which occur at L absorption edges..."

Other workers at SSRL remember her work: "Lieselotte Templeton, working together with her husband David, conducted pioneering research in the late 70's and 80's at the Stanford Synchrotron Radiation Laboratory (SSRL), studying anomalous dispersion and dichroism at the absorption edges of heavy metals. These experiments made special use of the tunable nature of synchrotron radiation to investigate the fundamental properties of anomalous dispersion. They measured single crystal x-ray anomalous scattering data using [a] diffractometer dedicated for crystallography studies. During the

David and Lieselotte at the experimental control area of beam line 1-5 at SSRL where many of their measurements were made. Photo courtesy of Keith Hodgson.



cont'd, next page

early years, the SSRL synchrotron beam was much less reliable [than now] and Lieselotte and David often spent several days (and nights) at the beam line. It was an adventurous time and one admires their energy, stamina, enthusiasm and resourcefulness in undertaking such experimental work so late in their careers, continuing working at SSRL well into the 1990's.² Their work at SSRL led to numerous publications.

It was this work that led to Lilo and David sharing the third Patterson Award in 1987, a significant event in both of their careers, though naturally enough not one that kept them from further research. Although I did not make an exhaustive search, I did find a 1997 paper authored by the Templetons.

Another of Lilo's talents that developed long before the Patterson award was her influence on the lives of young crystallographers, including myself. I was a student of David's from 1968 to 1972, and remember Lilo then only socially, but I came to appreciate her contributions more and more as my career as a crystallographer progressed and I saw the two of them at ACA meetings and read the papers they produced. What I saw in her at first, however, and continuously thereafter was that she did not allow her success as a scientist to get in the way of being a warm person. This same feeling has been expressed by Ken Raymond, a young assistant professor at Cal at the same time I was a graduate student, and by his students as well, including Keith Hodgson, who went on to collaborate with them at SSRL later in his career. I am sure, knowing Lilo, that it was not just the few students who worked closely with David who were encouraged and engaged by her example.

Frances Jurnak, now at U.C. Irvine, who was a few years behind me as a graduate student in David's research group, wrote: "I remember Lilo as a gracious lady who was years ahead of her time. In a world in which it was difficult for women to be professionals and mothers, she found a way to be intellectually engaged, continuing to make significant scientific contributions. Although I didn't see her as my type of role model back when I



Lieselotte and David in 1994 at the ACA Annual Meeting banquet.
Photo courtesy of Bill Duax.

was a graduate student, over my lifetime I came to appreciate just how successful she was in carving out a scientific niche for herself and for being a very close, intellectual companion to David, while being the mother of two children."

My appreciation of her worth as a crystallographer is that her contributions were not only what she did, in terms of research and publications, important though those are. As important, in the long run, will be what she was as a person, the epitome of a gracious scientific woman. She is survived by her husband, David and their two children, Diana Killen and Alan Templeton.

Frederick Hollander

(1) *Women in Crystallography* by Maureen M. Julien, p 349, *Women of Science, Righting the Record*, ed. by G. Kass-Simon and Patricia Farnes, Bloomington, Indiana: Indiana University Press, 1990.

(2) Keith Hodgson, private communication.

This memoriam has been written with major contributions from Dorothy Read from the office of *The Catalyst*, the newsletter of the College of Chemistry at U.C. Berkeley, Paul Phizackerley and Mike Soltis at Stanford University, Alan Templeton, Ken Raymond, Keith Hodgson and Frances Jurnak. Any mistakes or misinterpretations of their contributions are my own.

Index of Advertisers

ATPS, Inc	36
Bruker AXS, Inc.	inside front cover, 27
Dectris Ltd.	16
Emerald Biosystems	26
Hecus X-Ray Systems	31
MiTeGen	14
Oxford Diffraction	outside back cover
Rayonix	29, 33
Rigaku Americas, Inc.	inside back cover, 2
Wyatt Technology Corporation	9

Contributors to this issue

Ross Angel, Matt Beekman, Christian Betzel, Jim Britten, Marcia Colquhoun, Bill Duax, Howard Einspahr, Joe Ferrara, JuanMa Garcia Ruiz, Joerg Harms, Dirk Heinz, Keith Hodgson, Fred Hollander, Frances Jurnak, Judy Kelly, Armel Le Bail, Cora Lind, Virginia Pett, Paul Phizackerley, Ken Raymond, Dorothy Read, Bernie Santarsiero, Mike Soltis, Ian Swainson, Paul Swepston, David Templeton, David Watkin, Bomina Yu.

The Warren Diffraction Physics Award Lecture by Shih-Lin Chang



It is a great honor and pleasure to be here to receive the 2009 Warren Award. I would like to thank ACA and the Award Committee. Thanks also go to my past and present students, postdocs, colleagues, and collaborators for their help, support, and cooperation during my career. I would also like to take this opportunity to express my special gratitude to my thesis advisor, the late Prof. Ben Post of Brooklyn Poly. He taught me x-ray diffraction and crystallography and brought me into this field of research. His guidance has led me to this award. I would like to dedicate this talk to him.

I studied in the Fankuchen x-ray diffraction laboratory of the Polytechnic Institute of Brooklyn for a PhD degree in physics under the guidance of Ben Post from 1971 to 1975. I still remember that during my first year at Poly Ben gave lectures on the principles of x-ray diffraction and also taught the x-ray diffraction laboratory course, where I enjoyed very much his way of teaching and sense of humor. In four years of study, I learned various x-ray diffraction techniques, including powder, single crystal, topography, interferometry, fluorescence and multiple diffraction, and dynamical theory. I began to be interested in the fundamentals of the interaction of x-rays and crystals, such as the formation of wavefield, energy flow, extinction, phase, coherence, etc. My dissertation was on the theoretical and experimental aspects of Bragg-type multiple diffraction, where the dynamical diffraction effects were the main focus. This training has had a profound influence on my career of research and teaching.

Coherent Dynamical Interaction in X-ray Multiple Diffraction and Crystal Cavity Resonance

Coherence means the constant-phase relationship in space and time of wave propagation. Usually, temporal (longitudinal) coherence and spatial (transverse) coherence depend on the energy bandwidth and the transverse size of the source, respectively. *Longitudinal* and *transverse* mean parallel and perpendicular to the direction of wave propagation.

This constant-phase relationship applies in x-ray diffraction from crystals, giving rise to constructive or destructive interference. However, in a usual Bragg diffraction experiment, no information about the phase of the structure factor can be extracted from the intensity measurement of a single reflection. This is the so-called “phase problem”.

This difficulty can be overcome by using simultaneous 3-beam diffraction among many existing phasing methods, where two diffracted beams are generated in space and time. The interference between the two gives rise to intensity modification, thus providing the phase information. Hence, in part 1 I will address *Quantitative determination of x-ray phases using multiple diffraction*.

On the other hand, for x-ray optics, how to produce quasi coherent x-ray sources is one of the main themes of interest. More importantly, temporal coherence is not always attainable. In this case we may consider x-ray resonators (cavities) and x-ray free-electron lasers as candidates for providing quasi coherent x-rays. Therefore, in part 2 I will focus on *making x-ray Fabry-Perot resonators based on constant-phase relationships (coherence) in x-ray diffraction*.

Quantitative determination of x-ray phases using multiple diffraction.

In the literature, the idea of using multiple diffraction for phase determination has long been proposed and investigated, including the early work by W. N. Lipscomb, S. Miyake & K. Kambe, P. P. Ewald & Y. Heno, R. Colella, and B. Post, and the later studies of S.-L. Chang, H. J. Juretschke, R. Hoier, K. Hummer, F. Mo, Q. Shen, G. Thorkildsen, E. Weckert, Yu Stetsko, and S. L. Morelhaio, and many others.

Multiple diffraction occurs when several sets of atomic planes are simultaneously brought into position to diffract an incident x-ray beam. In real space, for 3-beam diffraction, the crystal is first aligned for a Bragg reflection G by adjusting the theta angle, and is then rotated around the reciprocal lattice vector of the G reflection, the azimuth ψ -scan, to bring another set of planes, L , also satisfying Bragg's law, into alignment. For clarity, we call G the primary, L the secondary, and $G-L$ the coupling between the primary and the secondary reflections. In reciprocal space, the reciprocal lattice point (rlp) G is first moved onto the surface of the Ewald sphere and then the rlp of the secondary reflection L is also brought onto the surface of the Ewald sphere by the azimuth ψ rotation around the reciprocal lattice vector of the G reflection. There are two positions at which 3-beam diffraction occurs, i.e., IN and OUT, when the rlp L moves towards and leaves the Ewald sphere, respectively.

Coherent dynamical interaction in 3-beam diffraction can be understood as follows: The incident beam is first diffracted into the G direction by the primary reflection and the transmitted beam is then successively reflected by the secondary L and the coupling $G-L$ back to the G -direction. The interaction of the Bragg reflected and the detoured diffracted beam modifies the intensity of the Bragg reflection G , leading to intensity variation. Therefore, the asymmetry of the relative intensity profile can be used to determine the phase d_3 of the structure-factor triplet $F_L F_{G-L} / F_G$.

Theoretical calculations show that for d_3 equal to $+90^\circ$ and -90° , the peak intensity decreases and increases, respectively. For $d_3=0^\circ$, the diffracted intensity first decreases and then increases, while for $d_3=180^\circ$, the profile asymmetry is reversed, i.e., first increasing and then decreasing. Hence the asymmetry depends on the cosine and the peak intensity is determined by the sine of the triplet phase d_3 .

For quantitative phase determination, according to first order approximation of the fundamental equations of the wavefield in dynamical theory, the relative intensity distribution of three-beam diffraction is given as the sum of the phase dependent I_D and phase independent I_K , where I_D is proportional to the sine and cosine of the triplet phase and I_K is a symmetric Lorentzian. To solve the two unknowns, $\sin d_3$ and $\cos d_3$, we need to measure intensity profiles of two 3-beam cases, which are inversion-symmetry related (ISR). That is, (OGL) vs (O, -G, -L). For simplicity, we call (OGL) the “+” case and (O-G-L) the

cont'd, next page

“-“ case. The corresponding phases are d_{3+} and d_{3-} of the triplets $F_{L}F_{G-L}/F_G$ and $F_{-L}F_{L-G}/F_G$. From the three-beam diffraction profiles of two ISR cases, the triplet phases can be obtained by fitting the experimental profiles with asymmetrical Lorentzian functions.

As an example, consider the determination of phase shift at resonance for a CdTe/InSb thin-film system, composed of a 500 Å thick MBE grown CdTe thin film on the (001) InSb crystal, by x-ray three-beam resonant diffraction. Resonance x-ray diffraction, utilizing the anomalous dispersion near the absorption edges of a constituent element, has recently become a powerful method for electronic and atomic structures characterization of materials. At an absorption edge, the anomalous dispersion corrections on the atomic scattering factors become important, leading to an additional phase shift which is called the resonance phase. This phase shift of a G-reflection can be expressed as the phase sum of the structure factors of the +G and -G reflections. Similarly, we could define the resonance triplet phases as the sum of the d_{3+} and d_{3-} . Far from the absorption edges, all the resonance phase shifts are nearly equal to zero, while at the absorption edges Friedel’s law is no longer valid. The values of all resonance phases can differ drastically from zero.

To determine the resonance phases quantitatively, we choose the (000) (002) (-3-11) “+” case and (000) (002) (1-31) “-” case for photon energies near the Cd L3 edge (3.538 keV), and the (000) (002) (331) “+” case and (000) (002) (3-31) “-” case for Te L3 edge (4.341 keV), where (002) is a symmetric Bragg (primary) reflection and {311} and {331} are the secondary reflections with the diffracted beams propagating along the crystal surface.

Since the absorption edges are in the soft x-ray region, the experiments are carried out at the double-crystal monochromator (DCM) tender x-ray beamline, 16A1, with photon energies from 1–9 keV at the National Synchrotron Radiation Research Center (NSRRC) in Taiwan. The energy resolution is about 0.2 eV. Because of the strong air absorption of soft x-rays, the whole experiment is performed in a high-vacuum environment ($\sim 2 \times 10^{-7}$ torr) and a UHV (ultrahigh vacuum) compatible six-circle kappa diffractometer (Fig. 1) is used.

the NSRRC, Taiwan, and Spring 8 and RIKEN, Japan. The collaborators are Y.-R. Lee, H.-H. Wu, S.-Y. Chen, M.-S. Chiu, W.-H. Sun and Y.-Y. Chang from my lab; Y. Stetsko, M.-T. Tang, and B.-Y. Shew of NSRRC; and M. Yabashi and T. Ishikawa from Spring 8 and RIKEN, Japan.

The Fabry-Perot resonator /interferometer has been frequently used in optics. It consists of two reflecting mirrors, with which the incident photons are reflected back and forth, thus leading to resonance, provided that the coherence conditions remain. In the case of hard x-rays, x-ray resonators (cavities) have long been proposed and, since 1967, pursued. (W.L. Bond, M. A. Duguay, & P. M. Rentzepis, *Appl. Phys. Lett*, **10**, 216 (1967)). However, observation of resonance fringes from an x-ray cavity has so far been very difficult, despite much excellent work reported in the literature. In 2005, x-ray interference fringes due to cavity resonance were observed by our group. In the following, I will report on this direct observation of interference fringes due to cavity resonance for hard x-rays and its related coherent interaction in



Fig.1: Six-circle soft X-ray diffractometer

the x-ray diffraction process involving two-crystals and multi-crystals.

A simplest geometry for an x-ray resonator is a two-plate cavity. Cavity resonance occurs when an incident x-ray is reflected back and forth coherently, both spatially and temporally, between the two plates, thus generating interference fringes, where x-ray back diffraction (Bragg angle=90°) is used.

We started the x-ray cavity study in 1997 by adopting the 2-plate Fabry-Perot type cavity in a normal incidence geometry for the back diffraction. To design the experiments, we first considered the required coherence conditions and the visibility of cavity resonance fringes. To observe well resolved resonance fringes in energy scans, the energy resolution ΔE of the incident beam should be smaller than the so-called free spectral range E_d (the separation between two adjacent fringes), and the width of a fringe. From the uncertainty principle and the definitions of longitudinal coherence length, the required

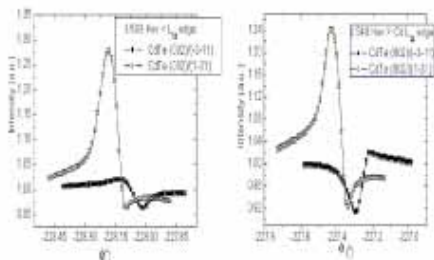


Figure 2, at left, shows the relative intensity profiles of the CdTe (002) reflection near the 3-beam diffraction positions of the ISR pair for the energies 3.533 keV (<Cd L3) and 3.548 keV (> Cd L3). Clearly, the asymmetry of the curve (solid

dots) in the “-“ case, is reversed when the photon energy is across the Cd L3 edge. There is no change of asymmetry of the curves (open circles) for the “+” case. Similar behavior is also observed for the 3-beam cases near the Te L3 edge. These measurements lead to 55° and 65° phase shifts at the Cd L3 and Te L3 edges, respectively.

We have shown the direct determination of resonance phase shifts near the Cd L3 and Te L3 edges in the CdTe/InSb thin-film system. This x-ray technique is capable of determining resonance phases for a variety of thin-film systems without restriction to any specific elements. Since in Bragg-surface three-beam diffraction the secondary reflected wave propagates along the interface, abundant interface structural information is carried by this surface-diffracted wave, which could be useful for interface structure analysis.

Making x-ray Fabry-Perot cavities based on constant-phase relationships (coherence) in x-ray diffraction. This research work results from the collaboration between my lab at NTHU and the research groups from

criteria for coherence are: (1) that the coherent time of the incident beam is larger than the circulation time of x-ray photons for a round trip inside the cavity; (2) that the longitudinal coherent length is greater than two times the effective gap distance d , which is the sum of the average thickness of the crystal plates and the gap. These two criteria are equivalent to each other. The key parameters are ΔE and the effective gap distance d .



To satisfy the required criterion, L (longitudinal coherent length) $> 2d$, $\Delta E/E$ should be as small as possible. Therefore we used a 4-crystal monochromator (at left), consisting of two pairs of (422) and (11 5 3) asymmetric reflections in a (+- -+) geometry, to provide an energy resolution

of the incident beam equal to 0.36 meV at 14.4388 keV, i.e., $\Delta E/E \sim 2.5 \times 10^{-8}$. Accordingly, the crystal gap should be of the order of a few 100 μm . We then chose cavity sizes of a few tens to hundreds of microns so as to satisfy the required coherence conditions. The crystal cavities are prepared on 4 inch Si wafers using the microelectronic lithographic technique. The size of 2-plate and 8-plate cavities is 800 μm wide and 200 μm high.

The diffraction experiments were carried out at the Taiwan undulator beamline, BL12XU, at the SPring-8 synchrotron radiation facility in Japan. The incident radiation impinging on the crystal cavity was first monochromatized by a Si (111) double-crystal and then by the four-crystal ultrahigh resolution monochromator at an energy $E = 14.4388$ keV. The Si (12 4 0) reflection was used as the back diffraction. The crystal cavity was placed at the center of a Huber 8-circle diffractometer which could be rotated around the vertical [001] and horizontal [-1 3 0] directions by varying the θ_v and θ_h , respectively. The transmitted diffracted and the back reflected beams were monitored by a pin diode and an ion chamber, respectively. Intensity oscillations due to cavity resonance were observed for the transmitted and the back reflected intensities in θ_v and θ_h scans. Also, interference fringes were clearly seen in energy scans of the transmitted beam through 2-plate and 8-plate crystal cavities.

At 14.4388 keV, a 24-beam diffraction takes place, which consists of 9 coplanar diffractions, including the direct (000) and the back reflected (12 4 0). Figure 3 shows the two-dimensional intensity distribution vs. angles θ_h and θ_v of the transmitted (000) beam for a 2-plate crystal cavity (70 μm thickness, 100 μm gap). As can be seen, the concentric rings are the interference fringes due to cavity resonance. The radial lines (lines L1 - L9) are the images related to the 9 coplanar diffractions of the 24-beam diffraction.

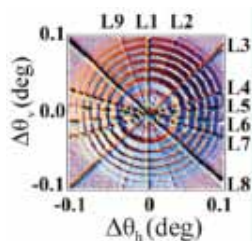


Fig. 3: Interference pattern of crystal cavity resonance and 24-beam diffraction at 0.8588 Å.

When cavity resonance takes place, x-ray standing-waves are expected to form inside the cavity. The calculations based on dynamical theory show the energy-dependence and position-dependence of the standing-wave intensity. The period is $\lambda/2$. Also, for every half-wavelength, the phase shift of the wavefield inside the cavity is π , indicating the characteristics of a standing wave. Moreover, the Fourier transform of the energy scans from 2-plate and 8-plate cavities shows time structures of periods 1.67 and 1.15 ps, respectively. This implies coherent trapping of x-ray photons in crystal cavities in the picosecond region. This result could be useful for time-resolved diffraction and spectroscopy experiments, if intensity is not a problem.

In summary, I have reported on the direct observation of resonance fringes in the (12 4 0) back reflection geometry from monolithic two and multi-plate silicon crystal cavities. The coherence required for cavity resonance may provide opportunities for developing new x-ray optics involving interferometers, narrow band filters, monochromators, intensity oscillators, etc.

The coherent dynamical interaction of x-ray multiple diffraction in single crystals, which has been used to determine crystallographic phases, dynamic phases, and resonant phase shifts, could be employed to develop new techniques for structural analysis. Consideration of the coherent interactions of x-ray back reflections in multi-crystals for the development of x-ray crystal cavity resonators may lead to new x-ray optics suitable for diffraction, spectroscopy, imaging, and microscopy applications.

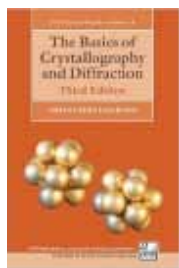
Acknowledgements: I am indebted to the late Ben Post for his guidance; to H.J. Juretschke of Poly; to Yu Stetsko and M.-T. Tang of the NSRRC for long-time collaboration; to H.J. Queisser of MPI-FKF for enthusiasm and continued support; to my graduate students and postdocs for their hard work and collaboration; to my colleagues of the NTHU, NTU (National Taiwan University), NSRRC, and RIKEN/SPring-8 for enlightening discussion and inspiration; and to the Ministry of Education and National Science Council for financial support. I am also very grateful to my wife for her understanding and support over the years.

Shih-Lin Chang.



Group photo of the X-ray Laboratory, Physics Department, National Tsing Hua University (NTHU)

IUCr monograph by Christopher Hammond: The Basics of Crystallography and Diffraction, 3rd Edition. Oxford Univ. Press, June 2009. Paperback, 352pp, \$53.00 ISBN-13: 9780199546459



The Third Edition of *The Basics of Crystallography and Diffraction* is a sound successor to the previous editions. The general layout of the book is unaltered, but many changes have been made throughout the text, and many illustrations have been re-drawn or replaced. The new chapter on Fourier series is clear and well illustrated; the new section on the Rietveld method stands a little isolated,

but perhaps is a pointer towards a more detailed description of optimization methods – and perhaps even single crystal structure determination – being saved for a 4th edition.

A casual glance at the book will give the impression that it is aimed at students mainly interested in inorganic (extended lattice) materials, or crystal physics. The discussion of organic materials is confined to six pages only. However, more careful reading shows that the book is a valuable “middle range” text for anyone carrying out diffraction experiments on any kind of material. For the molecular crystallographer it fits in well with the other *IUCr Texts in Crystallography* by Clegg *et al* and Giacovazzo *et al*. By covering a narrower field than these other texts, Hammond is able to develop concepts in more detail, and to provide helpful explanations of the mathematics.

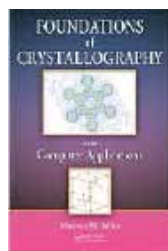
Structure analysis by single crystal x-ray diffraction is becoming a turn-key press-button technology, so that students have no exposure to fundamental crystallography until the automatic processes fail. This means that they have little opportunity to develop an understanding of the physics involved in the experiment. This book provides the insights needed for handling a wide range of non-standard problems, and is essential reading for a student wishing to become a competent crystallographer.

It is very likely now that almost everyone carrying out single crystal structure determinations will be using some form of area detector diffractometer to measure the structure intensities. These provide views of the reciprocal lattice, which for a randomly orientated crystal, are difficult to interpret. Hammond’s illustrations of the interpretation of diffraction patterns from orientated specimens may be referring to obsolete instrumentation, but they provide an insight into more general diffraction images. Most instrument makers now provide software for the synthesis of “pseudo-precession photographs”.

In the preface, the author notes that “many of the books listed in ‘Further Reading’ are very old. This is not incompatible with a recent straw poll in which ACA members were invited to suggest essential crystallographic reading. *The Basics of Crystallography and Diffraction* brings a lot of this classical information together into one place, and presents it in a way acceptable to a modern audience. It is well-structured, carefully written and a pleasure to read. There should be a copy on the shelves of every crystallography laboratory.

David Watkin

Foundations of Crystallography with Computer Applications by Maureen M. Julian. Taylor & Francis, 2008, 368 pp. Hardcover \$89.95. ISBN 9781-4200-6075-1.



The book is structured around a crystallography course the author has been teaching at Virginia Tech since 2000. It is a fully modern book in that the mathematical principles are explained by widely available symbolic programming languages and by a website developed by the author for the book. Two examples, hexamethylbenzene and anhydrous alum, are used

throughout the book. Numerous problems are provided at the end of each chapter to illustrate the principles learned. *The International Tables for X-ray Crystallography* are referenced frequently, although the reviewer notes the 4th edition are referenced rather than the more recent 5th edition.

The first five chapters are devoted to the elaboration of space group symmetry, starting with lattices and unit cells, two-dimensional and three dimensional groups and finally the reciprocal lattice. The sixth chapter discusses diffraction and the seventh covers the relationship between reciprocal and real space. The reviewer noted that the author made errors in some descriptions regarding symmetry; either they are wrong or oversimplified, and he provides a list of those errors.

Abstracted by Joe Ferrara from a full review by Mois I. Aroyo, in *Acta Cryst.* (2009). **A65**, 543–545.

Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology by Bernhard Rupp & Katherine Kantardjieff. Taylor & Francis, October 2009. Hardcover, 800pp, \$145. ISBN-13: 9780815340812.



This book has been referred to as an “epic tome” by Judith Flippen-Anderson, the “next Blundell & Johnson” by Jim Pflugrath and a paperweight by the author. I found this book to be a much needed compilation of the current state of the art of x-ray crystallography for structural biology. *BMX* is destined to become a classic and is worth reading cover-to-cover.

Among other features, *BMX* includes an extensive and descriptive main body; side bars with loads of useful information; and a key concepts section at the end of every chapter. The book provides many, many historical and current references. It is a first edition and there are a few typos and some awkward language, but I found only one math error and one historical error. It is very clear the community is supporting this book and has been most helpful in discovering the *errata*.

The only real complaint I have is that the page numbers are not associated with the figures and such, so it sometimes takes a while to find a non-adjacent figure or table. The book has thirteen chapters (no triskaidekaphobia here):

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Biomolecular Crystallography, cont'd: Chapter 1: This chapter is an abstract of the entire book, covering all the concepts and provides an outline for beginning your trek through a crystal structure analysis.

Chapter 2: Protein Structure. Basic protein structure is described here, although the chapter does include the basics of DNA and membrane protein structure.

Chapter 3: Protein Crystallization. I found this chapter to be a good survey of modern crystallization techniques with a good section on the physical chemistry of crystallization.

Chapter 4: Proteins for Crystallography. Provides a comprehensive listing of the methods available when the information in Chapter 3 is insufficient for success.

Chapter 5: Crystal Geometry. Here we learn about crystal geometry, crystal symmetry and the relationship between the symmetry of the real space lattice and the reciprocal space lattice.

Chapter 6: Diffraction Basics. This chapter provides a detailed description of the relationship between the real space lattice and the reciprocal space lattice, and hence the relationship between the electron density in the crystal and diffraction data.

Chapter 7: Statistics and Probability in Crystallography. I thought this was the best chapter because it provides a lucid discussion of the concepts in statistics and probability which are often misunderstood. Furthermore, the examples, as related to crystallography, make for easier understanding of these concepts.

Chapter 8: Instrumentation and Data Collection. While this is a good basic chapter on the subject, it is here that I found the historical error: imaging plates are reported as predating multiwire proportional counters, but to the best of my knowledge that is not true. A good description of crystal handling methods and cryo-crystallography is provided. Both synchrotron and home lab data collection are described, and there is an excellent section on data processing with modern tools.

Chapter 9: Reconstruction of Electron Density and the Phase Problem. Covers the solution of the phase problem and provides background information for the next two chapters.

Chapter 10: Experimental Phasing. Here is the current state of the art in phasing methods, MAD, SAD, SIR, SIRAS, MIRAS, initial refinement and density modification.

Chapter 11: Non-crystallographic Symmetry and Molecular Replacement. Provides a description of NCS and its usefulness in the solution and refinement stages. Molecular replacement, the most popular method for solving the phase problem, is also described.

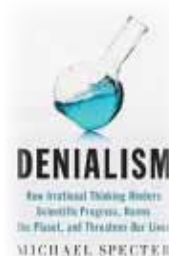
Chapter 12: Model Building and Refinement. The penultimate chapter describes in detail the refinement and model building stages using a couple of good examples and current software packages. A review of chapter 7 is appropriate for this chapter.

Chapter 13: Structure Analysis, Validation and Presentation. This final chapter details the pitfalls and traps of polishing and publishing a structure. Furthermore, a recent example of a falsified structure is presented with an explanation of the telltale signs of which every crystallographer should be aware.

Joe Ferrara

Denialism: How Irrational Thinking Hinders Scientific Progress, Harms the Planet, and Threatens Our Lives, by Michael Specter.
 Penquin Group, Hardcover, 304 pp, \$27.95.

ISBN-13: 9781594202308



In *Denialism*, New Yorker staff writer Michael Specter reveals that Americans have come to mistrust institutions and especially the institution of science more today than ever before. For centuries, the general view had been that science is neither good nor bad; that it merely supplied information; and that new information is always beneficial. Now, science is viewed as a political constituency that isn't always in our best interest. We live in a world where the leaders of African nations prefer to let their citizens starve to death rather than import genetically modified grains. Childhood vaccines have proven to be the most effective public health measure in history, yet people march on Washington to protest their use. In the United States a growing series of studies show that dietary supplements and "natural" cures have almost no value, and often cause harm. We still spend billions of dollars on them. In hundreds of the best universities in the world, laboratories are anonymous, unmarked, and surrounded by platoons of security guards - such is the opposition to any research that includes experiments with animals. And pharmaceutical companies that just forty years ago were perhaps the most visible symbol of our remarkable advance against disease have increasingly been seen as callous corporations propelled solely by avarice and greed.

As Michael Specter sees it, this amounts to a war against progress. The issues may be complex but the choices are not. Are we going to continue to embrace new technologies, acknowledging their limitations and threats, or are we ready to slink back into an era of magical thinking? In *Denialism*, Specter makes an argument for a new Enlightenment, the revival of an approach to the physical world that was stunningly effective for hundreds of years. What can be understood and reliably repeated by experiment is what nature regarded as true. Now, at the time of mankind's greatest scientific advances - and our greatest need for them, - that deal must be renewed.

I first heard of this book while listening to a Science Friday podcast. The author, Michael Specter, is a staff writer for the New Yorker. The author provides a number of examples where clear scientific evidence, for example the efficacy of childhood vaccines, is ignored and a final decision is made on ideological principles, much to the detriment of the decision maker. He goes further to examine how these decisions negatively impact society as a whole. I haven't read this book yet, but it is on my to read list.

Joe Ferrara



Snowcrystals. From the Patricia Rasmussen Collection 2002. © Rasmussen 2002

***The Strangest Man: The Hidden Life of Paul Dirac, Mystic of the Atom* by Graham Farmelo.** Basic Books, August, 2009. Hardcover, 560 pp, \$29.95, ISBN-13: 9780 4650 18277.



I am about 2/3 of the way through this book at the time I am writing this. I am really enjoying both the quality of the writing and the detail provided in the persona of Paul Dirac not to mention the history of quantum mechanics. I've always associated quantum mechanics with Schrödinger and Heisenberg, and never realized how about important Dirac was to its understanding. Dirac's equation describing the electron predicted, in a sense, the existence of holes and positrons, but it took experimental evidence from cloud chambers to make sense of the prediction.

***Stephen King Illustrated Companion: Manuscripts, Correspondence, Drawings, and Memorabilia from the Master of Modern Horror* by Bev Vincent.** Fall River Press, October 2009. Hardcover, 176pp \$32.62, ISBN-13: 9781435117662:



I thought I would add this one since Bev Vincent is not only a colleague of mine at Rigaku but also a well known crystallographer. I did not realize this book had been nominated for an Edgar award until I saw Bev on the front page of the local paper. I had read Bev's other works but not yet this one. Past writing has provided an incredible amount of detail and insight into

Stephen King's works, specifically *The Dark Tower* series. Since I have read just about everything Stephen King has written, (*The Dome* is in my queue), I look forward to reading *The Illustrated Companion* on some long flight in the near future.

Joe Ferrara joins RefleXions staff as Books Editor



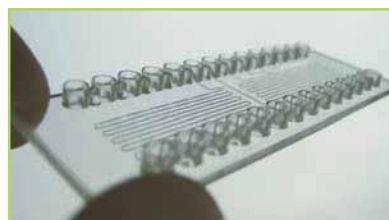
We are delighted to welcome **Joe Ferrara**, Rigaku Americas Corp, as our new (volunteer) editor of the *Books* section.

The winter 2009 *RefleXions* carried several of Joe's reviews. He has been writing book reviews for the Rigaku *Crystallography Times*, a monthly life sciences newsletter that has been published electronically since February 2009. Contact webmaster@Rigaku.com to subscribe.

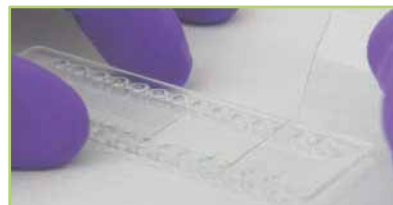
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Two international schools on crystal growth

International School on Biological Crystallization

International School of Crystallization
2009: Foods, Drugs and Agrochemicals



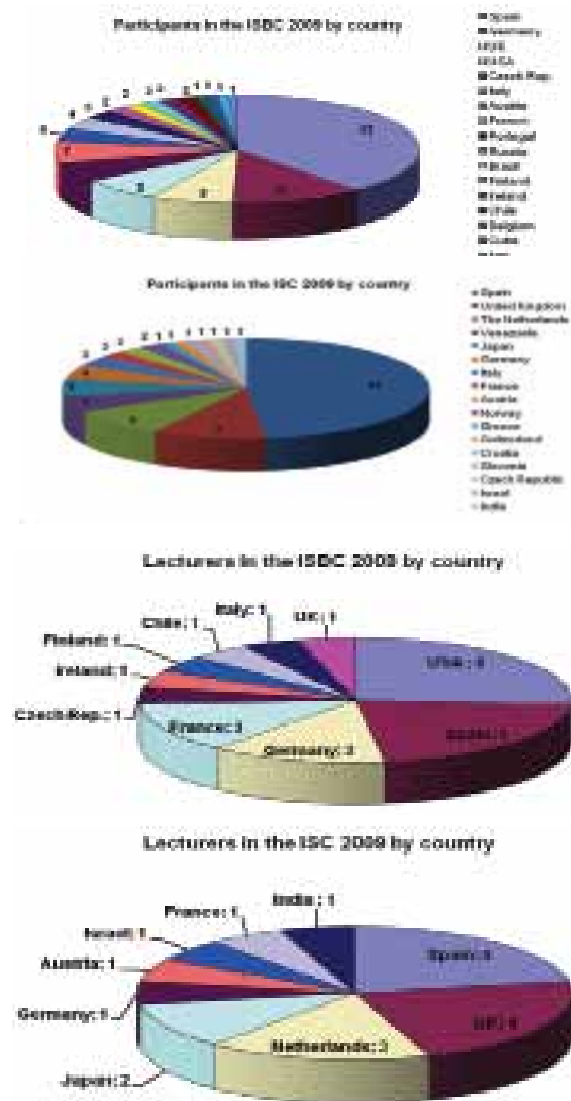
were held in Granada, Spain in May 2009 under the auspices of the IUCr Commission on Crystal Growth. The first was the second edition of the **International School on Biological Crystallization (ISBC)**, 18-22 May. Then, one week later, the first **International School of Crystallization** was held. Both schools were held at Hotel San Anton in the heart of the beautiful city of Granada.

The schools were designed for postgraduate and post-doctoral students as well as research scientists from industry and academia; all those who deal routinely with crystallization but seek fundamental knowledge of the crystallization phenomenon and the behaviour of crystallizing solutions.

Both schools dealt primarily with crystallization, but they addressed different topics. The ISBC focused on the crystallization of biological macromolecules, biominerals and biomimetic materials, with one full day devoted to case studies on the crystallization of membrane proteins and large macromolecular complexes. The ISC focused on the application of crystallization techniques to the fields of food and drug technology and to the agrochemical industry.

Considerable effort was made to provide financial help to as many students as possible and most of the students who applied were given a support grant. In total, 29 grants were given to ISBC students and 22 to ISC students. Remarkably, 94% of all students who came from outside Spain received some sort of funding.

The first day of the ISBC dealt with the fundamentals of crystallization from solution to protein crystals. Lectures included a wide range of topics from how to purify proteins, to the physicochemical properties of solutions, nucleation and light scattering theories, finishing with crystal growth techniques and handling of protein crystals. The second day was



devoted to the crystallization of large crystals, complexes and membrane proteins; the third day to a *Demonstration Fair*, at which 21 experts offered short (20-40 minutes) practical sessions, periodically, at scheduled times. Participants could choose what sessions they wanted to attend and in which order, so that they selected their own learning program *a la carte*. The fair proved to be an excellent teaching tool as it provided students with ample opportunities to interact on a personal basis with tutors and to watch closely how to perform crystallization experiments.

The fourth day's focal point was bio-mineralization, and this was followed in the afternoon with a seminar on publication of crystallization results. The final day went beyond structural biology to challenges such as large scale protein crystallization. The school ended with a round table discussion and the presentation of poster prizes offered by the IUCr and La Factoria. For additional information see www.isbcgranada.org/

The first day of ISC 2009 dealt with the fundamentals of crystallization from solution, nucleation theories, crystal growth kinetics, crystal morphology and analytical techniques. The second day covered classical and novel crystallization techniques such as gel growth, hydrothermal growth or crystallization from melts. Polymorphism occupied the third day, and the fourth day was fully dedicated to a *Demonstration Fair* similar to the fair held in the ISBC school. The last day featured special,

At the ISBC 111 participants came from 18 countries; at the ISC there were 91 attendants from 17 countries. Lecturers at both schools were from a variety of countries as well.

hot topics such as chiral crystallization, crystallization in space and the interface between drug substance and drug product. The school closed with the presentation of prizes offered by the IUCr and La Factoria. All the information about ISC 2009, including the list of teachers and the full program, is available at <http://lafactoria.lec.csic.es/iscgranada>.



The ISBC Poster Sessions featured 35 posters; there were 27 in the ISC Poster Session. An international panel of lecturers led by **Howard Einspahr** of the USA honored student teams from Germany, Japan, Cuba, Spain, UK, Slovenia and Norway with prizes. Five poster prizes were awarded in ISBC and four in ISC. Prizes consisted of volumes of *International Tables of Crystallography* provided by the IUCr, and crystallization devices, books on *Fractal Harmony* and shirts offered by La Factoria and Triana S&T.

Both schools started with a welcome cocktail party on Sunday, and participants were entertained later in the week by a night tour of the Moorish palaces of The Alhambra. On the last night everybody headed for the gypsy district of Sacromonte where, in one of its caves, participants were treated to a tapas dinner followed by flamenco music & dancing.

Two CDs, one for each school, that contain all the lectures and demonstrations performed and also posters and pictures, have been sent to the participants.

We are grateful to the Organizing Committee, especially **Luis Gómez Morales** and **José Gavira** for their substantial contributions to the schools, and to our sponsors and exhibitors. We are happy and proud to announce that the next ISC is already scheduled for **24-28 May 2010**. More information is available at www.iscgranada.org/.

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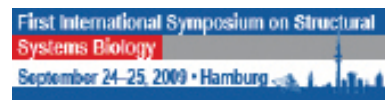
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First International Symposium on Structural Systems Biology

Hamburg, Germany, Sept. 24-25, 2009

The conference was organized and chaired by the committee of the **Centre for Structural Systems Biology (CSSB)** which will be built on the DESY Campus in Hamburg Bahrenfeld close to the new PETRA III storage ring (at right). The CSSB will be a collaborative research facility with about eight research groups focusing on infection biology, systems biology and structural biology. The symposium was held in the historic University Main Building located in the center of Hamburg, with more than 240 postgraduate and postdoctoral students and scientists from Europe, Asia and both North and South America in attendance. The rapidly emerging field of systems biology was featured with a strong focus on methods to analyze and image complex interactions in biological systems at molecular, cellular and organismal levels. Leading scientists in the fields of x-ray crystallography, NMR spectroscopy, electron microscopy and imaging, bio-Raman spectroscopy, cellular and molecular biology and bioinformatics addressed current and future developments in structural systems biology in 25 lectures over two days. For further details see www.cssb2009.de.



The latest technological advances in examining structures and dynamics of biological functions, such as signaling cascades and metabolic pathways, were addressed in stimulating sessions that featured applications of the unique light sources at Hamburg's world renowned Deutsches Elektronen Synchrotron (DESY), *i.e.* PETRAIII, the free-electron VUV laser FLASH and the soon-to-come X-FEL. The program featured present and future challenges in systems biology; key technologies and applications; and computational structural systems biology.



Keynote speakers were **Patrick Cramer**,

Ludwig Maximilians Univ., Munich, and **Greg Petsko**, Brandeis Univ. Patrick Cramer spoke in the first session on progress *towards molecular systems biology of gene transcription and regulation*; Greg Petsko ended the conference on a high note with his talk on *systems biology of neurodegenerative diseases*.

The need to establish an integrated structural biology infrastructure to support future development of cellular structural biology research was emphasized in a panel discussion chaired by **David Stuart**, Univ. of Oxford. Support for a number of centers across Europe which would allow scientists to access state-of-the-art equipment is anticipated from the **European Strategy Forum on Research Infrastructures**, within **Framework 7** of the EU.



Attendees had many opportunities to meet and interact in the central foyer where meals and refreshments were served and where more than 60 posters presented data on the structures and dynamics of biological interactions and cellular functions. Closing remarks and acknowledgments were combined with awards (sponsored by Molecular Dimensions) to authors of three outstanding posters which had been selected by an expert panel.

The organizers gratefully acknowledge the support of academic institutions, notably the University of Hamburg, DESY Hamburg and the Helmholtz Association, as well the industrial sponsors: MAR Research, Molecular Dimensions, Zinsser, and others, all summarized at www.cssb2009.de. This symposium was the first in a series to be held in Hamburg to highlight the latest structural aspects of systems biology.

Christian Betzel & Dirk Heinz

"Filler" photo courtesy of Paul Swebston, from <http://gallery.me.com/paulswebston#gallery>

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Abstracted from *Five Big Additions to Darwin's Theory of Evolution; #43 of top 100 stories of 2009* in the Jan/Feb 2010 issue of *Discover* magazine:

1. Evolution on the inside. Caltech biologist **Bruce Hay** is trying to harness the power of genetic cheaters, such as the “selfish” gene known as *Medea*, in the fight against malaria. Hay created a *Medea*-like DNA element that spreads through experimental fruit flies like wildfire, permeating an entire population within 10 generations. This year he and his team have been working on encoding immune-system boosters into those *Medea* genes, which could then be inserted into male mosquitoes. If it works, the modified mosquitoes should quickly replace competitors who do not carry the new genes; the enhanced immune systems of the new mosquitoes, in turn, would resist the spread of the malaria parasite.

2. Identity is not written just in the genes. The single rule that what is in the genes stays in the genes secured Darwin's place in the science books. But now biologists are finding that nature can break those rules. In 2009 **Eva Jablonka**, (Tel Aviv U), published a compendium of more than 100 hereditary changes that are not carried in the DNA sequence. This “epigenetic” inheritance spans bacteria, fungi, plants, and animals. For example, rats exposed to certain fungicides during pregnancy give birth to male progeny with lower sperm counts and an increased chance of developing diabetes and cancer. In each generation that follows, none of which were exposed to fungicides directly, the male offspring continue to suffer the same fate. Jablonka argues that environmental exposures— toxic substances, diet, and even stress— can affect the genome. In extremely high-stress cases, they could possibly rearrange it enough to create new species.

3. Mutations reveal surprising branches on the tree of life. Mutations give rise to new genes, but only some of those produce discernible changes that improve (or reduce) fitness. Many of them do nothing much at all, although they accumulate at a measurable rate. Generally, the more silent mutations two species have in common, the more closely related they are. Evolutionary biologist **Casey Dunn** (Brown) compared the genomes of 71 animal species and found that the common ancestor of all the animals on the planet may not have been as simple as a sponge, as previously thought. Instead, Dunn identified the more complex comb jellyfish as the earliest to diverge from the animal family tree. The idea that the simplest organism may not have come first upends the popular notion of an evolutionary march toward complexity. In 2009, Dunn and his team used a supercomputer to expand his revamped family tree, starting with *Acoelomorpha*, a flatworm that was long considered one of the most difficult animals to put in its evolutionary place. They were able to show that the worm is a product of the first split among bilateral animals more than half a billion years ago - a discovery that will help biologists understand the origins of the digestive and nervous systems.

4. The “missing link” is not missing. In October, 2009, paleontologists unveiled the earliest known skeleton of a potential human ancestor, the 4.4-million-year-old *Ardipithecus ramidus*, “Ardi,” who apparently walked on two feet with opposable toes and scampered through the branches on all fours. **C. Owen Lovejoy**, (Kent State), thinks that what made us human was the social switch from aggressive male to attentive mate. The diet of the male *Ardipithecus* suggests that by that time our ancestors had stopped fighting over mates - and started providing for their females and offspring instead. Walking upright, according to Lovejoy, is an adaptation to carrying food through the forest as gifts for potential mates.

5. We are closing in on how life began. In 2009 **Gerald Joyce** and **Tracey Lincoln** (Scripps), engineered a system of molecules that can sustainably replicate themselves and undergo Darwinian evolution in a test tube. Now Joyce says he wants to see “if we can get the molecules to invent novel function for themselves.” 2009 Nobel laureate **Jack Szostak**, (Harvard Medical School), has been packaging prebiotic chemistry into simple membranes to see how protocells could have self-assembled out of fatty acids.

See www.discovermagazine.com for the full story.

Update on the Anti-Global Warming Effort from the National Center for Science Education (NCSE)

House Concurrent Resolution 1009, now under consideration in South Dakota's legislature, borrows language from antievolution legislation in encouraging teachers to present "a balanced and objective" presentation of global warming, and two NCSE staffers reacted- **Steven Newton** at the *Huffington Post* (February 25, 2010) and **Joshua Rosenau** at the Center for American Progress's *Science Progress* blog (February 26, 2010). As the *Rapid City Journal* (February 24, 2010) reported, "The resolution, which does not have the force of law, asks schools that present the threats of global warming to balance the information with the skeptical view of climate change as well."

Analyzing HCR 1009 as it was introduced, Newton commented on the resolution's "startling lack of knowledge about the particulars of climate science and how science works," observing that it refers to "a variety of climatological, meteorological, **astrological, thermological, cosmological**, and ecological dynamics" (!) "Do they think glaciers melt slower when Virgo is ascending?" Newton then went on to say "Even more disturbing than these errors is the underlying premise of HCR 1009: the assumption that political bodies, rather than scientists, should have the final say over scientific issues. ... This political interference in science education is a problem that extends beyond merely getting the facts wrong. Students deserve better than to be pawns of science denialists."

After discussing the history of creationist activism and its increasing affinity for global warming denial, Rosenau noted that HCR 1009 was revised by the Senate to remove most of the scientific errors - including the reference to astrology, prompting a quip that *the stars were not aligned for the puzzling references to “astrological” and “thermological” explanations for global warming*. Some legislator must have seen the irony of decrying politically biased science while seeking to legislate a scientific result. Rosenau warned, however, that "the Senate strengthened the final line, insisting now that teachers offer a 'balanced and objective' presentation of global warming. However reasonable such advice may be in the abstract, the effect of the law will be chilling to teachers on the ground. Science is not and should not be resolved through the legislative process, and the details of what teachers present as science should not be dictated by legislators with no experience as scientists or teachers."

Crystallography Education Workshop for School Teachers

The U.S. National Committee for Crystallography (USNC/Cr) is pleased to announce a crystallography education workshop that will be offered in conjunction with the ACA 2010 meeting in Chicago. This one-day workshop is designed as a continuing education opportunity for high school teachers, and will supply teachers with theoretical background material and hands-on activities will provide ideas for lesson designs and experiment plans that can be taken back to the classroom. Instructors for the workshop include **David Goodsell**, Scripps, **Andrzej Joachimiak**, Argonne, **Cora Lind**, U.Toledo, and **Claudia Rawn**, Oak Ridge National Lab. Other members of the USNC/Cr will be available for small group discussions and hands-on exercises.

The workshop will address the need to improve science education in K-12 and hopefully instill an appreciation for crystallography in students of all ages, including K-12. While it is not possible to teach in-depth theory and background of diffraction and crystallography in K-12, many crystallographic concepts could be introduced at an age-appropriate level. Early exposure to the field may encourage students to learn more about crystallography when they enroll at a university.

Basic concepts of atomic connectivity and ordering will be introduced through materials matching games. Materials will be roughly grouped into the categories *metals*, *ceramics*, and *polymers*. Differences in bonding, density and properties will be discussed. Models illustrating basic crystal packing and structures will be constructed using spheres or legos. The more disordered nature of polymers will be visualized with yarn. The seven crystal systems will be introduced using models or minerals depicting characteristic crystal habits for each system. Using legos, the analogy between unit cells as smallest repeat units and external crystal habits will be introduced.

Diffraction basics will be introduced using lasers and gratings. Trigonometric constructions can be used to illustrate Bragg's law, and to explain constructive and destructive interference based on a simple wave model. Diffraction patterns observed with gratings will be correlated to the seven crystal systems.

The importance of understanding atomic level structure and the three-dimensional packing of atoms and molecules will be demonstrated using models of biological macromolecules, including proteins, DNA, viruses, and small molecule drugs. Crystallographic databases like the protein data bank will be introduced, and tools for searching and exploring the available information will be presented. Three-dimensional images will show how important crystallography is to understanding protein function and to applying that understanding in, for example, drug design.

Teachers are encouraged to register for this one day workshop. There are no registration fees associated with attending. Materials for classroom activities will be provided.

Cora Lind

Editor's note: see page 34 about the 2010 ACA meeting in Chicago.

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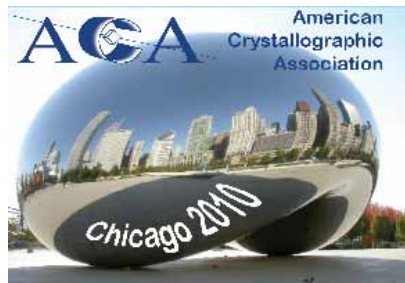
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ACA 2010 July 24 - 29

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Student and Young Scientist Travel Grant Applications: March 31, 2010

Advance Registration Deadline: May 31, 2010

Meeting website: <http://meeting2010.AmerCrystalAssn.org/>

Advance Hotel Registration for Conference Rates: June 24, 2010

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Submit abstracts; register; make hotel reservations; get Exhibit Show appl. ONLINE at www.AmerCrystAssn.org

EARLY BIRD SPECIAL

Director of Administrative Services Marcia Colquhoun has obtained an agreement from the Sheraton Chicago Hotel offering attendees an 'early bird special rate' for reservations made BEFORE APRIL 30. This would be \$189, a savings of \$40 per night (!). After April 30th, the rate increases to \$229 per night. The cost of the student rooms remains the same (\$127).



Local Chair

Bernie Santarsiero

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bds@uic.edu



Program Chair

Ross Angel

Virginia Tech
540 231 7974
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Workshops

PLATON

Organizer: Lee Daniels

Getting the Most out of the CCP4 Suite

Organizer: Charles Ballard

Crystallography: World of Wonders
(Note: this is an outreach workshop for Chicago Public Schools Science-Teachers, not ACA members.)

Organizers: Cora Lind, Christine Zardecki, David Goodsell, Claudia Rawn

GLOBAL Phasing Software Suite for Macromolecular Crystallography

Organizer: Gerard Bricogne

Sulfur-SAD Data Collection and Phasing Organizers: B.C. Wang, Albert Fu, John Rose

Award Symposia

Trublood Award in honor of Anthony Spek

Fankuchen Award in honor of David Watkin

*Margaret C. Etter Early Career Award**
in honor of Ray Triebel

* The Etter symposium is exclusively for young scientists. Young scientists are encouraged to submit their abstract, in any field of crystallography, directly to this symposium. Questions should be sent to the YS-SIG chair Ryan Jackson (ryjacks@gmail.com).

Plenary Lectures

Jim Ibers, and

Nobel Laureates Ada Yonath, Thomas Steitz and Venkatraman Ramakrishnan

Transactions Symposium

The First Element : in Memory of Bob Bau

Organizers: Christine Hoffman, Larry Falvello, Thomas Proffen, Nobuo Niimura

Photo of the Chicago skyline from the lakefront courtesy of Bernie Santarsiero.

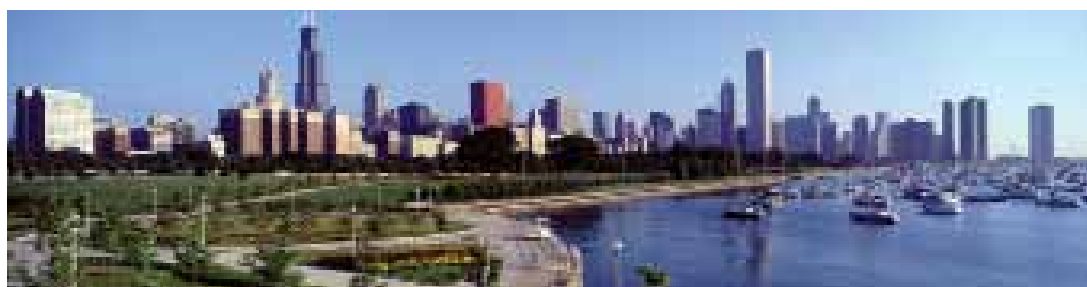


Exhibit Show 2010

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 on the evening of Saturday, July 24 in conjunction with the Opening Reception. The 2010 Show will run through Tuesday evening July 27th. The exhibit show will be closed on Wednesday July 28th but posters will remain accessible. The Advertising and Exhibits Div. of the AIP is managing the show. For further information contact Bob Finnegan, AIP, rfinneg@aip.org, tel 516-576-2433. Not-for-profits groups are eligible for a discounted booth fee of \$400 for one booth. Booth rental is \$1,400 for all others. ACA Corporate Members will receive 10% off one booth fee.

Not a member? Join now!



*Photo of the "BEAN" in Chicago's Millenium Park.
Courtesy of Bernie Santarsiero.*

Staying Green: We will once again be distributing the full set of abstracts only on CDs with a hardcopy Program Schedule. We will not have a new meeting bag so if you would like one you should remember to bring your favorite from an earlier meeting. These 'greening' measures have proven both popular and cost effective, and allow us to continue offering morning and afternoon coffee breaks as well as food at the opening reception and snacks at the poster sessions, all without a major increase in registration costs.

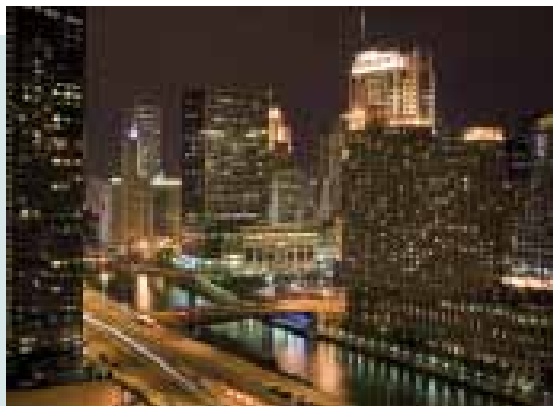
Financial support for young scientists will be available through the sponsorship of the IUCr and other sources. Applications for support should be made by the abstract deadline on the meeting web site.

The Organizing Committee will observe the basic policy of non-discrimination and affirms the right and freedom of scientists to associate in international scientific activity without regard to such factors as ethnic origin, religion, citizenship, language, political stance, gender, sex or age, in accordance with the Statutes of the International Union.



Scenic photos of the city from www.dreamstime.com/. At right, Summer Day in Chicago, © Dmitri Mihhailov/Dreamstime.com; below, River East, © Robert Wojtow / Dreamstime.com; at left, View from the Top, © Kenneth Sponsler / Dreamstime.com.

*Sunday morning, July 25th: The Bio-Mac SIG has organized **Lighting the Way**: a session (1.01) to commemorate the work and honor the memory of Louis Delbaere, a passionate researcher, mentor, and pioneer in the field of protein x-ray crystallography. – John Allingham will chair the session.*



MAY 2010

24-28 **ISC Granada 2010 2nd International School of Crystallization**, Hotel San Ant3n, Granada, Spain. **Juan Manuel Garcia-Ruiz, Director**. www.iscgranada.org/



25-29 **2010 Chemical Crystallography Workshop**, McMaster University, Hamilton, ON, Canada. www.chemistry.mcmaster.ca/facilities/mcmaster-analytical-x-ray-diffraction-facility-max/251.



JUNE 2010

3-13 **Structure and Function from Macromolecular Crystallography: Organization in Space and Time** Erice, Italy. **Directors: Tom Blundell and M. Armenia Carrondo**. www.crystalalice.org/erice2010/2010.htm.



6-11 **Gordon Research Conference in Crystal Engineering**, Waterville Valley Resort, Waterville Valley, NH. www.grc.org/programs.aspx?year=2010&program=crystaleng.

JULY 2010

18-23 **Gordon Research Conference in "Diffraction Methods in Structural Biology"** Bates College, Lewiston, Maine **Chair: Andrew Leslie, Vice-chair: Ana Gonzales**. www.grc.org/programs.aspx?year=2010&program=diffrac.

24-29 **ACA2010, Chicago, IL. Local chair: Bernie Santarsiero (bds@uic.edu); Program chair: Ross Angel (rangel@vt.edu)**. See pages 34-35.



AUGUST 2010

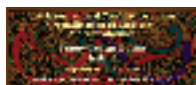
22-27 **XXIVth ICMRBS** (International Council on Magnetic Resonance in Biological Systems), Cairns, Australia. www.icmrbs.org.

29-2 **ECM26**, European Crystallographic Association Meeting in Darmstadt, Germany. www.ecm26.org/.



SEPTEMBER 2010

12-16 **13th ICCBM**, Crystallization Workshop, Trinity College, Dublin, Ireland. www.iccbm13.ie.



20-23 **XTOP2010, The International Conference on High-resolution X-ray Diffraction and Imaging**, University of Warwick, UK, www2.warwick.ac.uk/go/XTOP2010.



OCTOBER 2010

1-3 **AsCA2010**, Asian Crystallographic Association Meeting, Busan, Korea. www.asca2010.org.



NOVEMBER 2010

9-10 **APC2010, Advances in Protein Crystallography**, Florence, Italy. www.selectbiosciences.com/conferences/APC2010/ **Deadline for abstracts: 14 May 2010**. Register early and save.



MAY 2011

21-26 **ACA 2011**, Sheraton Hotel New Orleans, New Orleans, LA. **Program Chair: Chris Cahill; Local Chairs: Cheryl Klein-Stevens & Ed Stevens**.

AUGUST 2011

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



JULY 2012

28-2 **ACA2012**, Westin Boston Waterfront Hotel, Boston, MA.



Chicago lakefront. Courtesy of Bernie Santarsiero.

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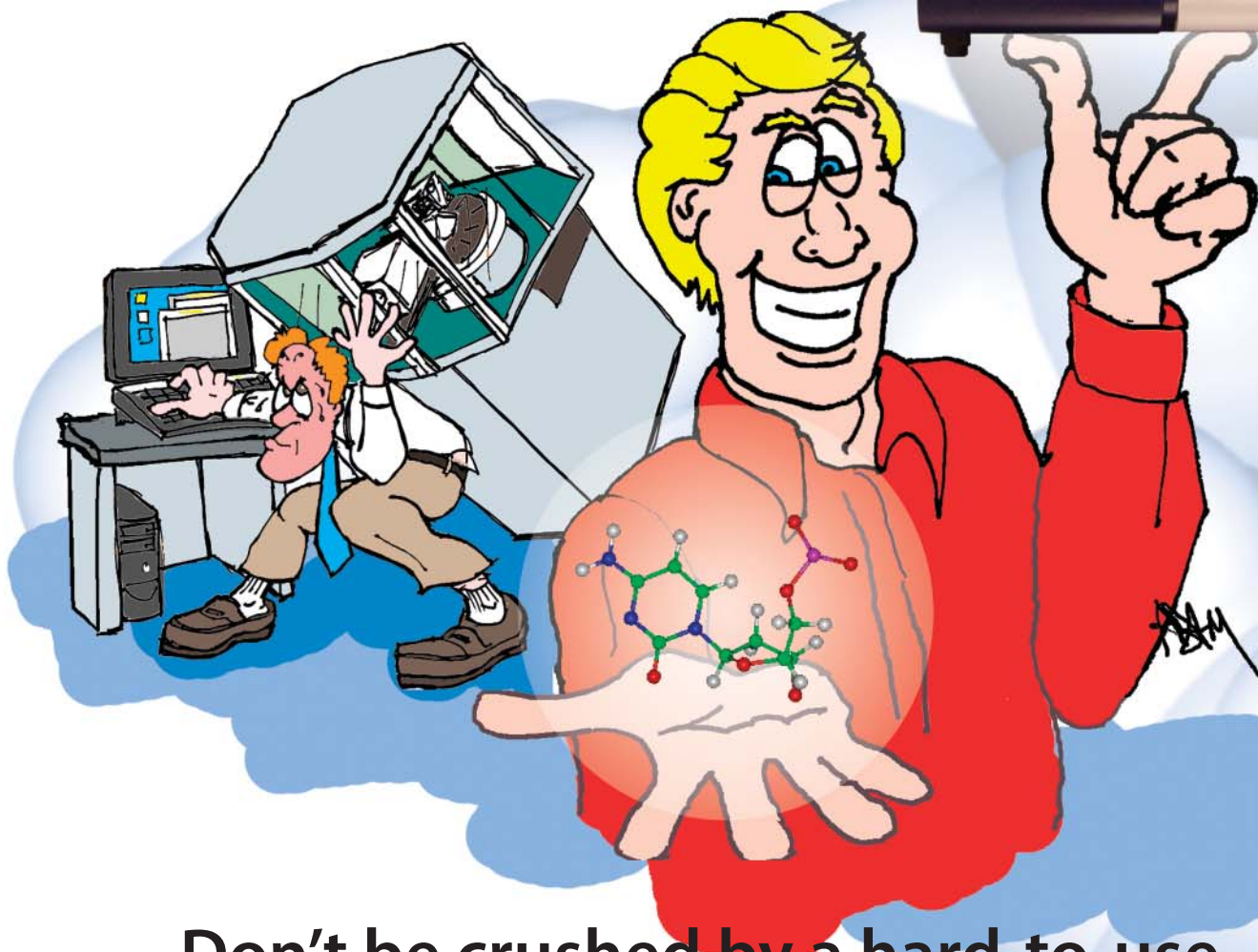
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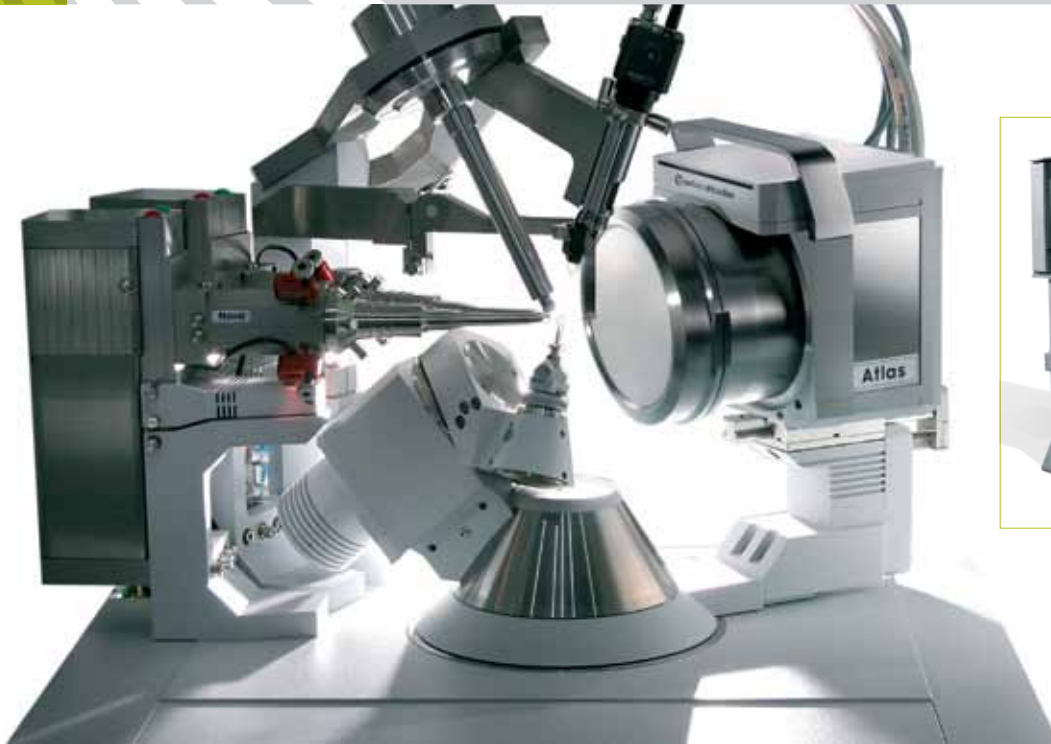


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