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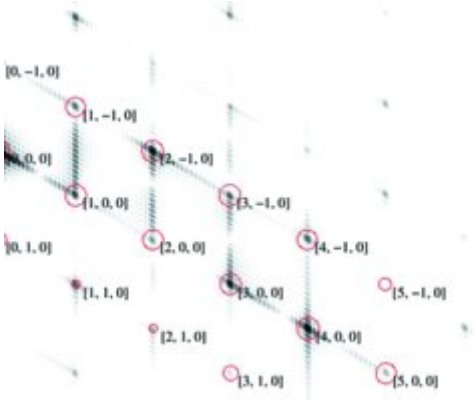
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IUCR JOURNALS NEWS

Structure-factor analysis of femtosecond microdiffraction patterns from protein nanocrystals

Acta Cryst. (2011). A67, 131–140 (doi.org/10.1107/S0108767310050981)



Simulated femtosecond microdiffraction pattern from membrane protein nanocrystal, showing 'shape-transform' fringes running between Bragg partial reflections. These are expected to provide new solutions to the phase problem [*Optics Express* (2011). **19**, 2866].

The invention of the pulsed hard X-ray laser is providing new opportunities for structural biology. Here Kirian and co-workers describe their 'Monte Carlo' data analysis method, developed for merging millions of 'partial' femtosecond snap-shot diffraction patterns from individual protein nanocrystals, running in a fine liquid jet in random orientations across the Linac Coherent Light Source at SLAC. This 'diffract-before-destroy' method is expected to be powerful for time-resolved crystallography, for proteins which don’t grow large crystals, and as a means to minimize radiation damage. Experimental results for this work (and for LCLS diffraction and imaging of a single virus) were published recently in *Nature* by Chapman *et al.* and by Siebert *et al.*

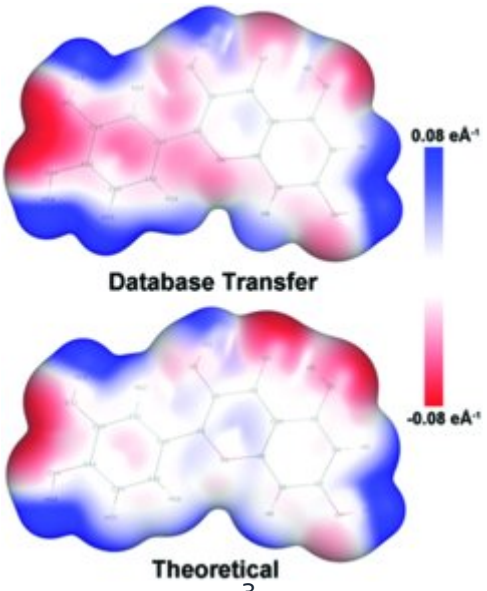
R. A. Kirian, T. A. White, J. M. Holton, H. N. Chapman, P. Fromme, A. Barty, L. Lomb, A. Aquila, F. R. N. C. Maia, A. V. Martin, R. Fromme, X. Wang, M. S. Hunter, K. E. Schmidt and J. C. H. Spence

See related article on Workshop on X-ray Lasers for Biology.

IUCR JOURNALS NEWS

Structural analysis and multipole modelling of quercetin monohydrate – a quantitative and comparative study

Acta Cryst. **(2011). B67, 63–78 (doi.org/10.1107/S0108768110041996)**



Electrostatic potential mapped on the 0.001 e bohr^{-3} isosurface of the electron density in the quercetin molecule.

The application of the aspherical structure factors computed from the extended experimental database of the electron-density parameters is presented. The multipolar charge density was transferred to the new crystal structure of quercetin monohydrate. The improvement of the geometrical parameters over the independent atom model was assessed with respect to the average neutron *X*–H distances. The resulting electron density was compared with the multipolar atom model obtained from the theoretical calculations. Comparison of these two models shows good correlation between electron-density distributions and derived quantities.

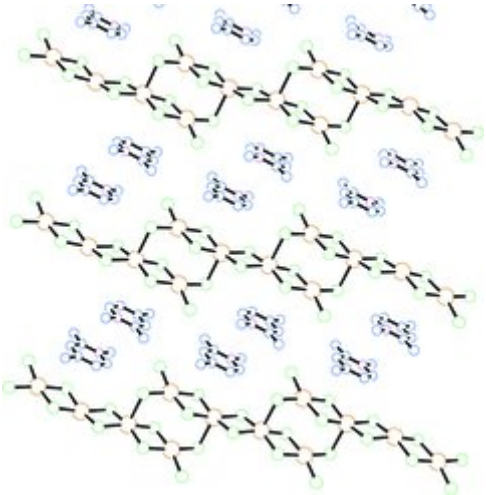
S. Domagala, P. Munshi, M. Ahmed, B. Guillot and C. Jelsch

IUCR JOURNALS NEWS

Nine compounds containing high-nuclearity [CunX2n+2]2- (n = 4, 5 or 7; X = Cl or Br) quasi-planar oligomers

Nine compounds containing high-nuclearity $[Cu_nX_{2n+2}]^{2-}$ (n = 4, 5 or 7; X = Cl or Br) quasi-planar oligomers

Acta Cryst. **(2011). C67, m22-m34 (doi.org/10.1107/S0108270110049024)**



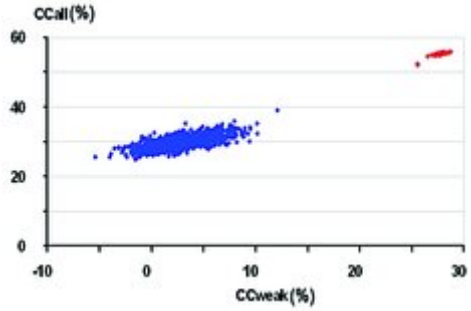
These structures almost double the number of known high nuclearity, quasi-planar $[Cu_nX_{2n+2}]^{2-}$ oligomers. Included is the first fully halogenated pentacopper complex, $(C_6H_7Cl)_2Cu_5Br_{12}$, now also the highest nuclearity oligomer with isolated stacking. All but one of the seven reported $A_2Cu_4X_{10}$ structures are derived from the parent CuX_2 layer structure in which organic monocation pairs replace $[Cu_nX_{2n-2}]^{2+}$ fragments. Differences in oligomer stacking patterns in chemically similar di- and trimethylpyridinium salts illustrate the subtle interplay of competing forces present in these structures.

A. Kelley, S. Akkina, G. K. Devarapally, S. Nalla, D. Pasam, S. Madhabushi and M. R. Bond

IUCR JOURNALS NEWS

Multi-crystal anomalous diffraction for low-resolution macromolecular phasing

Acta Cryst. (2011). D67, 45-59 (doi.org/10.1107/S0907444910046573)



SHELXD correlation coefficients (CCall *vs.* CCweak) from 1000 Se substructure tries. Successful solutions (45 in red) from multi-crystal data (8 data sets here) are well separated from random solutions (rest in blue). Multi-crystal data supported structure solution whereas all single-crystal data failed.

Phase evaluations from MAD and SAD diffraction data typically require the acquisition and analysis of weak anomalous signals. Here, limitations on data accuracy, largely due to radiation damage, are overcome by carefully merging the data from several crystals. The method was tested in selenomethionyl SAD phasing of a relatively large structure (1456 ordered residues) at relatively low resolution (3.5 Å). The results show that data from multiple crystals robustly support structure determination where attempts from single-crystal data sets fail.

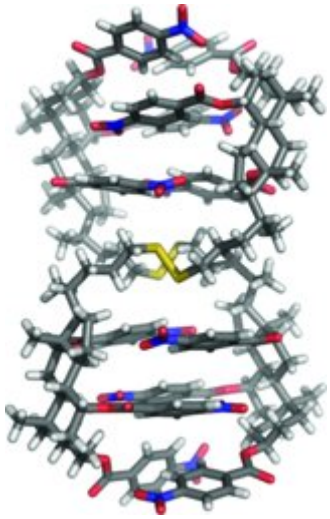
Q. Liu, Z. Zhang and W. A. Hendrickson

IUCR JOURNALS NEWS

Bis[3α,7α,12α-tris(4-nitrobenzoyloxy)-5β-cholan-24-yl] disulfide-ethyl acetate-n-hexane (4/4/1)

Bis[3α,7α,12α-tris(4-nitrobenzoyloxy)-5β-cholan-24-yl] disulfide-ethyl acetate-*n*-hexane (4/4/1)

Acta Cryst. (2011). E67, o74-o75 (doi.org/10.1107/S1600536810050385)



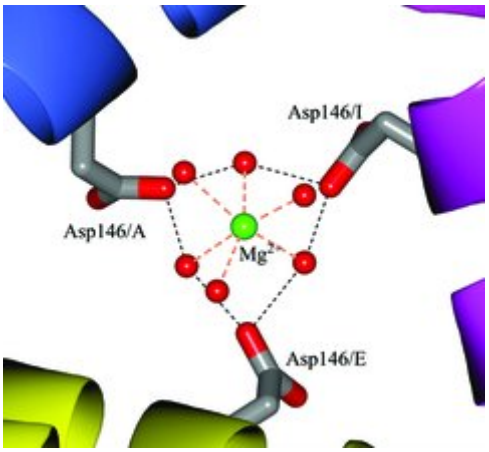
The absolute configuration of a *per*-4-nitrobenzoyl bile acid derivative has been established with diffraction data collected with high-energy synchrotron radiation, despite a very small anomalous scattering effect from the sulfur atoms. The two symmetry-independent disulfide molecules in the asymmetric unit, with their centrally placed disulfide bridges, exhibit different helicity and intertwine to form a tight dimer having a double-helix-type structure.

K. Brzezinski, A. M. Tomkiel, Z. Lotowski, J. Morzycki and Z. Dauter

IUCR JOURNALS NEWS

Structures of the SEp22 dodecamer, a Dps-like protein from Salmonella enterica subsp. enterica serovar Enteritidis

Acta Cryst. (2011). F67, 17-22 (doi.org/10.1107/S1744309110043113)



An Mg^{2+} ion at the entrance of the Asp channel. The threefold axis of the octahedrally hydrated Mg^{2+} ion is almost coincident with the threefold axis at the Asp channel.

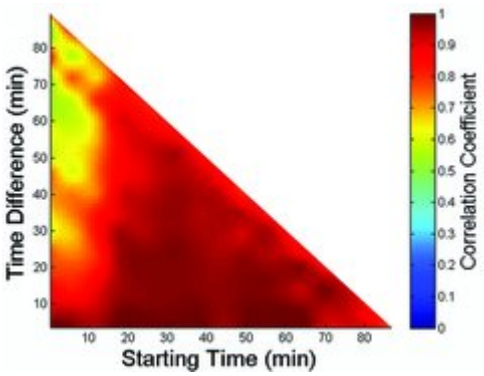
SEp22 from *Salmonella enterica* prevents the production of the reactive oxygen species (ROS) by sequestering Fe^{II} ions into the cavity of the dodecameric shell with 23 symmetry. The anti-ROS activity is crucial for the survival of *S. enterica* infection in humans. Structures of SEp22 dodecamers revealed the distorted octahedral geometry of Fe^{II} ions at the ferroxidase centers in high detail. Hydrated Mg^{2+} ions were located near the entrances of the Asp channels, which suggests how Fe^{II} ions pass through the channels and flow into the cavity.

T. Miyamoto, Y. Asahina, S. Miyazaki, H. Shimizu, U. Ohto, S. Noguchi and Y. Satow

IUCR JOURNALS NEWS

NIST and Argonne researchers develop new USAXS-XPCS tool at APS

J. Appl. Cryst. (2011). 44, 200-212 (doi.org/10.1107/S0021889810053446)



Correlation coefficient map quantitatively describes how 1D USAXS–XPCS scans from an advanced dental composite sample change during slow cooling from an annealing temperature of 388 K.

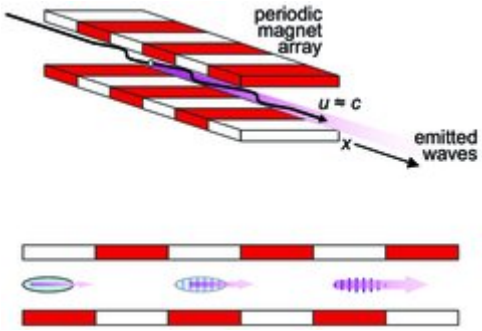
Taking advantage of 2D-collimated Bonse-Hart-type crystal optics, NIST and Argonne researchers have developed a new ultra-small-angle X-ray scattering (USAXS)-based X-ray photon correlation spectroscopy (XPCS) measurement technique at the Advanced Photon Source. This technique probes low-frequency equilibrium and nonequilibrium dynamics in optically opaque materials containing prominent features that scatter in a q range between those of dynamical light scattering and conventional XPCS. To date, USAXS-XPCS has been successfully applied to study colloidal suspensions and incipient structural changes in advanced dental composites.

F. Zhang, A. J. Allen, L. E. Levine, J. Ilavsky, G. G. Long and A. R. Sandy

IUCR JOURNALS NEWS

A simplified description of X-ray free-electron lasers

J. Synchrotron Rad. (2011). 18, 101-108 (doi.org/10.1107/S090904951004896X)



Can the working mechanism of free-electron lasers (FELs) be understood with basic arguments and simple mathematics? The question is relevant because of the recent commissioning of the first X-ray FEL and the fast progress in this field. The answer is positive: we derive the basic FEL equations - including gain and saturation properties - with elementary arguments. We explain, in particular, the counterintuitive fact that electron microbunching with the very short periodicity required for X-rays is much more difficult than for long-periodicity infrared FELs.

G. Margaritondo and P. Rebernik Ribic

MEETING REPORT

Methods of high-pressure single-crystal X-ray diffraction

Darmstadt, Germany, September 2010



Participants at the High-pressure Single-crystal X-ray Diffraction Workshop

Single-crystal diffraction provides the most accurate structural data on the compression of crystalline solids. The methods for high-pressure diffraction developed over the last 3 decades are mature and easy to use in both the laboratory and at synchrotron sources, but are not well known throughout the crystallographic community. In summer 2008 a group of high-pressure crystallographers from Europe and the USA met in Padova, Italy to discuss how to promote high-pressure single-crystal methods. On the occasion of a second meeting a year later in Copenhagen, Denmark, we agreed to meet on a regular basis and decided to offer an open workshop in association with the 26th European Crystallography Meeting held in Darmstadt, Germany (September 3-4, 2010).

The workshop, hosted on the campus of TU Darmstadt and organised by R. Miletich, A. Grzechnik and H. Ehrenberg, attracted 50 participants. A general overview of the entire workflow for a high-pressure experiment, and the additional challenges to be overcome compared to ambient-pressure measurements, was given by R. Angel. The first morning featured presentations by R. Miletich, C. Hejny and B. Periotto on diamond cells, how to load them, and then perform the data collections on the diffractometer. In the afternoon M. Alvaro reviewed software for data integration, before the workshop split into separate sections in which R. Angel, D. Gatta, T. Balic-Zunic and A. Grzechnik showed how to integrate high-pressure data with several commercial and freeware software packages. The second day was devoted to the separate subjects of equations of state (T. Boffa-Ballaran) and intensity data reduction and refinement (K. Friese, R. Angel), followed by structure validation and structure analysis (T. Balic-Zunic, K. Friese). The majority of the second afternoon was devoted to discussing detailed data issues with the participants, along with a demonstration by the research group of R. Miletich of preparing and loading diamond-anvil cells. The workshop was concluded with a short presentation by H. Ahsbahs on the design of a new generation of diamond cells, and a review of synchrotron beamlines available for single-crystal diffraction.

The workshop participants included researchers from many fields (chemistry, physics, geology, and materials science) at all levels of experience with high-pressure single-crystal X-ray diffraction. More than one third of the participants were PhD students. Comments on the presentations are available at www.crystal.vt.edu/crystal/hpworkshop.html.

We would like to acknowledge the generous support of Agilent Technologies (formerly Oxford Diffraction), Stoe & Cie GmbH, Incoatec GmbH and Scimed GmbH that allowed us to offer travel grants to some student participants, and to cover catering costs.

Ross Angel and Andrzej Grzechnik

MEETING REPORT

COSPAR 38th Assembly

Bremen, Germany, July 2010, http://cosparhq.cnes.fr/



From the right: Gerda Hornick (Germany), Ruedi von Steiger, Chair of COSPAR Scientific Commission D, Hannu Koskinen, Finnish representative, Werner Schmutz, Swiss representative, and Hanna Dabkowska, IUCr representative to COSPAR.

COSPAR was established in 1958 by the International Council of Scientific Unions (now the International Council for Science), with the main objective of promoting international collaboration on various levels of research in space. Emphasis has always been on the exchange of results, information and opinions as the development of world standards for the space environment, and its protection, requires cooperation at both national and international levels. With this in mind it should be stressed that IUCr representation at the COSPAR General Assembly increases our visibility as well as providing us an opportunity to monitor emerging trends and to see future changes in this global area of research and to position our own approach accordingly.

The majority of COSPAR activities are devoted to space topics (such as astronomy, space travel and exploration or climate research). The most interesting for the IUCr division of COSPAR is the Scientific Commission on Materials Science in Space (MSS, Commission G) which deals with scientific experiments on materials performed in reduced gravity environments. Different experiments on the growth of crystals and dendrites in microgravity have been part of these programs. Currently the stress is more on combustion and biotechnology. The MSS Commission reviews fundamental theoretical and experimental approaches, helping to understand emerging fields and recommends promising avenues for future research. It also coordinates the exchange of information on scientific subjects. The MSS Commission is chaired by V. Shevtsova (Belgium), with vice-chairs being S. Amiroudine (France) and S. Yoda (Japan). The presentations dealt mostly with microgravity experiments conducted in drop towers, parabolic flights, photon satellites and on the International Space Station. Four half-day symposia reported on effects of gravity on physico-chemical processes. The local Organizing Committee, headed by Hans J. Rath, did an excellent job. The official statistics are as follows: final number of participants: 4836, which

included 586 students and 1000 local visitors. Overall, 64 countries were represented and 4503 abstracts were received.

Outreach events included: a public lecture by the scientific director of the MPI for Plasma Physics, providing insight into modern astrophysical research on cosmological objects and phenomena; a Mars exhibition at the Bremen town hall; an art exhibition: Genesis and Dreams; and Bremen’s 'Children reach for the stars' exhibition. The financial situation of COSPAR is satisfactory and recommendations were made to hold a multidisciplinary general symposium every other year starting in July 2013. The symposium will focus on training and education with special activities dedicated to teachers, students, young professionals and the general public.

'Advances in Space Research' (ASR), an official journal of COSPAR, covers all areas of space research including – but not limited to – space studies of the earth’s surface, meteorology, climate, fundamental physics in space, materials physics in space, space debris, weather and earth observation of space phenomena. The journal home page is http://ees.elsevier.com/asr.

The COSPAR President for the period 2010-2014 is G. Bignami (Italy) and the Vice-Presidents are R. Lin (USA) and J. Wu (China). Members of the Bureau are: I. S. Batista (Brazil), K.-H. Glassmeier (Germany), A. Jayaraman (India), S. Sasaki (Japan), J.-P. St.-Maurice (Canada), and L. Zelenyi (Russia).

The next COSPAR Assembly will be held in Mysore, India, July 14-22, 2012, whereas the following one (2014) is planned for Moscow, Russia.

Hanna Dabkowska

MEETING REPORT

19th Slovenian-Croatian Meeting

Strunjan, Slovenia, June 2010, http://abra.fkkt.uni-lj.si/fn01leban/slkr19/



Two of the meeting organizers, I. Leban and S. Popović.



Plenary lecturers (from left) Z. Dauter, A. Višnjevac, I. Arčon and T. Spek.

The meeting was held in Strunjan, home to one of the most northern salt works on the Mediterranean that supplied the salt (NaCl) for the Venetian republic between 15th and 17th century. The four plenary lectures were: 'Why Crystal Structure Validation?' (A. L. Spek, Utrecht, The Netherlands), 'Nobel Prizes Related to Crystallography' (Z. Dauter, Argonne, USA), 'Single-Crystal X-ray Crystallography as a Method of Choice in Biomimetic Modelling (A. Višnjevac, Zagreb, Croatia), and 'Analysis of Ordered and Disordered Materials with X-ray Absorption Spectroscopy' (I. Arčon, Nova Gorica, Slovenia).

Over 60 participants from seven countries presented forty oral contributions on crystallography of macromolecules, organic, organometallic and inorganic compounds, metallurgy, solid solutions, small-angle scattering, synergy of diffraction and other methods, structure and properties, and nanocrystallography. There were interesting talks on Friedel opposites, jumping crystals (very easy to lose), explosive compounds, protein aggregation, solar cells, complexes of copper paddle–wheel building blocks and potential anticancer agents. We learned how to use X-ray absorption spectroscopy to study order-disorder and how to locate selenium atoms using just a few intensities.

The social aspect of the meeting included a visit to the Salt Works to see crystallization in action at the macro level, a wine cellar tour, and the conference dinner. We wish to thank the sponsors, Slovenian Research Agency and the Faculty of Chemistry and Chemical Technology, U. of Ljubljana whose financial support allowed us to organize and hold this meeting without registration fees.

The Croatian Crystallographic Association and the Slovenian Crystallographic Society cordially invite you to attend the 20th CRO-SLO Meeting which will be held June 15-19, 2012, on the Island of Krk, in the north Adriatic Sea. For more information contact S. Popović, spopovic@phy.hr, or I. Leban, ivan.leban@fkkt.uni-lj.si.

I. Leban and S. Popović

MEETING REPORT

Spreading the word: An intensive Course on Biological and Chemical crystallography

Manchester, January 2011www.chemistry.manchester.ac.uk/aboutus/events/crystallography/index.html





From left to right going clockwise: Chris Muryn, Dora Gomez, Stefan Kofler, Marco Martinez, Kaenket Surasak, Nerea Gallastegui de la Rosa, Madeleine Helliwell, John Helliwell, Simon Tanley, Jim Raftery and Robin Pritchard.

These are challenging times for crystallographic education as undergraduate courses are constantly under pressure to streamline content. Crystallographic results that make the headlines are still often included in such courses, along with the core basics of crystallography, and sometimes the latest methods research such as at synchrotrons or FEL X-ray or neutron sources.

After graduation new PhDs and postdocs, in addition to on-the-job training , can go to annual or biannual courses or workshops run by our various crystallographic associations, usually of 1 to 2 weeks duration, and mainly focused on a single discipline such as macromolecular or chemical crystallography. Excellently run and productive workshops are also run at the synchrotron and/or neutron facilities. There are also exemplar institutions like Birkbeck College, University of London, that have a long tradition in crystallographic education and now have online courses as well.

Can we do more? I know that the ECA is marshalling efforts in Europe towards a masters in crystallography. and Massimo Nespolo (Nancy) has taken the lead in applying for European funds to support this project. A notable national initiative, that has been run for several years, is the Spanish masters in crystallography and crystal growth led by Juan Ma Garcia-Ruiz.

At the University of Manchester, encouraged by an across-campus course of lectures to PhDs on macromolecular crystallography that I gave during my sabbatical 3 years ago, and by the head of our school, Christopher Whitehead, as well as helpful input from our NMR colleague Vasudevan Ramesh, we launched a 2-day intensive school for biological and chemical crystallography. Our vision for the course is to emphasise the unity of crystallography across these two disciplines and thus reverse the trend of

separate courses. Our course also comprised both lectures and practicals, including using the latest software and CCD diffractometers. The practicals used the School of Chemistry PC Cluster and our Bruker Apex CCD diffractometer. Tutorials were given on publishing macromolecular papers at resolutions of 1.4 Å and 3.2 Å and at 30 Å by combining EM and SAXS data and a chemical crystal structure at 0.8 Å. A tutorial demo on Laue diffraction was also provided using the Daresbury Laue software package. The combined use of neutrons and X-rays featured prominently in a core lecture, which underpinned the subsequent chemical and biological crystallography. There was also a lecture each on powder diffraction and on biological and chemical databases (PDB, MESPEUS and CSD). Practicals were available on the use of small molecule graphics, twinning, structure solving, refinement software and CSD database usage, as well as macromolecular isomorphous replacement and metal atom occupancy refinement. The course lecturers and tutors/demonstrators were John Helliwell, Madeleine Helliwell, Robin Pritchard, Chris Muryn and James Raftery. The weblink is http://www.chemistry.manchester.ac.uk/aboutus/events/crystallography/index.html

A Course dinner was held at our University's premier dining place, Christie's Bistro, located in the old library (pictured). A quiz on crystallography kept the brain cells whirring throughout the evening, especially with the prize being a two volume set of IUCr's *Crystallography Across the Sciences*.

Did we succeed? We chose our course dates to be just before our NMR 2-day workshop, mentioned above, and to be a few days after the 2-day CCP4 annual study weekend (this year held at Warwick University, about 90 minutes by train from Manchester). The participants in our course included one person who also attended the NMR workshop as well as another who had attended CCP4. The countries of origin of the participants were Austria, Mexico, Spain/Germany, Thailand, Venezuela and UK. One participant took in the Manchester United *versus* Liverpool match during the weekend but we cannot guarantee such a fixture every year! The feedback from participants, written and verbal, was very positive. One person stayed a third day to do more work on the practicals, a feature we plan to add to next year's course to be held January 10–12, 2012. The NMR course will be held January 12-13, 2012.

How can we improve the course? We started advertising the course too late. We posted notices on the CCP4 and X-rayMan Bulletin Boards and sent emails to our contacts in industry and other collaborators at the same time. We have started much earlier this second time around and posters will also be put on display at BCA Keele and IUCr Madrid. Could we reduce the fees? These were approx £500 for an academic and nearly £1000 for industry. These are set by the continuing professional development policy of the University, and ours were basically the same as the NMR Workshop. Are the fees justifiable? With our staff time, including secretarial and admin as well as IT support, as well as the use of equipment including the computer cluster and an X-ray diffractometer, and lecture rooms, I would imagine the fees are not far out. That's just what it costs!

Acknowledgements are due to CCP4, *COOT*, *OLEX*, *SHELXTL* and *WinGx* whereby permission for free download and access to their software was readily given. Bruker kindly sponsored a PhD student bursary and Mitegen donated crystal mounting and manipulation packs, one for each participant. The IUCr donated the two *Crystallography Across the Sciences* books. We are very grateful for their help and generosity. We are also grateful to the PDB and CSD for their databases curation, which we all appreciate (and also to CSD for their *Mercury* software).

John R. Helliwell

MEETING REPORT

Minutes of the AsCA Council Meeting 2010

Busan, South Korea, November, 2010. www.asiancrysassn.org



The IUCr Executive Committee (EC) held its annual meeting in Busan, South Korea, prior to AsCA 2010. Sine Larsen presented a report from the EC outlining the history and management of the regional associates to the IUCr (ACA, ECA, and AsCA). She discussed the actions taken at the EC meeting, and a proposal for an International Year of Crystallography (IYCr) in 2013. She also presented an update on the IUCr Congress and General Assembly to be held in Madrid in August 2011. The IUCr is currently seeking support from the UN (through UNESCO) for the IYCr. The IYCr will involve the development of a website, educational materials, exhibits and activities, and the participation of the Regional Affiliates, National Adhering bodies, IUCr Commissions and crystallographic resources including synchrotron and neutron radiation centers and crystallographic databases. An open competition will be announced shortly for the design of an official logo for the IYCr.

Organizing chair Se Won Suh outlined the statistics of AsCA 2010. There were 415 presentations (83 oral and 332 poster). The distribution of presentations was: 155 biological, 156 non-biological, 90 technology, and 7 others. Attendance was the highest yet for an AsCA meeting, and the ratio of students to full registrants was very high (approximately 2:3). A week prior to the meeting 626 had registered, of which 229 (36.6%) were Korean and 235 were students. Exhibitors had taken 31 booths. Nine of 58 applications for travel support were honored. Eight of 38 rising star applications were awarded, and five poster prizes were awarded (IUCr, AsCA and RCSB Protein Data Bank). Jenny Martin served as program chair.

Proposals for future AsCA meetings

Alice Vrielink presented a proposal from Adelaide, Australia, to host a joint AsCA/SCANZ conference and Bragg centenary celebration in 2012 to mark the centenary of the presentation of Lawrence Bragg’s paper defining Bragg’s equation to the Cambridge Philosophical Society. The dates for the meeting are proposed for December 2-6. The Bragg symposium will be a public forum with speakers including descendants of Lawrence Bragg, his former students and high profile scientists. The conference will be held in the Adelaide convention centre. Direct flights are possible from many Asian cities. The IUCr President noted that the meeting would be perfectly timed as a curtain raiser for the 2013 IYCr.

AsCA President Mitchell Guss has received a formal expression of interest from Singapore to hold the 2016 meeting. However, it was noted that if Iran is soon to be included within the AsCA region, a future committee may wish to solicit a bid from that country.

Election of new executive officers for the 2010-2013 term: President, Se Won Suh (Korea); Vice-President, Pinak Chakrabarti (India); Secretary-Treasurer, Alice Vrielink (Australia).

Se Won Suh

MEETING REPORT

First North African Crystallographic Conference

Casablanca, Morocco, November 2010. http://nacc1.univ.ma/



Opening ceremony of First North African Crystallographic Conference. Left to right: Abdelmalek Thalal, President, Moroccan Association of Crystallography; Santiago García-Granda, President, ECA; Sine Larsen, President, IUCr; Abdelaziz El Jazouli, Chair, NACC1 Organizing Committee.



Participants at NACC1.

On November 23–26, 2010, over 120 scientists gathered in Casablanca, Morocco, for the First North African Crystallographic Conference (NACC1). The Conference attracted a world-wide audience, with researchers coming from Algeria, Australia, Denmark, Egypt, Ethiopia, France, Germany, India, Iran, Iraq, Japan, Jordan, Malaysia, Morocco, Netherlands, Nigeria, Poland, Portugal, Russia, Saudi Arabia, Senegal, Spain, Sudan, Switzerland, Tunisia, UK, and USA.

The Conference was organized by Abdelaziz El Jazouli, Chair, along with Rahma Adhiri, Said Benmokhtar, Saida Krimi, Mouna Lamdaouar, Mohamed Mousseted, and Abdelmalek Thalal, Driss Zakaria, Abdella Boukhris, Lahcen El Anmari, and Mohamed El Azhari, all members of the Executive Committee of the Moroccan Association of Crystallography. The aim of this First NACC was to contribute to the development of crystallography in North Africa.

The conference was attended by Sine Larsen, President of the International Union of Crystallography (IUCr); Judith Kelly, President of the American Crystallographic Association (ACA); Mitchell Guss, Past President of the Asian Crystallographic Association (AsCA); and Santiago García-Granda, President of the European Crystallographic Association (ECA). These representatives of international crystallographic associations expressed their great satisfaction with the scope and scientific aspects of the meeting, as well as its organization, and the commitment of their associations to the development of crystallography in Africa.

The topics presented were as diverse as the countries of the attendees. There was a major focus on the crystal structures of materials, nanomaterials and minerals, as well as sessions on fundamentals of crystallography, instrumentation and synchrotron resources, biological macromolecular crystallography, and crystallographic education. Accompanying over forty oral presentations were more than one hundred posters, the majority presented by student attendees. This international assembly provided a

wonderful opportunity for broad-ranging discussions among researchers interested in the full gamut of diffraction science. People were able to share their results and explore possibilities for new collaborations. Topping off the scientific program was a tour of the fascinating city of Casablanca and a closing dinner at the Hotel Suisse, just off the Cornishe. Five poster prizes were awarded to students as the finale of the evening. The winners were: Youssef Aboufadil (Marrakech, Morocco), Meriem Benslimane (Canstantine, Algeria), Saida Kaoua (Casablanca, Morocco), Anissa Mansour (Monastir, Tunisia), and Laura Menéndez Taboaba (Oviedo, Spain).

The Conference enjoyed broad financial sponsorship from the International Union of Crystallography, the European Crystallographic Association, le Centre National de la Recherche Scientifique et Technique, Université Hassan II Mohammedia, Faculté des Science Ben M'Sik-Casablanca, Cambridge Crystallographic Data Center, Springer, Agilent Technologies, Bruker, Radaco, Rigaku, PANalytical, XENOCX, and Groupement d'Assurance du Superior_GASUP–MAMDA–MCMA.

Future NACC meetings are planned for 2011 in Algeria and for 2012 in Tunisia.

In parallel with NACC1, the second edition of a series of meetings titled 'Materials for Energy, Health and Environment: Research and Education - MEHERE' was held. MEHERE-2 was co-organized by Abdelaziz El Jazouli, from the University Hassan II Mohammedia-Casablanca; Abdou Lachgar, from Wake Forest University, USA; Mohamed Eddaoudi, from the University of South Florida and King Abdullah University of Science and Technology, Saudi Arabia; and Santiago García-Granda from the University of Oviedo, Spain. The meeting was sponsored by the CNRST and by the European Office of Aerospace Research and Development (EOARD). The main motivation for the organization of the MEHERE series of meetings is to bring together academic and industrial researchers and experts from Morocco, the European Union, and the United States of America to discuss recent advances in research and education related to materials with potential applications in the fields of energy, environment, and health. At the end of the MEHERE-2 meeting, the participants agreed to create a Research and Education Network on Materials.

Judith Kelly

MEETING REPORT

International Congress on Nanotechnology and Research Infrastructures

Barcelona, Spain, May 2010. http://www.gennesys2010.eu



'Future Challenges in Nanomaterials Design'. From left to right: H. Hahn, N. Casañ, P. Ordejón, C. Miravitlles, W. Kaysser, L. Malier, J. Samitier.

The Congress was organized under the Spanish EC Presidency, by PRUAB (UAB Research Park, Barcelona, Spain, http://parc.uab.cat); DESY (Deutsches Elektronen-Synchrotron, Hamburg, Germany, www.desy.de), ICMAB (Institut de Ciència de Materials de Barcelona del Consejo Superior de Investigaciones Científicas (CSIC), www.icmab.es); and INL (International Iberian Nanotechnology Laboratory, Braga, Portugal, http://inl.int). Attendees included representatives from the US National Science Foundation (NSF), the US Dept of Energy (DOE), the European Commission, research directors from major European research centres, and representatives from the chemicals industry, car manufacturers and semiconductor developers.

The starting point of the congress was the White Paper[1], which addresses the grand challenges of modern science and technology and emphasizes potential solutions based on the development of advanced nanomaterials with novel properties and the role of modern research infrastructures for the fine analysis of matter. The congress was officially opened by Spanish authorities, A. Mas-Colell (General Secretary of the European Research Council, ERC), who gave an overview of the ERC, and H. Dosch (Director General of DESY and GENNESYS Chair), who set the framework for the discussion of the grand challenges in the fields of energy and environment, health, sustainable transport, and information and communications technologies. Dosch stressed the important role that nanotechnology can play in facing these challenges and the need for coordinated efficient use of large research infrastructures such as neutron and synchrotron light sources.

At a session on 'Nanotechnology and Research Infrastructures - European and Global Challenges' chaired by R. Pascual, Chairman of the executive commission of the ALBA Synchrotron, keynote speaker C. Marrett, Deputy Director of the NSF, emphasized the resonance between the NNI (National Nanotechnology Initiative) in the US and the GENNESYS initiative in Europe. M. Takamura described research infrastructures and nanotechnology plans in Japan. I. Mattaj, Director General of EMBL, identified the challenges in nanosciences including securing financial support for infrastructures, and presented examples of relevant work at the EMBL. R. Batterham, Chair of the International Energy Agency (IEA) Expert Group on Science for Energy and President of the Australian Academy of Technological Sciences and Engineering, concluded that 'much more science for energy is needed to face future challenges', and H. Pero, Director of directorate B of the European Commission, discussed how to integrate research in Europe in a consistent manner.

In a session on 'Future Challenges in Nanomaterials Design', M. Roco, NSF, described examples of nanotechnology. P. Fratzl (Max-Planck Inst. of Colloids and Interfaces), G. Brasseur (Climate Research Center, Germany), E. Issacs (Argonne National Lab.), W. Kaysser (GKSS-Forschungszentrum), L. Malier (LETI Inst., Grenoble), and J. Samitier (Inst. for Bioengineering of Catalonia IBEC) described applications of nanotechnologies. Finally, H. Hahn (Director of the Inst. of Nanotechnology, KIT), N. Casañ (Inst. of Materials Sciences, Barcelona), and P. Ordejón (Centre of Research in 'Nanociencia y Nanotecnología') presented new strategies for nanomaterials design.

In a session on 'Advanced Photon and Neutron sources and Laser Research Infrastructures', M. van der Rest, SOLEIL, delivered an overview of the last technical advances in analytical facilities. H. Ohno described both the newly constructed beam lines and the status of the new XFEL facility at Spring-8. M. Gibson, Director of the Advanced Photon Source, discussed the need to study materials under real conditions in real time. J. L. Martinez Peña, Director of Inst. Laue-Langevin (ILL) in Grenoble, noted that the ILL and the ESRF share the vision of providing opportunities for cutting-edge research on the structure and dynamics of matter, either with neutrons or X-Rays. C. Vettier presented exciting experimental prospects for the future European Spallation Source in Sweden, and M. Altarelli, Managing Director of the European XFEL, emphasized that X-Ray Free-Electron Lasers have about 8 orders of magnitude more brilliant light than synchrotron sources with ultrashort pulses (<1 ps).

The next two sessions and the final session covered 'Industry Challenges in the World of Open Innovation' (chair, W. Riess, IBM, Zurich) and 'Nanotechnology: Societal Challenges' (chair, J. Chevrier, Grenoble Universities Consortium), and 'European and International Needs' and 'Towards a European Action Plan' were panel discussions directed by F. Fedi and J. M. Labastida, with panelists C. Rizzuto (ESFRI and ELETTRA), C. Tokamanis (EC), and M. Van Rossum (IMEC, Belgium).

The GENNESYS International Congress in Barcelona reemphasized key barriers to meeting future challenges in Europe.

C. Miravitlles, H. Dosch, J. Marquet and Jose Rivas

(1) GENNESYS White Book. Editors: H. Dosch, M. H. Van de Voorde. Max-Planck Institute for Metals Research. ISBN: 978-3-00-027338-4

MEETING REPORT

Workshop on X-ray lasers for Biology

Menlo Park, CA, USA, January 2011



John Spence, Uwe Weierstall, Rick Kirian, Petra Fromme, Bob Schoeman and Lukas Lomb prepare nanocrystals for the liquid jet injector.



John Spence, Henry Chapman, Inger Andersson, and Janos Hajdu, delighted and amazed to find that destructive readout crystallography actually works!



The control room at LCLS on Dec 13, 2009, as the first patterns arrive on the big screens from Photosystem I nanocrystals.

In mid-2009 the world's first hard X-ray laser, the Linac Coherent Light Source (LCLS), became operational at SLAC near Stanford, CA, USA. Later that year it was first applied to biological samples by a large collaboration between Heidelburg MPI, DESY (Hamburg), Arizona State University, Uppsala University, SLAC, LLNL, LBNL, and others. At that time the LCLS produced about 1E12 photons in each 70 femtosecond pulse, at 60 Hz and 1.8 kV with a 7 micron diameter beam. The group was thus able to record and read out snapshot diffraction patterns at 60 Hz using the fast 1K×1K detector at 8.5 Å resolution, from both single viruses and protein nanocrystals, producing terabytes of data and millions of diffraction patterns. The samples were sprayed across the X-ray beam in a liquid column, single-file synchronized droplet, or gas jet, and so can be fed from a liquid phase. The results depend on the fact that such a brief, intense X-ray pulse terminates before the samples are vaporized, giving excellent diffraction patterns by a 'diffract-before-destroy' mechanism. The results were first published in *Nature* in two papers on February 3, 2011, the first led by H. Chapman, J. Spence, P. Fromme, I. Schlichting, J. Ulrich and others on diffraction from membrane protein nanocrystals, the second led by J. Hajdu and M. Seibert on single virus diffraction and image reconstruction. (Both papers have about 80 additional co-authors, many common to both papers, including the team which made the remarkable chamber and detector system). Many more experiments have been done since this work was completed in December 2009, such as pump-probe time-resolved diffraction, with the LCLS now running up to 12 kV at higher repetition rate, limited by the detector read-out time. A sub-micron beam diameter is promised for the near future. Many papers have already been published concerning the problems of single-particle orientation and conformation determination from diffraction patterns, on the dynamics of the damage process, and on nanocrystal data indexing, phasing (using oversampling), and merging (see Chapman, *Nature Materials*, **8**, 299 (2009), Kirian *et al. Optics Express*, **18**, 5713 (2010), and the two *Nature* papers for reviews and references).

John Spence

See related article in *Acta Crystallographica Section A*, IUCr journals highlights.

MEETING REPORT

ISFC2010

Montevideo, Uruguay, November 2010. http://cryssmat.fq.edu.uy/ISFC2010



(From left to right) Massimo Nespolo, Mois Aroyo, Robert Burrow, Sebastián Píriz, Ernesto Estévez-Rams, Raimundo Lora-Serrano, Eduardo Granado and Leopoldo Suescun during farewell dinner.



Participants at the ISFC2010 conference in Montevideo, Uruguay.

The International School on Fundamental Crystallography (ISFC2010) was held at the Facultad de Química, Universidad de la República in Montevideo, Uruguay. The School was organized by the Crystallography, Solid State and Materials Lab. (Cryssmat-Lab)/DETEMA/Facultad de Química and the IUCr Commission on Mathematical and Theoretical Crystallography (MaThCryst) and sponsored by the IUCr, the Universidad de la República through CINQUIFIMA, CSIC and Facultad de Química, PEDECIBA and ANII from Uruguay and the ACA and ICDD that provided funds and folders for participants.

Fifty-one participants with backgrounds in chemistry, materials science, physics, structural biology and geology from Argentina (4), Brazil (25), Chile (2), Colombia (2), Mexico (2) and Uruguay (16) attended lectures by Massimo Nespolo (Nancy Université, France), Mois I. Aroyo (U. del País Vasco, España), Ernesto Estévez-Rams (U. de La Habana, Cuba), Eduardo Granado (UNICAMP, Brazil) and Gustavo Echeverría (UNLP, Argentina) on fundamental aspects of crystallography in direct and reciprocal space. All participants received some degree of support ranging from free lunch to full travel, lodging and expenses with 65% of the available funds devoted to support students.

The school was preceded by a preparatory session covering fundamental mathematics such as matrix algebra and Fourier series (led by Ricardo Faccio and Leopoldo Suescun from UR, Uruguay) and followed by a one-day workshop on representation theory of space groups led by Mois Aroyo.

The participants presented 30 posters. Six poster prizes were awarded, five consisting of a one-year complimentary membership to the ACA (Luciana Fernández Werner, Uruguay; Nicolás Ignacio Neuman, Argentina; Rodrigo Correa, Brazil; Hugo Javier Serrano Posada, Mexico; and Lorraine Andrade Malaspina, Brazil) and a special poster prize awarded to Eduardo Bittar (Brazil). The event was deemed highly useful for participants, 39 of whom replied to the on-line post-event evaluation. Many felt that their attendance at the ISFC2010 will improve their research activities and that they would recommend the next school to others.

The organizer of the next International School on Fundamental Crystallography in Latin America â€“ ISFC2012 - will be Raimundo Lora-Serrano (U. Federal de Uberlandia, Brazil).

More information is available at the MaThCryst Commission website or the local portal for the ISFC2010 (http://cryssmat.fq.edu.uy/ISFC2010). More pictures are at http://picasaweb.google.com/isfc2010/isfc2010 and www.iucr.org/gallery/2010/fundamental-crystallography-montevideo.

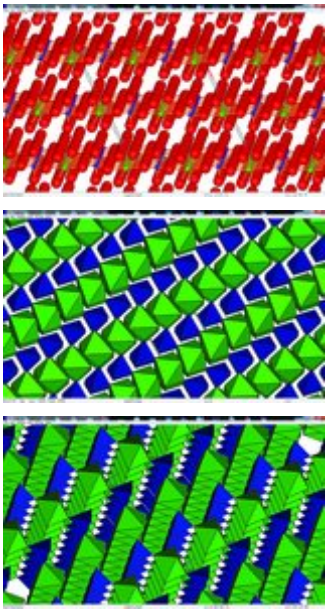
Leopoldo Suescun and Massimo Nespolo

OBITUARY

Lachlan Cranswick (1968-2010)



Lachlan Cranswick, a National Research Council scientist at the Chalk River Laboratories, Ontario, Canada, disappeared in January of 2010. An extensive search conducted at that time was fruitless and it wasn't until six months later that his body was discovered in shallow water by two people canoeing on the Ottawa River near Welsh Bay. What happened to him remains a mystery.



Images of Cranswickite $MgSO_4.4(H_2O)$, a new mineral from Calingasta, Argentina. Cranswickite is described in a paper by Ron Peterson (Queen's U.), submitted to *The American Minerologist*.

Lachlan was extraordinarily active in distributing powder and single-crystal computer programs throughout the world. He organized satellite workshops at international congresses and round robins concerning the Rietveld method, Structure Determination by Powder Diffractometry (SDPD), and Search/Match. He was one of the original founders of the SDPD and Rietveld mailing lists and various internet news groups including sci.techniques.xtallography. He chaired the Commission on Crystallographic Computing for the IUCr and was webmaster for the Canadian National Committee for Crystallography and for the 2009 ACA meeting in Toronto. He edited Newsletters produced by IUCr Commissions on computing, powder diffraction and teaching. From 1998 to 2003 the CCP14 gave him an opportunity to apply his talents cataloguing the most efficient computer programs. Although not a developer of programs, he constantly cajoled developers to make improvements in their algorithms, and to provide better documentation. His concern about the difficulties of doing science in developing countries prompted him to distribute his NEXUS CD to many countries, including Cuba, where internet access is difficult or impossible. His regularly updated CD contained a huge list of open software and documentation about crystallography. Lachlan was also interested in philosophy, history, literature and poetry. 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 chose to move to Chalk River, Canada, with its spectacular natural beauty, over another job opportunity at Berkeley. An avid dinghy sailor on the Ottawa River, Lachlan also enjoyed walking, cross-country skiing and curling.

From an article by Armel Le Bail and Ian Swainson

MISCELLANY

Stereographic projection cakes



Crystallographers in the Dept. of Crystallography, Faculty of Chemistry, A. Mickiewicz U. in Poznan, Poland, periodically hold parties (a 'special seminar' series), celebrated with a 'crystallographic cake'. Test your knowledge of crystallography and identify the point group and form represented in a stereographic projection on this delicious cake made by Agnieszka Paul!

Mariusz Jaskolski (photo Mirek Gilski)

AWARDS AND PRIZES

James awarded Honorary Degree

U. of Manitoba awarded Canadian scientist Michael N. G. James of the U. of Alberta with the DSc honorary degree this June during their 132nd Spring Convocation.

AWARDS AND PRIZES

Cotton Award to Dahl

Lawrence Dahl, R. E. Rundle and Hilldale Prof. of Chemistry at the U. of Wisconsin-Madison, was named winner of the 2010 F. Albert Cotton Award by the American Chemical Society. Dahl, who is now a Prof. Emeritus, was honored for the challenging synthesis and crystallographic characterization of large metal clusters.

AWARDS AND PRIZES

Kavli nanoscience prize to Seeman

The Kavli Prize is a joint venture between the Norwegian Academy of Science and Letters, the Norwegian Ministry of Education and Research, and the Kavli Foundation (US). The prizes in astrophysics, nanoscience, and neuroscience are awarded biennially. Among the eight 2010 Kavli Prize Laureates, Nadrian Seeman was recognized for his invention of structural DNA nanotechnology that could be harnessed to create raw materials for new nanoscale circuits, sensors and medical devices. Seeman shares this year’s prize in nanoscience with Donald Eigler of IBM’s Almaden Research Centre in San Jose, 'for their development of unprecedented methods to control matter on the nanoscale'.

AWARDS AND PRIZES

Bau Neutron Diffraction Award

Robert Bau (1944-2008) was an esteemed faculty member of the Chemistry Dept. at the U. of Southern California (1969-2008) and President of the ACA in 2006. The Bau Neutron Diffraction Award to recognize exceptional research achievement in neutron diffraction has been established by his widow Margaret Churchill. The Bau Award will be presented triennially, with the first award to be given in 2013.

AWARDS AND PRIZES

Aminoff Prize 2011: biological minerals inspire for the future



Lia Addadi



Stephen Weiner

The Royal Swedish Academy of Sciences has awarded The Gregori Aminoff Prize in crystallography 2011 to Lia Addadi and Stephen Weiner, both at the Weizmann Institute of Science, Rehovot, Israel, 'for their crystallographic studies of biomineralization processes, which have led to an understanding of mechanisms of mineral formation.'

Biomineralization refers to the processes by which organisms form minerals. Addadi and Weiner have been the leading researchers in this field since 1980, particularly in the area that concerns the calcification of organisms. This process reflects the biologically formed calcium-containing minerals and is a very important feature of marine life forms. They have challenged the most fundamental problems in biomineralization: nucleation, crystal-protein interaction, crystal growth and stability of different types of biomineralization polymorphs.

Weiner and Addadi induced biological mineralization by forming nucleation domains of metabolic products. These nucleation domains are carbohydrate-bound sulphates at the nucleation site, which is composed of structured arrays of protein-derived carboxylic acid groups achieving a cooperative activity with the nucleation domain. Addadi and Weiner successively identified the biologically controlled texture of biominerals that occurs along specific crystallographic planes on the protein crystals, which in all aspects control their formation, orientation, size, shape and assembly, and give rise to the complex shapes of many beautiful marine organisms. This also has implications for our understanding of the development of the various functions of biominerals.

An important aspect of crystallization of calcium carbonate is the occurrence of amorphous precursors that Addadi and Weiner have shown lead to different polymorphs: calcite, aragonite, vaterite and less stable disordered forms that are important for growth of exoskeleton shell structures.

Biomineralization research is of great importance not only for understanding processes in biology, geology and medicine but also as a source of inspiration for material science through the exciting field of biomimetics.

The Prize will be awarded at the Royal Swedish Academy of Sciences' Annual Meeting on March 31, 2011. Prize amount: SEK 100 000, to be shared equally between the two Laureates.

Lia Addadi became Dean of the Feinberg Graduate School in 2008 and is also a Dorothy and Patrick E. Gorman Professor.
More information: www.weizmann.ac.il/sb/faculty_pages/Addadi/

Weiner has a Walter and Dr Trude Borchardt Professorial Chair in Structural Biology, and is the Director of the Kimmel Center for Archaeological Sciences at The Weizmann Institute of Science.
More information is available at www.weizmann.ac.il/sb/faculty_pages/Weiner/

The Gregori Aminoff Prize, awarded for the first time in 1979, is intended to reward documented individual contributions in the field of crystallography, including areas concerned with the dynamics of the formation and determination of crystal structures. The prize may be awarded either to an individual Swedish or foreign researcher, or to a joint research group of no more than three persons.

Erik Huss