



# e-newsletter

Issue 2, 2011

Australian X-ray Analytical Association

## President's Address

Dear AXAA Members and Readers,

Welcome to winter!

I'd like to congratulate several of our members at this time for their outstanding achievements. Firstly, Mark Raven won the prestigious 2010 5<sup>th</sup> Reynolds Cup. Notably, this Newsletter includes a report on Mark's achievement from Brian O'Connor, who was recently announced as a Distinguished Fellow of the International Centre for Diffraction Data at their 2011 Spring Meeting (which I had the pleasure of attending). Congratulations to both.

The Newsletter is distributed to members and those interested in AXAA activities to provide information on upcoming events, news (as the name suggests), but also to inform about matters potentially important to our community. In our last Newsletter we called for interest in proposed changes to the way ARPANSA controls X-Ray sources in Australia. Thank you for your feedback, which was used in developing a statement made to ARPANSA on this issue (again, read on in the Newsletter for details). We encourage you to provide feedback on this and any other matter in the Newsletters to AXAA. I take this opportunity to remind our members and readers who may not be members that our membership rules have changed. Please read further for details.

Vanessa Peterson  
National Council President

## Editorial

The council have decided to introduce a new section to the Newsletter, aimed at promoting exciting X-ray, neutron and light scattering-related research being carried out in Australia, particularly by students and early career researchers. Keep an eye out for "Matters for Scatterers" in future editions. If you know of a good candidate to have their research X-posed, please forward your suggestion to me.

Nathan Webster  
Newsletter Editor

## AINSE Awards Honorary Fellowship to Brian O'Connor of Curtin University

The Australian Institute of Nuclear Science and Engineering (AINSE) is a joint Australian-NZ universities & ANSTO organisation devoted to facilitating use of ANSTO facilities by university students and staff. Importantly for AXAA this includes the use of neutron scattering/diffraction equipment with the OPAL reactor and, prior to that, HIFAR. AINSE Honorary Fellowships are awarded by the AINSE Council to individuals for distinguished and dedicated services to the Institute.



AINSE Honorary Fellowship recipient  
Professor Brian O'Connor.

Professor Brian O'Connor's 2011 Honorary Fellowship recognises his AINSE leadership (including Council Member from 1990-2007; member of Council Executive from 2003-2007 and AINSE President in 2007; and member of Neutron Scattering Specialist Committee from 1991-2003), as well as his AINSE-related research achievements (which have included authorship of 27 refereed publications, commencing with a neutron diffraction study of  $\text{NiSO}_4 \cdot 6\text{D}_2\text{O}$  which was one of the early single crystal studies performed with neutrons at the HIFAR research reactor). Previous awardees include Professor John White of ANU (2009) and Dr. Trevor Hicks of Monash University (2007).

## Brian O'Connor Announced as a Distinguished Fellow of the ICDD

Professor O'Connor has also been recognised by the ICDD Board of Directors as the 2011 Distinguished Fellow, an award given to a member who has given long and meritorious service to the ICDD. Professor O'Connor was named as an Honoree during the recent ICDD Spring Meetings. Further details can be found at: <http://www.icdd.com/newsletter/icdd-v-9-i-3.htm>

## 2010 Reynolds Cup Awarded to Mark Raven and Peter Self

Mark Raven of CSIRO Land and Water and Peter Self of the University of South Australia have been announced as the winners of the 2010 Reynolds Cup. The Reynolds Cup competition is organised on a biennial basis by the American Clay Minerals Society. The competition is named after Bob Reynolds for his pioneering work in quantitative clay mineralogy and his great contributions to clay science. The aim of the competition is to quantify as accurately as possible the mineral content of three clay-bearing samples supplied blind to the competitors.

See <http://www.clays.org/SOCIETY%20AWARDS/5thRCresults.html> for full details.

Winning the Reynolds Cup is said to be the clay characterisation equivalent of winning a gold medal at the Olympics or winning the soccer World Cup. For the 2010 and 5<sup>th</sup> Reynolds Cup, 76 sets of three samples were distributed to 63 participants from 22 different countries. The blind round robin format affords participants an unrivalled opportunity to test their given methods in complete honesty and thereby identify both strengths and weaknesses.



(Left) Mark Raven, (middle) Peter Self, and (right) the certificate in recognition of winning the Cup.

Mark Raven is the leader of the Mineralogical and Geochemical Services group at the CSIRO Land and Water, Adelaide, South Australia and has almost 30 years practical experience in XRD and XRF analysis. He undertakes research and development of methods of mineralogical analysis specialising in identification and quantification of minerals in rocks, soils and industrial materials. Mark was awarded a Master of Applied Science (Physics) from the Curtin University, Perth, Western Australia in 1989 under the supervision of Professor Brian O'Connor, after which he joined CSIRO. At Curtin he published one of the first papers in the international literature on Rietveld phase composition analysis - B.H. O'Connor and M.D. Raven (1988): *Application of the Rietveld refinement procedure in assaying powdered mixtures*. *Powder Diffraction*, **3**, 2-6.

Brian O'Connor  
Curtin University

## Ericé 2011 – The Power of Powder Diffraction

The 44<sup>th</sup> Crystallographic Course, "Ericé 2011 – The Power of Powder Diffraction", was held in Ericé, Sicily, from 2<sup>nd</sup> to 12<sup>th</sup> June. Ericé, sited on a hilltop, 751 m above sea level, is an ideal place for specialised meetings with a limited number of participants. Isolation, a wealth of archaeological sites, and the echoes of 3,000 years of history and prestige are the main attractions on this mountain, dominating Trapani and the extreme north-western edge of Sicily.

The meetings in Ericé are very highly regarded within the crystallographic community, and for some is a once-in-a-lifetime opportunity to learn from, and interact with, world-leading experts in a particular field of crystallography. The purpose of the 2011 course was to serve as a comprehensive introduction to the field of powder diffraction, and provide a solid grounding upon which to build future research pursuits and achievements. A diverse range of topics were covered - in lecture, demonstration and workshop format - including powder diffraction fundamentals, experimental techniques and instrumentation, structure solution, texture analysis, quantitative phase analysis, and crystal-ball gazing into the future of powder diffraction.



(Top left) View of the Mediterranean Sea and the northern coast of Sicily from the balcony behind the San Michele lecture theatre, (top right) entrance to the San Michele lecture theatre where most of the powder diffraction sessions were held, (bottom left) the paved streets of Ericé, and (bottom right) bon vivant and bear about town Dr. X-ray Ted checks out the beer and menu for some fine Sicilian food in Ericé.

The course was co-organised by Bill David (ISIS) and Kenneth Shankland (University of Reading), and was attended by other luminaries in the powder diffraction world such as Lynne McCusker, Christian Baerlocher (both ETH Zurich), and Bob Von Dree (Advanced Photon Source) to name but a few. Australians were well

represented among the participants with five students and one lecturer.

The days were long but rewarding; there was always a beer, a laugh and some hearty Sicilian food in the evening to recharge the batteries. After particularly tough lectures, one only had to stand on the balcony during the morning and afternoon tea breaks and contemplate the magnificent view behind the lecture theatre.

I encourage other members to consider future Ericé meetings – they are a truly wonderful and inspiring event. See <http://www.crystalerice.org/Erice2011/2011pd.htm> for further details.

Ian Madsen  
CSIRO

## Update - Code of Practice for Protection Against Ionizing Radiation Emitted from X-ray Analysis Equipment

Dear AXAA members,

As you will remember from the last newsletter I reported on ARPANSA's intent to re-write the aforementioned code of practice so I wanted to give you a quick update. Hopefully you downloaded it and provided comment to ARPANSA as it has the potential to affect most of you. ANSTO is regulated by ARPANSA and so we provided very detailed feedback to the organisation on the draft they produced. To date we have not heard back from ARPANSA in any form, I don't know if this is good news or bad news. When we do hear something I'll inform the membership so that hopefully if more feedback is required you will have the opportunity to give it.

Gordon Thorogood  
National Council Treasurer

## Membership Matters

We remind readers that AXAA-Inc membership is for the 3-year period starting from the last AXAA National Conference (existing membership will be re-approved in 2014).

Membership is free. Candidates should provide their CV and a short sentence about what they intend to do in the organisation, and a nomination letter from an existing AXAA member (if possible). Please send these to National Council Secretary Natasha Wright (contact details overleaf). Council votes on membership at periods no longer than 6 months.

## Upcoming Events

### **1. National XRD Course** ***X-ray Powder Diffraction Analytical Methods,*** **Curtin University, Perth** **Saturday 10 Sep – Tuesday 13 Sep, 2011**

**Venue:** Department of Imaging and Applied Physics, Curtin University, Bentley (Perth), Western Australia. [Client-specific version of the course can be presented at the customer's site].

**Duration of Curtin Course:** 4 days

**Course Presenters:** Professor Brian O'Connor and Dr Robert Hart

**Enquiries and further information:**  
B.O'Connor@curtin.edu.au

**Cost:** \$2,420 including GST

**Availability of places strictly limited – 5 places remaining as of 30<sup>th</sup> May**

**Overview:** The course has been designed to give participants a theoretical and practical grounding in the principal characterisation methods which make use of X-ray powder diffractometry data. Approximately 60% of the course involves hands-on instruction. Participants personally collect diffractometry data sets and then process these, both manually and with PCs, in exercises on various analytical methods, including Rietveld analysis. Public domain software will be used, including *WINPLOTR* and *Rietica*. The course also includes overviews and demonstrations of the commercial software packages *X'Pert HighScore Plus* and *Diffraclus Topas*. While the course is relevant to the analysis of all classes of crystalline materials, attention will be devoted mainly to materials relevant to the mining and mineral processing sector.

### **2. Internet XRF Course: Series 4, 2011**

The course provides XRF analysts, particularly those new to the field, with on-site instruction in the practical principles of wavelength dispersive XRF. Features of course include -

- Start at any time, subject to the availability of places in the course.
- Self-paced instruction to accommodate the needs of busy people.
- Study materials transmitted as e-mail attachments in the form of 11 modules; with an assignment being set for each module.



➤ Feedback on the assignments provides excellent mentoring.

The course now has a substantial number of international participants, as well as Australians.

Course availability: Starting date by arrangement.

**Approximately 5 places will become available in August for the XRF I-Course.**

Course director: Dr Brian O'Connor

Course fee: \$2,420 including GST

**Further information and enrolment:**

brian\_oconnor@iprimus.com.au

(Tel 08 9291 7067)

Brian O'Connor

**3. New Synchrotron and Neutron Users Symposium**

**Venue:** Seminar room M17, Chemical Sciences Building F10, University of New South Wales, Kensington Campus, Sydney.

**Date:** Friday 8 July 2011, 9AM to 6PM

Topics include:

- Neutron scattering
- Protein crystallography
- Biomedical Imaging
- X-ray fluorescence microscopy and mapping
- Single crystal and powder diffraction
- X-ray absorption spectroscopy

**Enquiries and further information:**

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**AXAA Website and Contacts**

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**Events, Conferences and Deadlines**

Date	Event	Location	Further Information
Start at any time, subject to place availability	XRF I-Course	Internet delivery	brian_oconnor@iprimus.com.au
8 July 2011	Synchrotron and Neutron New Users Symposium 2011	The University of New South Wales	<a href="http://www.ansto.gov.au/talks_and_workshops/synchrotron_and_neutron_new_users_symposium">http://www.ansto.gov.au/talks_and_workshops/synchrotron_and_neutron_new_users_symposium</a>
22-30 August 2011	22 <sup>nd</sup> Congress and General Assembly of the IUCR	Madrid, Spain	<a href="http://www.iucr.org/iucr/cong/iucr-xxii">http://www.iucr.org/iucr/cong/iucr-xxii</a>
6-9 September 2011	Powder Diffraction at Australia's Synchrotron and OPAL Facilities: Experiment Planning to Data Analysis	The Australian Synchrotron, Clayton, VIC	<a href="http://www.synchrotron.org.au/index.php/news/events/australian-events/event/77-pd-workshop">http://www.synchrotron.org.au/index.php/news/events/australian-events/event/77-pd-workshop</a>
10-13 September 2011	National XRD Course	Curtin University of Technology, Perth	B.O'Connor@curtin.edu.au
15 September 2011	2012/1 OPAL Proposal RoundFor instrument time 01 January 2012 to 30 June 2012	OPAL, ANSTO	<a href="http://www.ansto.gov.au/research/bragg_institute/users/call_for_proposals">http://www.ansto.gov.au/research/bragg_institute/users/call_for_proposals</a>

### PANalytical makes nanoparticle sizing even easier with EasySAXS 2.0



PANalytical has launched new hardware and software for small-angle X-ray scattering (SAXS) measurements on its range of X-ray diffraction (XRD) systems. The new multi-purpose sample stage that fits the Empyrean and X'Pert Powder is easy to use and provides superior data quality. Further, with the release of EasySAXS v2.0, a major new software version for SAXS analysis, PANalytical makes nanoparticle analysis even easier than ever.

Small-angle X-ray scattering (SAXS) is a versatile technique that is used for the structural characterization of solid and fluid materials in the range of 1-100 nanometers. It is applicable to crystalline and amorphous nanomaterials alike. Typical applications of SAXS comprise nanoparticle or pore size distribution determination, particle shape analysis and nanostructure analysis.

SAXS delivers complementary information to X-ray diffraction, also known as wide-angle X-ray scattering (XRD, WAXS), which is applied for qualitative and quantitative analysis of the crystalline phases that are present in a material. With the Empyrean and the X'Pert Powder instruments, PANalytical offers multi-purpose platforms that support the application of these and several other experimental techniques.

The new multi-purpose and factory pre-aligned SAXS/WAXS sample stage removes the need for a user to align samples – they simply attach the stage and insert their prepared sample. Supplied with sample holders and preparation tools for liquids, powders, and thin solid objects, the stage also uses disposable quartz capillaries for liquid sample measurement. An adjustable precision SAXS anti-scatter slit attachment is available to extend the low-angle resolution limit, and a semi-transparent beamstop for fast low-angle diffraction measurements completes the hardware upgrades.

With EasySAXS v2.0 researchers can analyze liquid nanoparticle dispersions, nanopowders, nanocomposites, and porous materials. The package features both automatic and GUI-based interactive modes. Automatic mode enables non-expert analysis of nanoparticle size distributions and specific surface areas using templates of predefined parameters. Results are summarized in automatically created reports.

Major improvements have been made to the interactive mode covering primary data handling, Guinier and Porod analyses, determination of scattering invariant, model simulations, and fitting to particle size distribution and pair distribution function analyses.

For more information on how EasySAXS v2.0 can work for you, please visit [www.panalytical.com](http://www.panalytical.com) or contact your local PANalytical specialist.

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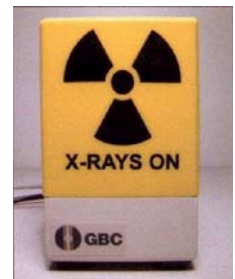
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**Bruker AXS**

Bruker recently launched a new series of high-performance X-ray crystallography systems, including the D8 QUEST™ and the D8 VENTURE™ instruments. Both systems incorporate next-generation X-ray source and novel detector technology to deliver unrivalled performance, ease of use, reliability and value. The D8 QUEST is a compact and economical, yet high-performance, single X-ray source configuration for typical applications in chemical crystallography, while the D8 VENTURE provides the platform for all dual wavelength combinations for chemical and biological crystallography.

The D8 QUEST and D8 VENTURE systems both feature the newly-developed PHOTON 100™ detector, the first CMOS-based detector for chemical crystallography. The PHOTON 100 represents a paradigm change in area X-ray detector technology with respect to sensitivity, speed, dynamic range, resolution and detector size. The PHOTON 100 detector is based on a large, research-grade CMOS sensor with an active area of 100 cm<sup>2</sup> that is four times larger than typical CCD chips commonly used for X-ray detection today. This new CMOS detector offers a detection efficiency significantly better than any other available detector. Also, because of the outstanding reliability of low-voltage CMOS detector technology, the PHOTON 100 is the first detector to carry a full 3-year warranty.

The new D8 crystallography systems offer a range of X-ray source and optics options, including the proven performance of sealed-tube X-ray generators with the unique TRIUMPH™ curved crystal monochromator, or the exceptional brilliance and long lifetime of the new I $\mu$ S™ microfocus X-ray source with now up to 60% higher intensity. All new D8 system configurations feature a new beam path design that allows easy alignment with the X-ray enclosure doors closed in order to comply with the latest radiation safety regulations.

The D8 systems also offer the widest range of proven goniometer options, including the open access and convenience of the FIXED-CHI, or the ultimate performance and flexibility of the KAPPA geometry. Both new goniometers are driven by a new collision-avoidance program, based on the latest robotic trajectory-planning algorithms, which makes experiment planning easier and more efficient than ever.

Dr. Michael Ruf, Global Product Manager for Single Crystal XRD at Bruker AXS, stated: "Fifteen years ago, Bruker pioneered CCD-based area detectors that revolutionized X-ray crystallography. Most of the chemical structures published worldwide since that time have been measured using Bruker instruments with CCD detectors. However, today customers are looking at ever more difficult problems, from micro-crystals to electron charge density to metal-oxide frameworks. With its advanced CMOS detector technology, cutting-edge X-ray sources, innovative software and flexible, modular design, the new D8 QUEST and D8 VENTURE crystallography systems offer even more powerful capabilities to deal with these challenging scientific problems."

For further information, please contact Bruker on (03) 9474-7000 or email [sales@bruker.net.au](mailto:sales@bruker.net.au)



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