2009 ANNUAL REPORT

ARC CENTRE OF EXCELLENCE FOR
COHERENT X-RAY SCIENCE

CXS

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COHERENT X-RAY SCIENCE

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FUNDAMENTAL PHYSICS OPENING A NEW WINDOW ON THE BIOLOGICAL WORLD

CXS would like to acknowledge the support of the Australian Research Council. We would also like to acknowledge the financial and in-kind support provided by our collaborators –University of Melbourne, La Trobe University, Monash University, Swinburne University of Technology and the Australian Commonwealth Scientific and Industrial Research Organisation (CSIRO). We are grateful for the financial support received from the Science, Technology and Innovation (STI) Initiative coordinated by the Office of Science and Technology within the State Government of Victoria.

CXS would like to thank the School of Physics at the University of Melbourne, Mr James Gibbons of Monash University, Ms Fabienne Perani of La Trobe University and Ms Tatiana Tchernova of Swinburne University of Technology for their support.

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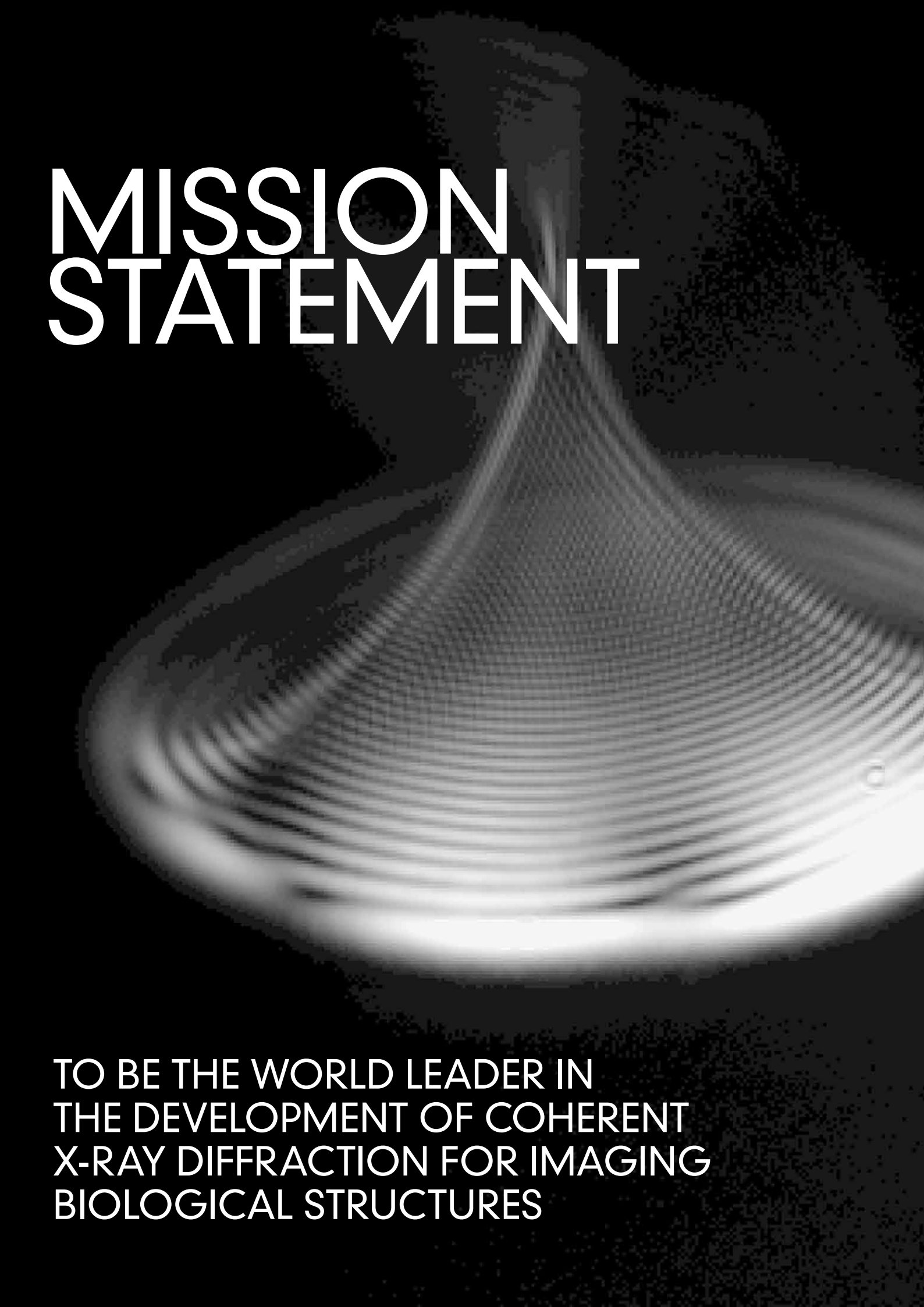
ABOUT CXS

The Australian Research Council (ARC) Centre of Excellence for Coherent X-ray Science (CXS) brings together leading Australian researchers in the fields of X-ray physics; the design and use of synchrotron radiation sources; and the preparation, manipulation and characterisation of biological samples.

Its aim is to open a new frontier in biotechnology – the non-crystallographic structural determination of membrane proteins. These proteins mediate the activity of pharmaceuticals in human medical therapies. Their structures, however, are still mostly unknown because they do not form crystals suitable for analysis using the conventional crystallographic techniques that have driven almost all the progress in structural biology. A breakthrough in this area would revolutionise rational drug design through the insight gained into the function of membrane proteins. This would have far-reaching consequences for the pharmaceutical industry. CXS's research is driven by its access to existing third-generation synchrotron light sources and to the Australian Synchrotron. We are also exploring the application to imaging problems of short wavelength high-harmonic generation sources and free-electron X-ray lasers that are under development worldwide.

When combined with non-crystallographic diffractive imaging techniques, the brightness and intensity of these sources gives us the opportunity to take snapshots of biomolecules. We are exploring the fundamental issues in the use of these light sources, including the nature of the interaction between intense coherent X-rays and electronic matter. The efficiency of diffraction processes in these highly coupled light-matter systems, the detection of the scattered light, the preparation and handling of suitable biological samples, the management of radiation damage throughout the interaction, and the design of algorithms to extract structural information from diffraction data is also under exploration.

It is an ambitious interdisciplinary program of research.



MISSION STATEMENT

TO BE THE WORLD LEADER IN THE DEVELOPMENT OF COHERENT X-RAY DIFFRACTION FOR IMAGING BIOLOGICAL STRUCTURES

DIRECTOR'S REPORT

2009 was a great year for CXS. It began with the news that we had done very well in the ARC review at the end of 2008 and that our funding level is to be increased and extended until December 2013. This is very exciting for us and we celebrated in a joint event with another University of Melbourne led centre, the CoE for Free-Radical Chemistry and Biotechnology which also had a similarly successful review outcome.

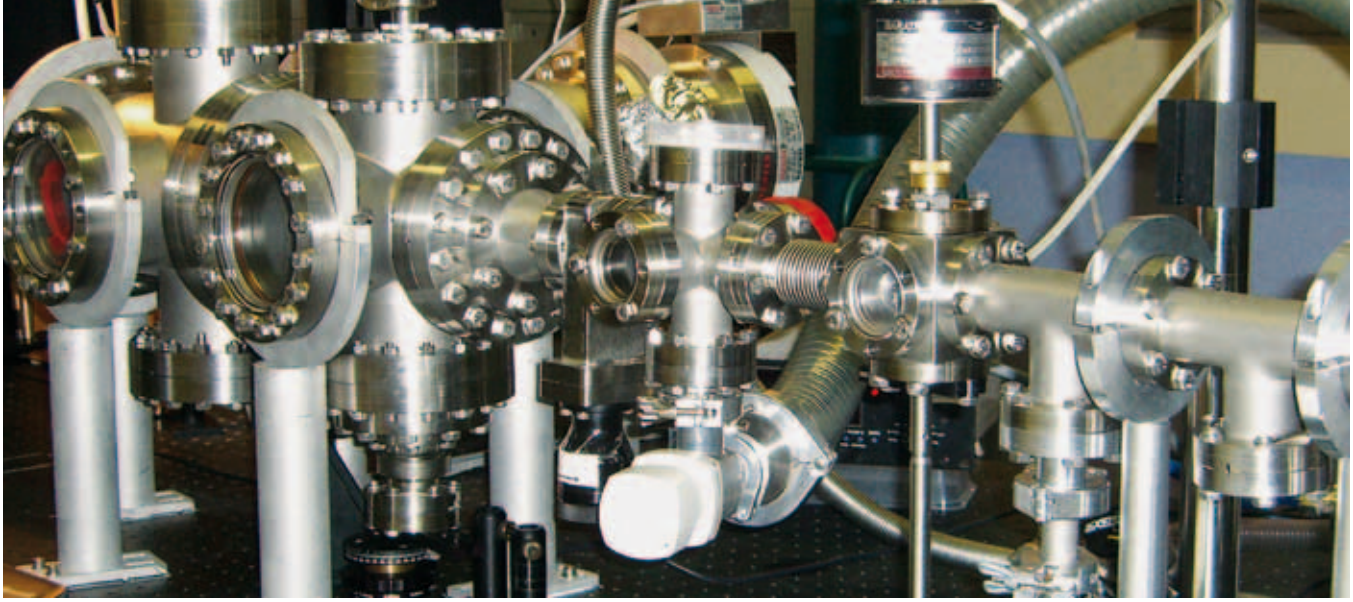
The acquisition of guaranteed funding for a further five years means that we can re-focus on the long-term goals that should be at the centre of the planning of an organisation such as CXS. With this in mind, in September, CXS held a very enjoyable and productive planning retreat in Beechworth in which we gave considerable thought to the directions we should take. With the able assistance of the members of our Scientific Advisory Board, well-informed decisions were made and we are already seeing many of these bearing fruit.

Another response to the review was our decision to do some re-casting of the directions of the centre. Accordingly, we invited a group led by Dave Kielpinski from Griffith University to join us so that we can enhance our experimental work in the study of the interaction of high-fields with atomic structures, an important aspect of our long term goal of enabling the analysis of molecular structures using X-ray free electron lasers. We have named this new part of CXS the Attosecond Science Program as it will concentrate on the interaction of extremely short light pulses with atomic systems. An attosecond is extremely short – there are 10^{18} attoseconds in one second , which is a 1 followed by eighteen zeroes, and this is the same as the number of seconds in the age of the universe.

As part of this re-structuring, we also have elected to close down the Detectors & Beamline Development Program based at Monash University. This decision was made easier by the news that Chris Hall had been offered an ongoing position at the Australian Synchrotron with the result that the program was no longer viable. Rob Lewis also took the opportunity to resign from CXS so as to enable him to re-focus on his work related to biomedical imaging. We wish both of these former CXS members well in their future research and fully anticipate an ongoing relationship with both of them. Our association with work on detectors will continue as we deepen our relationship with the Cooperative Research Centre for Biomedical Imaging Development.

Scientifically, the centre continues to perform superbly. CXS members continue to be highly productive and publishing high-impact science. There are a number of measures of the impact of our work but one that is notable is the number of our papers that are featured on the covers of journals. This year, three CXS papers were featured on the cover of the journal in which they were published. This is an exceptional result and indicates that world continues to take note of the quality of our science.

A centre is more than the sum of its parts and the sum of its outputs. We have continued to ensure that members of CXS have access to a vibrant program of centre activities, meetings, workshops and visitors. We want CXS members to be able to meeting the



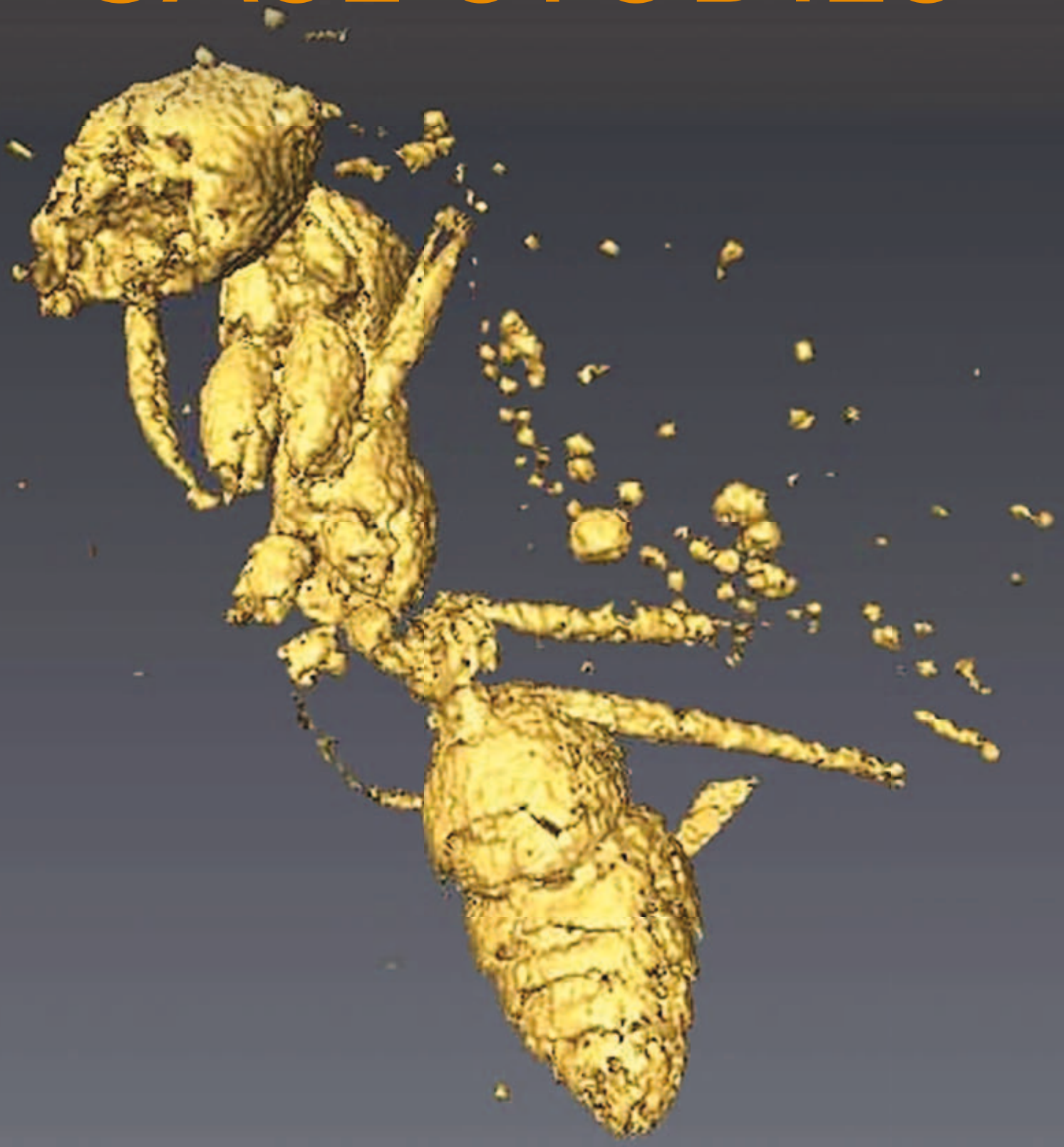
leading scientists in the world and discuss their ideas with them and with each other. This has led to a number of very productive workshops, also outlined in this report, as well as innovative ideas such as the "Talking Backwards" workshop in which physicists were asked to explained biology to CXS members, and biologists asked to explain physics. This is in addition to CXS workshops on commercialisation, intellectual property, careers and science. We thank our active IP and Advisory Board members for their contributions to all of these activities.

2009 was also a year in which some of our outreach activities hit a new level of achievement. The movie project continues to proceed well and we were able to see a preview of it at our end-of-year function. We also formed a partnership with Santa Maria College, Northcote which we have called *Growing Tall Poppies*. This program was supported by the Catholic Education Office and the University of Melbourne through a Knowledge Transfer grant, and it went on to be selected as the winner of the Victorian State Impact Award from the new *Schools First* grant system sponsored by the National Australia Bank and the Federation of Young Australians. As a result, the partnership was awarded a cash grant of $100,000 to support its further development. This award has led to considerable publicity for CXS and Santa Maria College and will lead to further exciting developments over the coming years.

We have had some staff depart from CXS and so we wish them well. In particular, Garth Williams has been with CXS since its beginning and he has now moved on to an ongoing position at the X-ray free electron project at the SLAC laboratory run by Stanford University in California. We wish Garth well, but expect to continue to work with him in the coming years.

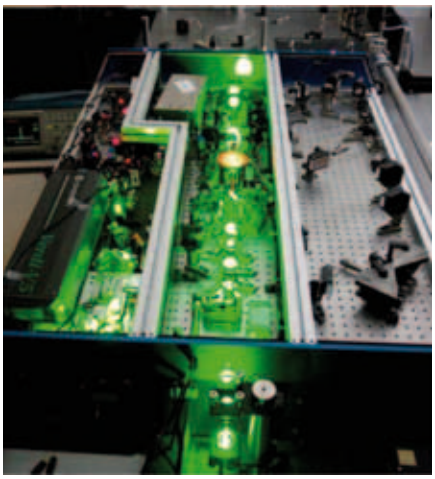
PROFESSOR KEITH NUGENT
DIRECTOR

RESEARCH PROGRAMS & CASE STUDIES



RESEARCH PROGRAMS & CASE STUDIES

ATTOSECOND SCIENCES PROGRAM



The heart of the Australian Attosecond Science Facility: a laser system producing phase-locked optical pulses of 6 fs duration with 30 GW peak power.

The Attosecond Science Program in CXS, which began collaborating with CXS in June 2009, offers new opportunities for coherent X-ray science that are unique within Australia. The new and rapidly expanding field of attosecond science is based on recent revolutionary developments in ultrafast optics that resulted in the award of the Nobel Prize in 2005. It is now possible to generate high-energy infrared light pulses consisting of only a few cycles of the electric field and to control the optical electric field waveform within the light pulses. Such optical pulses have been used to generate isolated soft X-ray bursts with durations below 100 attosecond (1 as = 10^{-18} s). They can also provide information on atomic and molecular dynamics on the attosecond timescale and have been used to map the electronic structure of molecules. The Australian Attosecond Science Facility (AASF) is the unique tool in Australia for attosecond science investigations. The facility is directed by A/Prof Kielpinski, leader of the CXS Attosecond Science Program as of January 2010. The heart of the facility is a laser source providing 6 fs, 300 μJ, phase-stabilized laser pulses, commissioned in 2007 through an ARC LIEF grant.

In 2009, the AASF experimental group began a close collaboration with the CXS Theory and Modelling group on the response of atomic hydrogen to strong few-cycle laser pulses. Atomic and molecular dynamics in strong optical fields plays a crucial role in many CXS activities, from the Biological Sciences Program's goal of molecular structure retrieval from single-molecule X-ray diffraction to the high-harmonic generation work of the Short Wavelength Laser Source Program. However, theory and experiment in this area rarely give quantitative agreement. As the only attosecond science group with access to atomic hydrogen, the AASF group has a unique opportunity to benchmark strong-field theories with the help of the Theory and Modelling group.

As part of CXS, the AASF group will also pursue the generation of isolated attosecond X-ray pulses, which have already proved useful as tools for probing electronic structure of atoms, molecules, and surfaces. Currently only four research groups in the world have this capability. Isolated attosecond pulses can help unravel the problem of nonlinear X-ray backaction on molecular diffraction imaging, a key step in realising CXS goals in biomolecular structure determination. Modelling of backaction during the long X-ray pulses

Attosecond Sciences Program team.

from synchrotrons and free-electron lasers (FELs) requires simultaneous incorporation of several mutually interacting many-body effects, a highly challenging task. In contrast, attosecond pulses provide a window into the short-time dynamics, effectively decoupling the many-body effects. Attosecond interactions can also selectively incorporate or exclude particular processes. Although the total energy delivered in an attosecond pulse is much lower than that expected at an FEL, the peak X-ray intensity can be nearly as high because of the short pulse duration.

GOALS

The goals of the Attosecond Science Program are twofold:

1) We will generate isolated attosecond pulses of XUV light for time-resolved X-ray science. Such pulses are presently the unique means of access to attosecond dynamics and are currently available at only four laser facilities worldwide. We anticipate that XUV pulses of duration <500 as and peak intensities of 100 GW/cm^2, with wavelength in the 10-20 nm range, will be achievable in the next two years. Isolated attosecond pulses have already proved useful as tools for probing electronic structure of atoms, molecules, and surfaces. We will extend these studies to specific chemical and biological applications of interest to CXS members. Because attosecond science is so new, basic experimental methods are still under development. Close collaboration between our group and end-users in CXS will prove essential in realising the promise of attosecond science and new methods will be rapidly taken up worldwide. We have already generated XUV radiation at wavelengths as short as 30 nm by focusing the AASF laser through an argon gas jet and are preparing to investigate the temporal properties of the XUV light. Nonlinear X-ray processes in helium gas have been observed in other laboratories with isolated attosecond pulses and will be readily observed for the much larger dipole moments of chemical and biological samples. Generalising commonly used ultrafast pump-probe techniques to the attosecond domain will eventually enable us to evaluate the full dynamic structure factor of chemical and biological samples under X-ray irradiation for detailed comparisons with backaction models.

2) We will investigate the effects of atomic structure on strong-field interactions through quantum control of the ultracold metastable neon atoms currently generated in our laboratory. HHG data on the exotic electronic structure of metastable neon will be critically sensitive to poorly-understood atomic physics effects in HHG. Quantum state control of the atoms involved in HHG isolates specific atomic processes for detailed tests of theoretical HHG models. The novel computational techniques of the CXS Theory and Modelling group will transform our data into optimised designs for HHG-based X-ray sources of specific spectral and temporal characteristics. The Short Wavelength Laser Source Program can take advantage of these designs for their XUV imaging source, tailoring the XUV source to their particular goals.

The single-atom dipole response to a strong IR field is a crucial input for optimisation of HHG sources. A recent experiment has shown that interference between the dipole amplitudes of different atomic species in a mixture of gases can boost HHG by over three orders of magnitude. However, the standard theory of HHG is inadequate for describing atomic structure effects and numerical predictions of the HHG spectrum vary by a factor of 2 according to the exact methods used. The CXS Theory and Modelling group has developed a new theory of atomic HHG based on free-field atomic states. Our current experiment examines ionisation of atomic hydrogen with few-cycle laser pulses, and we are now working with the CXS Theory and Modelling Group to interpret these results. Because the hydrogen atom is so simple, subsequent HHG studies in hydrogen will be an excellent benchmark for HHG modeling.

Dr Matthew Dixon imaging malaria parasites.

BIOLOGICAL SCIENCES PROGRAM

Methods for imaging cellular architecture and ultimately macromolecular complexes and individual proteins, within a cellular environment, are an important goal for cell and molecular biology. The Biological Sciences Program involves the participation of biochemists, structural biologists and cell biologists who are undertaking specific research in the biomedical area. As part of work undertaken within CXS, Biological Sciences Program members collaborate closely with members of the Experimental Physics Program (EPP) in the development and implementation of novel imaging techniques to provide new insights into the structures of membrane-enclosed compartments within cells. Members of this program also interact with members of the Structural Determination Methods Program to optimize techniques in determining the structures of membrane proteins and membrane protein complexes.

The groups within this program conduct world-class research in the following areas:

MALARIA AND REMODELLING OF THE RED BLOOD CELL

The most deadly of the human malaria parasites, *Plasmodium falciparum,* invades red blood cells and initiates a remarkable series of morphological rearrangements. The mature red blood cell (RBC) is effectively a floating sack comprising a membrane that encloses the oxygen-transporting protein, haemoglobin. Unlike other cells, RBCs have no DNA and cannot make or traffic proteins. In order to colonise and remodel the red blood cell, the parasite generates a series of novel structures that are involved in the export of virulence proteins to the surface of the host cell. These include extensions of the parasite's vacuolar membrane, known as the tubulovesicular network, and structures referred to as Maurer's clefts. These membrane structures play an important role in the trafficking of virulence proteins to the host cell surface, however their ultrastructure is only partly defined and there is on-going debate regarding their origin, organization and connectivity. Parasite endocytic processes are also poorly understood. The parasite consumes host haemoglobin in order to support its own growth. Packets of haemoglobin are transferred from the host cell cytoplasm to a parasite digestive vacuole for haemoglobin digestion and heme detoxification however the precise mechanism for uptake is debated. One of the aims of CXS is to image these compartments and to develop an understanding of their function and the way in which they are formed. Such research can lead to new avenues for drug and vaccine design to inhibit the growth of malaria in RBCs.

MITOCHONDRIA: UNDERSTANDING THE POWERHOUSE AND THE POISON CUPBOARD

Mitochondria are the generators within our cells, synthesizing chemical energy in the form of the molecule ATP. They also act as poison cupboards, where upon opening of the mitochondrial outer membrane, certain proteins become released that kill cells as part of programmed cell death. Defects in mitochondria cause energy-generation disorders and are also implicated in other diseases including Parkinson's and Alzheimer's diseases. In addition, efforts to activate the machinery involved in mitochondrial permeabilization can act as anti-cancer agents. Work within the CXS is to understand some of the events involved in remodeling mitochondrial membranes during disease and to provide potential new insights into the formation of pores that lead to cell death. In addition, work is being undertaken to provide insights into the structure of mitochondrial membrane proteins and their complexes.

GOALS:

- Prepare and optimize cellular samples for use as test-beds for X-ray coherent diffraction imaging and for other pioneering imaging techniques

Biological Sciences Program team.

- Use X-ray imaging and other imaging modalities to gain novel insights into cellular architecture and function
- Prepare samples of soluble and membrane proteins and determine their structural characteristics using both conventional and novel X-ray-based approaches

ACHIEVEMENTS

The malaria parasite *Plasmodium falciparum* has been used as a test system for X-ray coherent diffraction imaging (CDI), and the data have been correlated with other imaging modalities, including light and electron microscopy and scanning and transmission X-ray microscopy. In particular, the group has performed pioneering efforts in the development of whole cell electron tomographic imaging, X-ray tomographic imaging and super-resolution fluorescence imaging.

IMAGING INSIDE CELLS

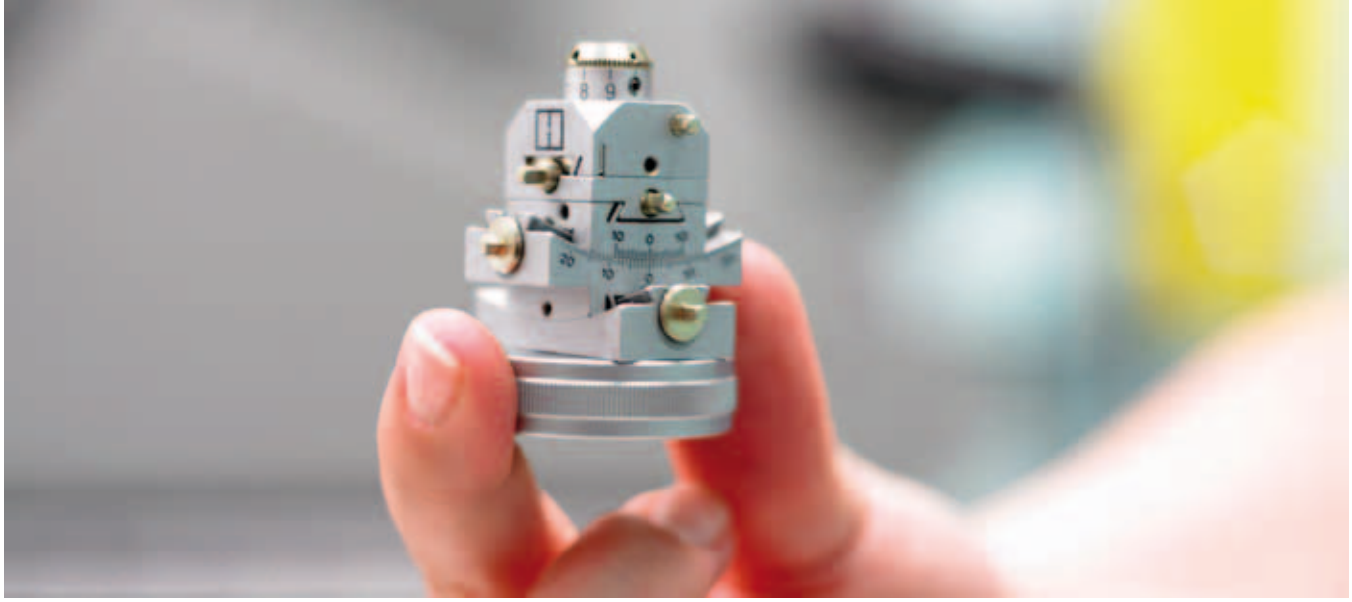
Three-dimensional structured illumination microscopy provides resolution beyond the optical diffraction limit and permits analysis of fluorescently labeled whole cells. Cryo transmission x-ray microscopy in the "water window" of photon energies has recently been introduced as a method that exploits the natural contrast of biological samples. Immunoelectron tomography offers the possibility of high resolution imaging of individual ultrastructural features in a cellular context. Combined with serial sectioning and immunogold labeling, this technique permits precise mapping of whole cell architecture.

P. falciparum develops within human red blood cells (RBCs). As it grows the parasite establishes a membrane network outside its own limiting membrane in the cytoplasm of its host cell. These membrane structures play an important role in the trafficking of virulence proteins to the host cell surface. Using electron tomography and super-resolution optical microscopy Dr Eric Hanssen and Dr Nick Klonis showed that the exported secretory system of *P. falciparum* is composed of a series of modular units, comprising flattened cisternae, known as Maurer's clefts, tubular connecting elements, two different vesicle populations and electron-dense structures that have fused with the erythrocyte membrane. The membrane network is not continuous, pointing to an important role for vesicle-mediated transport in the delivery of cargo to different destinations in the host cell. Two genes encoding Maurer's cleft-located proteins were disrupted; that this induces disorganization of the trafficking compartments and affects delivery of the virulence determinant, PfEMP1, to the RBC surface.

The electron tomography studies have also provided novel insights into the process of haemoglobin digestion by the malaria parasite. The work shows that haemoglobin digestion is initiated in the early ring stage of development in pre-digestive vacuoles which then fuse to form a mature digestive vacuole. The timing of the onset of haemoglobin digestion has implications for the action of antimalarials.

With Prof Carolyn Larabell, National Center for X-ray Tomography, Lawrence Berkeley Laboratory, USA, we have used tomographic x-ray imaging of whole hydrated cells at different stages of growth of *P. falciparum*. The hemoglobin degradation product, hemozoin, and lipid-rich structures in the developing merozoites show high x-ray absorption. Quantitative analysis of changes in the density of material in the parasite cytoplasm during intraerythrocytic development reveals a previously unrecognized change in ribosome packing density. We observed novel invaginations of the parasite surface that may play a role in hemoglobin uptake. We used immunospecific labelling with gold/silver aggregates to confirm the identify of compartments in the host cell cytoplasm.

We have also undertaken techniques to image mitochondria and their remodeling within cells. This has been performed using electron microscopy and novel confocal techniques that utilize photoconversion of specific fluorescent proteins to track intracellular movements. PhD students Laura Osellame and Catherine Palmer have investigated the function of two novel membrane proteins that are located on patches on the mitochondrial surface and are involved in causing mitochondrial fission. In order to analyse these patches in more detail, we have commenced collaborations with Assoc Prof Trevor Smith and Dr Liisa Hirvonen (Laser Source Program) to undertake structured illumination microscopy. These studies will also investigate the localization of other proteins – including cell death proteins – on the mitochondrial surface.

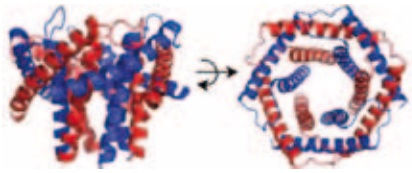


STRUCTURAL AND BIOCHEMICAL STUDIES OF MEMBRANE PROTEINS

Using biochemical methods, we have investigated the association of the cell death protein, Bak, at the mitochondrial surface. We have found that that Bak is prevented from undergoing accidental activation by binding to a membrane protein termed VDAC2 (voltage-dependent anion channel 2). We are now purifying and reconstituting the Bak-VDAC2 complex to understand how they interact together. This is being conducted by Dr Diana Stojanovski and Mr Boris Reljic.

Lynn Liang, a PhD student supervised by Connie Dharmain (CSIRO) and Leann Tilley, has been optimising conditions to express and purify G-protein coupled receptors (GPCRs) in baculovirus/insect expression system and receptors. These receptors represent ~40% of drug targets yet little is known about their mechanism of action. Lynn has been optimising both the expression in other insect cell lines and assays for function. She has also been carrying out detergent screening in attempts to extract the GPCRs from insect cell membranes.

We have also optimised the expression and purification of new proteins involved in the assembly of the first mitochondrial generator, Complex I. These proteins are now being used in crystallisation trials for conventional protein structure determination and can be used as future test beds with complex I assemblies in novel X-ray approaches.



Structure of the yeast Tim9-Tim10 complex (Baker et al, Mol. Cell. Biol. 2009).

BIOLOGICAL SCIENCE PROGRAM CASE STUDY

GUIDING PROTEINS ACROSS MEMBRANES

The Tim9-Tim10 complex plays an essential role in maintaining mitochondrial function by chaperoning hydrophobic proteins into the inner membrane. How the complex interacts with these proteins is not clear, although it has been proposed that Tim10 acts in substrate recognition, whereas Tim9 acts in complex stabilization. Jacqui Gulibis and Chaille Webb (WEHI), determined the structure of the yeast Tim9-Tim10 hexameric assembly to 2.5 Å and we performed mutational analysis in yeast to evaluate the specific roles of Tim9 and Tim10. Each Tim9 and Tim10 subunit contains a central loop flanked by disulfide bonds that separate two extended N- and C-terminal tentacle-like helices. Buried salt-bridges between highly conserved lysine and glutamate residues connect alternating subunits. Mutation of these residues destabilized the complex, causes defective import of membrane proteins and caused cell growth defects. Truncation analysis revealed that in the absence of the N-terminal region of Tim9, the hexameric complex no longer trapped incoming substrates. Our results demonstrated that Tim9 plays an important functional role that includes facilitating the initial steps in translocating precursor substrates into the intermembrane space. Our future goals are to analyse protein binding to the complex using small angle X-ray scattering at the Australian Synchrotron.

Detector and Beamline Development Program team.

DETECTOR AND BEAMLINE DEVELOPMENT PROGRAM

The Detector and Beamline Development team (DBD) at Monash University are striving to design and build the optimal detector for X-ray coherent diffractive imaging. We are also partially responsible for the delivery of a high technology end station, which will control the Coherent X-ray Diffraction Imaging (CXDI) optics, sample, and detector positioning.

The CXS DBD project team are addressing the limitations of current couple-charged device (CCD) based X-ray imaging devices for CXDI. CCDs are well-established detectors for this area of research. They are integrating devices, which accumulate information about the X-ray field during an exposure period. The signal read out is related to the total charge released in a pixel as each X-ray photon interacts with the silicon. This method is a simple and reliable means to measure the X-ray intensity that falls on the detector. However, there are penalties to be paid for this simplicity. The signal-to-noise ratio and the dynamic range in integrating detectors are sub-optimal for a technique as demanding as CXDI. For successful CXDI image reconstruction the precise number of photons that hit a pixel should be recorded. Errors in this value should be less than 1% in order to allow the reconstruction algorithms to converge in reasonable time. The estimate provided by an integrating detector is usually not good enough for imaging applications. Readout noise and other detector artefacts increase the measurement error especially when only a few photons are being measured. This is always the case in the high scattering angle regions of the CXDI image.

A better alternative is to count individual X-ray photons as they arrive at the detection plane. Given full quantum efficiency, the measurement of flux in this case is accurate with almost no noise. An important limitation to the counting technique arises when the flux is high. In this case the electronic circuits can struggle to keep up with the rate of arrival of the photons. The rate limit can be increased if the area for which the counting is taking place is very small. Using very large scale integrated circuit (VLSI) technology, the readout circuitry for a given pixel can be made very small. Using modern integrated circuit processes it is now feasible to place all the readout circuitry for an individual X-ray detector in an area of less than 100 microns square. It is also possible to reproduce this circuitry many times and devise a means to multiplex the outputs into just a few electronic channels. Using this technique a matrix of readout nodes can be fabricated covering the whole of the sensitive area required. Placing an X-ray sensitive material above this matrix circuit and connecting to it electrically, or even optically, produces a versatile and accurate X-ray detector. The general name given to such a device is a hybrid pixel detector (HPD), or simply 'pixel detector'. The particular demands of CXDI are highest in the specification of sensitivity and dynamic range. High sensitivity is required to detect the faint scattered X-ray flux at high angles from the sample. The difference in flux between the central region of the image and the diffraction region is many orders of magnitude, therefore requiring a large dynamic range in the detector. For both sensitivity and dynamic range the HPD has the potential to provide superior performance to CCDs; this is the device of choice for a future CXDI detector.

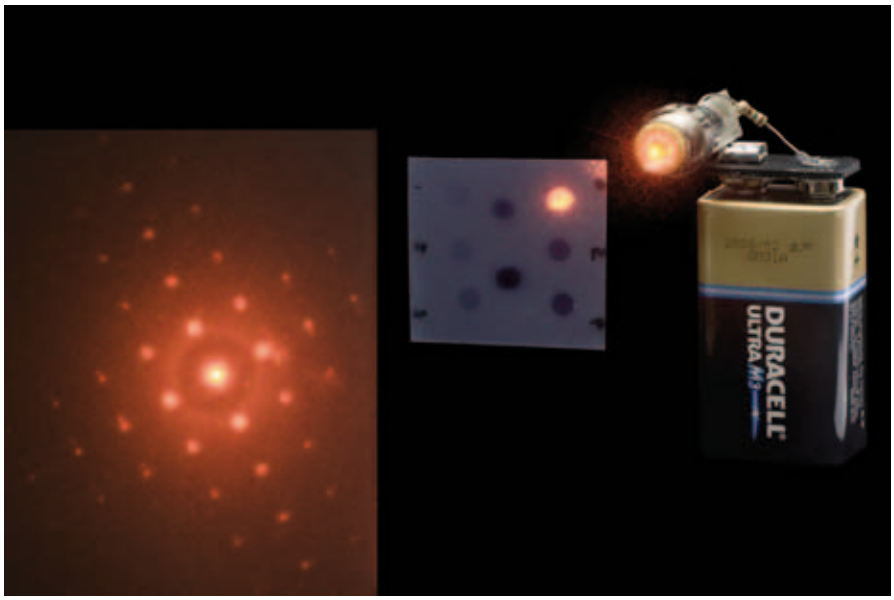


Figure 1: Scatter of coherent light from radiation-induced optical centres can be the basis for ionizing radiation detection. Here a laser illuminates a piece of self-developing X-ray film that has been contact-shadowed with a fine metal mesh. The far-field shows the diffraction pattern of the original mesh arising from coherent optical scattering by the film. It demonstrates that coherent optical scatter from radiation-induced centres can serve as the basis for X-ray detection. The coherence of the scattered light can serve as the basis for powerful new coherent X-ray diffraction developments. In the context of Bragg's X-ray microscope the scattered coherent light would be used to optically compute the structure of the X-rayed object, making it directly visible, but at the spatial resolution corresponding to the original X-ray wavelength.

ACHIEVEMENTS

During this year the DBDG focussed on two aspects of its research program. A continued study of a prototype photon counting pixel detector and early development of methods using optical readout. Testing of the detectors at low x-ray energies was facilitated after the commissioning of an evacuable detector test chamber. This facility allows testing with x-rays having energies around the silicon k edge at 1.83 keV without attenuation from long air paths. This apparatus is also well suited to testing the novel optical readout materials designed for high dynamic range ultra fast detection of CXDI fields.

It is clear that a photon counting detector, with its very low noise readout would suit a CXDI end station well. A table of specifications, derived from consultation with the imaging scientists was published by our group in 2008. This highlighted the need for detector sensitivity accompanied by high dynamic range. A small silicon sensor, the Medipix2 which operates by photon counting was trialled as a potential CXDI detector during the year. Two aspects of the device were measured: the room temperature limit to the lowest photon energy detectable and the spatial resolution limit due to signal sharing. The published limit of 6 keV at 21 degrees Celsius was verified by our tests. The next step would be to cool the device so that the lowest detectable energy more closely matches that in the specifications

A novel form of charge sharing analysis was developed using the Medipix2 detector this year. A low flux of photons was collected in 10,000 frames of 1 second exposure each. Each frame was analysed for expected neighbouring registration of events. A cluster analysis algorithm was used to generate a histogram of cluster size in each image versus frequency. During data collection the detector discriminator threshold was set close to the noise so that signal sharing would perturb the cluster histogram from that expect by chance alone. As expected the variation from chance was small when photons of 6 keV were used. Only events which deposited energy very close to the pixel border generate 'split' events. Modelling of this effect will be informed by the results of these experiments. The group is working towards a complete model of a CXDI pixel detector which will be used to predict performance of this and other potential detectors under a variety of x-ray fluxes.

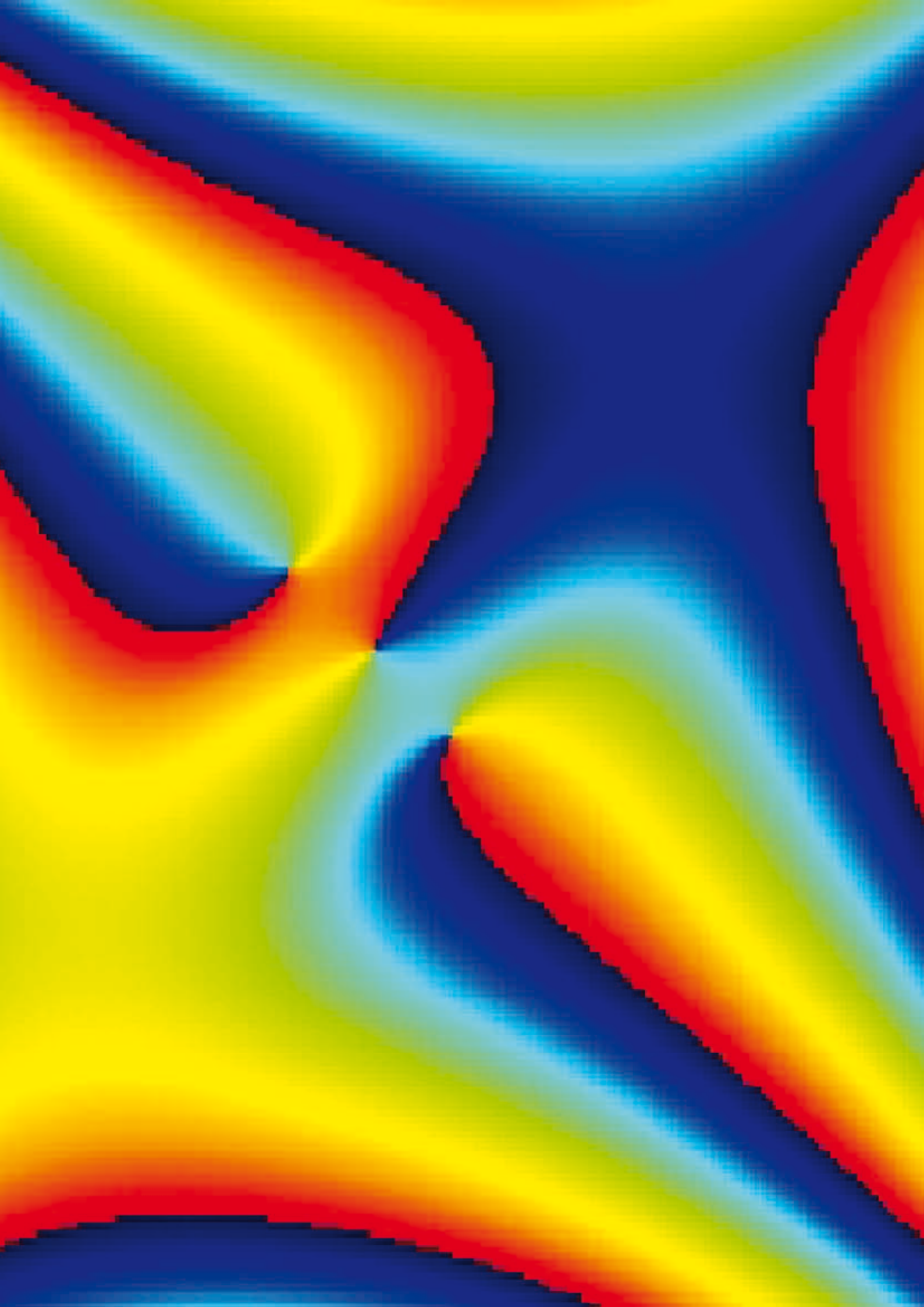
Our other focus involves investigations into optically active materials which respond to a soft x-ray flux. Absorption features in the optical or near optical wavelength range are created in certain materials after interaction with x-rays. The absorption centres mimic the intensity pattern of the x-ray flux and can be read out with an optical light source and an optical detector. The electro-chemistry of the creation of these absorption features leads us to believe they will potentially have an exceptionally high dynamic range when used for x-ray imaging. Due to the wide range and availability of fast, sensitive optical detectors this provides a multiplicity of options for CXDI detector development. Furthermore the iterative procedure for calculating the phase of the x-ray wavefield may well be implementable with optical computing.

Wilfred holding an ultrasonically driven miniature bubble chamber being prototyped for use with ultrashort pulsed X-ray sources.

DETECTOR AND BEAMLINE DEVELOPMENT PROGRAM CASE STUDY

The issue of signal sharing in small pixel x-ray detectors has been studied during the year. A solution has been proposed which involves segmenting the pixels to deliberately share photon induced signals was developed which involved deliberately sharing signals across electrodes. If this is done in a controlled and known way, an interpolation can be used to determine photon interaction positions to less than the pixel pitch. Even complex interpolation calculations are within the capability of modern pipelined digital processing circuits and so can be made fast enough to cope with the rate requirements from CXDI. With current technology the minimum physical size of a pixel in such a detector is around 50 microns. This limitation is due to the integrated device sizes required to execute the functionality required for each pixel. In order to achieve a sub pixel resolution in the final image a scheme has been modelled by the DBDG. The scheme involves both electronic network analysis using MicroCap 9, a Monte Carlo calculation of the physics of the photon interaction using Geant4, and analysis of the transport of the charge carriers which forms the detected signal.

Bubble chambers are one of a few technologies that allow the development of transient optical gratings formed by ionising radiation, particularly famous for their sensitive optical scattering measurements of individual particle tracks traversing condensed matter in high energy physics. The picture above shows Wilfred holding an ultrasonically driven miniature bubble chamber being prototyped for use with ultrashort pulsed X-ray sources. As with all bubble chambers, a state of near-cavitation must be achieved; acoustic pressure is a method for doing this that offers synchronisation to pulsed X-ray sources. Pending successful acoustic cavitation in the device, coherent optically probed radiation-triggered cavitation experiments of the type motivated in Figure 1 and its caption will be investigated.



Corey Putkunz, Keith Nugent and Rob Scholten working on FRIEND, December 2009.

EXPERIMENTAL METHODS PROGRAM

The Experimental Methods Program (EMP) develops imaging methods using coherent and partially coherent light sources. The research profile of EMP includes the design of experimental systems, sample handling and nano-fabrication techniques, tomographic imaging of three-dimensional objects, the detailed characterization of radiation sources and the development of novel imaging methodologies using diffraction data. These are the key experimental techniques required to undertake the CXS mission. In particular, the EMP has developed a dedicated endstation that will greatly facilitate the investigation of biological samples. It is the first instrument of its type that provides sufficient stability to apply the imaging methods developed for CXS.

The EMP group has members based at La Trobe University, the University of Melbourne and Monash University. Through its broad spectrum of members and activities, the EMP is ideally suited for interaction with the other programs of CXS. Through regular interaction with the Theory and Modelling Program, the EMP has established standing research activities with most of the other programs in CXS:

- Biological Sciences Program (BSP) – this is a fundamental CXS interaction. The work of the EMP is to image biological samples in three-dimensions. This basic work is assisted by both groups and by the Theory and Modelling Program in analyzing imaging data obtained from biological samples. With the bulk of their membership based at La Trobe University, EMP and BSP staff regularly meet to develop imaging methods. To further facilitate the mutual translation of physics and biology BSP staff attend EMP experiments at overseas facilities, which has led to the exploration by BSP of access to other imaging techniques and facilities around the world. EMP and BSP also hold seminars and meetings designed to encourage interaction between students and staff from the two groups.
- Theory and Modelling Program (TMP) – TMP and EMP regularly cross-fertilize. EMP provides experimental data that TMP can apply new methods of analysis to and TMP provides new directions for the experimental work. Members of TMP are co-located at the University of Melbourne with several of the EMP group so that interaction is frequent.
- Short Wavelength Laser Source Program (SWLSP) – the SWLSP provides a novel source of coherent photons at wavelengths approaching X-ray. Again, with strong interaction from TMP, the EMP and SWLSP have a standing experimental activity based around pursuing the limits of imaging with these sources.
- Ultra-Cold Plasma Source Program (UCP) – the UCP was formed within CXS to exploit techniques developed by EMP and TMP to demonstrate imaging using a bright coherent source of high-energy electrons. Again with membership based at the University of Melbourne UCP and EMP have a high degree of interaction.
- Detector and Beamline Development Program (DBD) – the DBD has significant interaction with EMP in the development of experimental facilities. In particular, the endstation developed for CXS experiments was a joint activity and budget share for the DBD and EMP.

ACHIEVEMENTS

In 2009 the Experimental Methods Program conducted a wide range of experiments at several facilities (synchrotron sources in three different countries and the Swinburne High Harmonic Generation source) as well as consolidating its activities in commissioning the Fresnel Imaging ENDstation (FRIEND) at the Advanced Photon Source in Chicago. In this time EMP published several results demonstrating new optical techniques. We have also made major strides forward in understanding the systematics involved in making FRIEND achieve its goal of keeping a sample stable at 3 nm root mean square with respect to an optics stage that is about 10 cm away. This is equivalent to keeping a laser spot inside a 1 mm target at a distance of 30 km – try it!

Data taken on FRIEND showing reconstruction of the phase of a test structure performed without (top) and with (bottom) the incorporation of a priori knowledge.

A FRIEND IN NEED

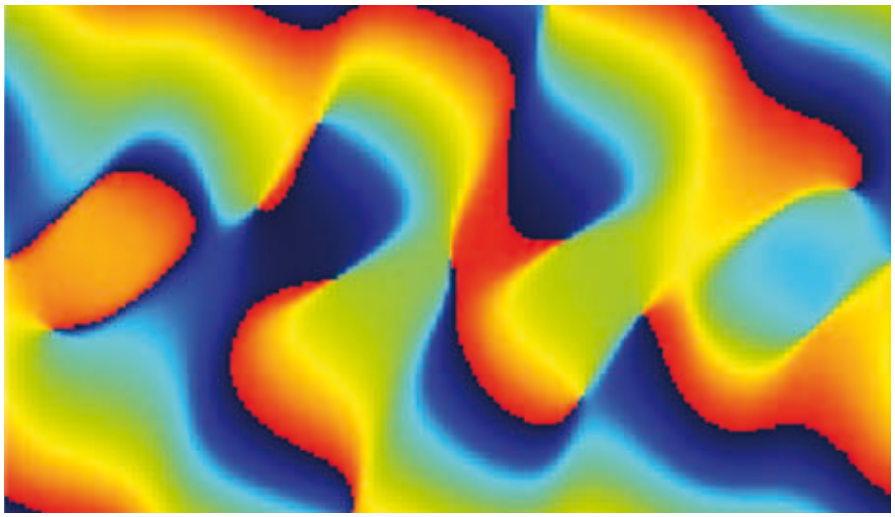
FRIEND uses a clever arrangement of lasers and geared down weak-link stages in order to implement a position feedback loop that can correct for motion at the nanometre scale. This type of work is notoriously difficult to implement typically taking teams of researchers and technicians months or years of 100% access time to resolve. It is a credit to the dedicated post-doctoral researchers and students in EMP (in particular Garth Williams, David Vine Mark Pfeiffer, Jesse Clark and Corey Putkunz) that from a distance of over 15,000 km and with only a handful of trips during the year that headway has been made. The progress of FRIEND in 2009 has been the story of much of experimental physics, but with over $1,000,000 invested it is a story writ large. At the time of the 2008 CXS annual report all seemed well. As x-ray data progressed it became apparent that an unknown heat source was causing the "stable" components to drift. By the end of the year the heat source was identified and correctional steps discovered that allow the system to operate in a stable fashion. Data taken in December indicates stable measurements with x-rays can be taken (see image) With this the development of FRIEND for our coherent diffractive imaging experiments and the planned upgrade to allow for scanning transmission x-ray microscopy (STXM) experiments is back on track. In the coming year an EMP postdoc (David Vine) will move to Chicago to increase our coverage for experiments and to support external users. In addition we will appoint another researcher to oversee the upgrade to STXM capability and the relocation of the instrument to the branch line of the soft x-ray beamline at the Australian Synchrotron.

EMP FACILITIES

In addition to FRIEND EMP maintains laboratory facilities for microfabrication (Eugeniu Balaur) where bespoke samples for experiments are created; for optics (Garth Williams) where student projects can be tested prior to a synchrotron visit; and for tomography (Benedicta Arhatari) where conventional x-ray imaging and 3D methods can be trialled. In 2009 all of these laboratories were very productive in producing papers, data and samples for CXS researchers.

TOMOGRAPHY

Our studies into the process of image formation in x-ray tomography have allowed us to experimentally verify the development of the contrast transfer function through a high resolution x-ray tomography system, to model the effects of a polychromatic laboratory source and to implement our methods in application to external user samples (papers led by Benedicta Arhatari).



The phase distribution of a charge three vortex distorted by two cylindrical lenses.

HIGH HARMONIC GENERATION SOURCE DIFFRACTIVE IMAGING

The HHG source developed by the Short Wavelength Laser Source Program at Swinburne has allowed us to demonstrate key imaging results using a new approach, developed in collaboration with the Theory and Modelling Program, to coherent diffractive imaging (CDI). In this approach a modal expansion of the incident beam in terms of the harmonic peaks in the source spectrum is used to break down the net incoherent wavefield into an incoherent sum of coherent modes. This allows us to treat the analysis of the data using tools previously established for single mode CDI. In work led by Bo Chen image reconstructions of test samples have been obtained and published.

PTYCOGRAPHICAL FCDI

In Fresnel Coherent Diffractive Imaging a probe beam defines a region of illumination on a sample. In work led and published by David Vine multiple overlapping positions of the beam are used to create redundant sets of data. This greatly improves the iterative reconstruction. The approach is similar to the ptycographical method employed by groups working in CDI but is potentially more flexible here by using a defocused beam from a zone plate as the probe.

A COMPLEX CONSTRAINT FOR FCDI

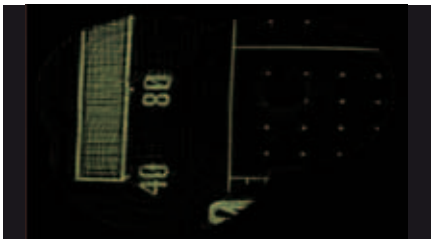
Even using the CXS approach of Fresnel Coherent Diffractive Imaging reconstructions of a diffraction pattern can be degraded by artefacts due to systematic present in the experiment. In work forming part of Jesse Clark's PhD thesis the possibility of improving results by incorporating some *a priori* knowledge of the sample into the algorithm was explored. In work published in 2009 we showed that a modest amount of prior knowledge can have a significant impact on th equality of the reconstruction (see image on page 18).

VORTEX

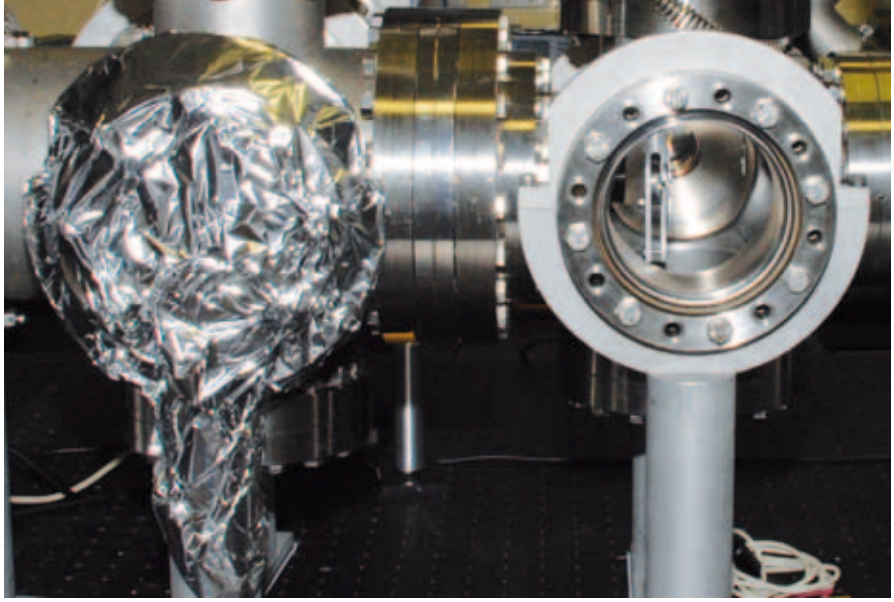
Vortex beams are a fascinating state of light characterised by a donught shaped ring of intensity around a dark core and a spiral phase along the direction of propagation. While there are many possible applications for such a state of light (for instance as an optical spanner!) vortices are of interest in studies of coherence and phase retrieval as they represent a pathological object that resists analysis by conventional phase retrieval methods. In part of her PhD work Clare Henderson working with Harry Quiney from the Theory and Modelling Group has been able to show that by using cylindrical lenses certain symmetries in the beam can be broken and correct phase retrieval performed. Her work was also featured as a "front cover" image for the online journal Optics Express.

EXPERIMENTAL METHODS PROGRAM CASE STUDY

Part of the core business of CXS is coherence. In a range of experiments we have been able to show that it is possible to characterise the coherence function of the light from a synchrotron beamline. As part of Sam Flewett's PhD work a study demonstrating this based on measurements taken at the APS was published during 2009. In a fine example of synchronicity we were then able to use these measurements and combine them with the ideas developed in the HHG work described above. Specifically, the coherent spatial modes of the total wavefield are treated separately in an algorithm (just like the coherent spectral modes in the HHG work) to recover the partially coherent diffraction pattern from a test object and reconstruct an image of the sample. The measurements for this work were conducted using FRIEND as part of Lachlan Whitehead's PhD work and the analysis was conducted in conjunction with the Theory and Modelling Group. The images show the diffraction measured, a reconstruction performed using "conventional" CDI and a reconstruction performed using the new modal approach.



Data taken on FRIEND showing high resolution reconstruction due to stability of the system.



SHORT WAVELENGTH LASER SOURCE PROGRAM

The Short Wavelength Laser Source Program has investigated the generation of extreme ultraviolet (XUV) and soft X-ray pulses by high harmonic generation (HHG) and applied these sources in atomic and molecular spectroscopy, condensed matter physics, and imaging on the micron- and submicron-scale. These compact (table-top) femtosecond pulsed sources will complement larger installations such as X-ray free-electron lasers (XFELS) currently under development.

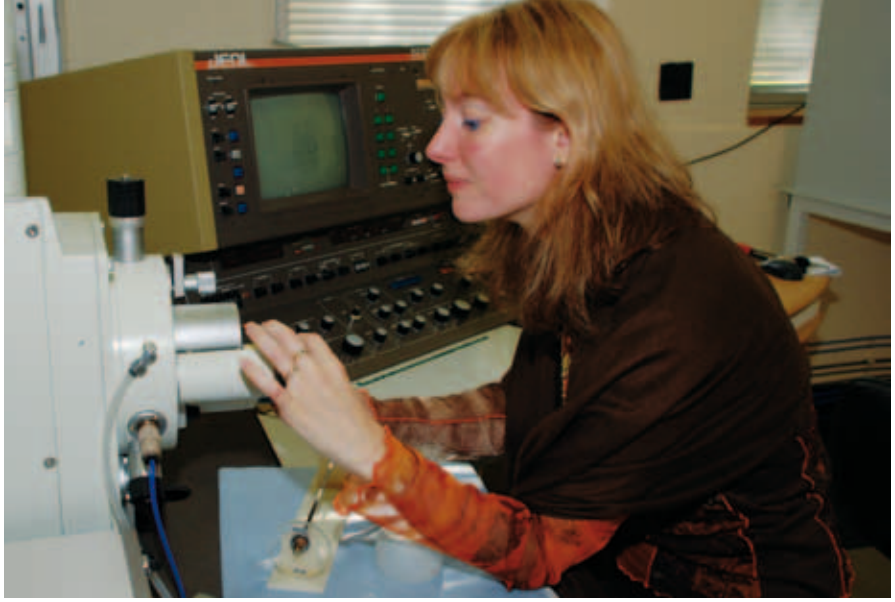
By their nature, HHG sources produce a laser-like beam that consists of a number of harmonic orders. Therefore a harmonic source with just a few intense orders (ideally a single harmonic order) would be advantageous for many applications because they can be used directly without additional spectral selection optics.

The high harmonic generation process can be explained in terms of a semi-classical three-step model. In this model, under interaction of a strong laser field the active electrons first tunnel through the potential barrier, are then accelerated in the first half of the optical cycle of the laser field, and then are pulled back and finally recombine with parent ions to emit high-energy photons in the second half of the cycle. The acceleration process of an electron in a continuum and the variation of the molecular or atomic ground state by the interaction with the driving laser field should play an important role in such quantum systems and need to be studied in more detail.

Unlike atoms, molecules are not isotropic systems. For randomly aligned molecules, the HHG has been shown to have characteristics similar to that of atoms, but for aligned molecules, which can be realized by using another laser field, the HHG is influenced by the angle between the molecular frame and the polarization vector of the femtosecond laser field. An investigation to clarify the roles of intramolecular quantum processes in field-free aligned molecules is highly desired, in order to obtain an improved understanding of the underlying physics which is the basis of future applications.

Due to the low efficiency of the HHG process, phase-matched propagation of the fundamental and harmonic radiation throughout a macroscopic sample is required to obtain a measurable signal. The degree of phase-matching depends on the harmonic order and several experimental parameters including the focusing characteristics of the laser beam, the absorption coefficient of the target gas at the harmonic frequencies, the ionization fraction of the gas, and the difference in the refractive index at the fundamental and harmonic wavelengths. We have been investigating ways of optimizing the phase matching.

The high harmonic spectrum and intensity contains information about the electronic structure of the atom or molecule and other quantum processes involving the free and bound electrons. Studies of the process of high harmonic generation provide a better understanding of the microscopic and macroscopic process and may lead to additional information about the electronic structure of the atom or molecule.



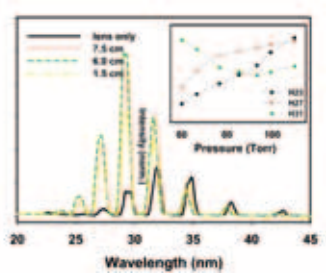


Figure 1: HHG spectra for three different distances between the axicon and the lens (7.5, 6.0 and 1.5 cm). The solid line shows the HHG spectrum for the case without the axicon. The inset shows the intensity of different harmonic orders versus gas pressure when the distance between the axicon and the lens is 6.0 cm.

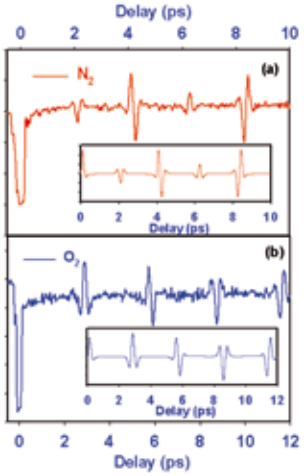


Figure 2: Intensity of harmonic H27 of aligned N_2 molecules (a) and H21 of aligned O_2 molecules (b) versus delay between the two beams. The insets show simulations of the change of the nonlinear refractive index.

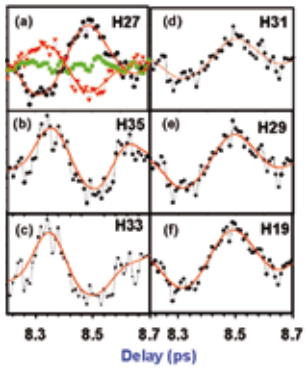


Figure 3: (a) Intensity of harmonic H27 from aligned N2 molecules around T ≈ 8.4 ps versus delay between the two beams for different relative polarizations of the second beam (circles – parallel, triangles – crossed, and squares – 54.7^0). (b-f) Intensity of different harmonics from H19 to H35 for N_2 versus time delay between two parallel polarized beams at T≈ 8.4 ps. The symbols are experimental data and the line is a smoothing curve.

ACHIEVEMENTS

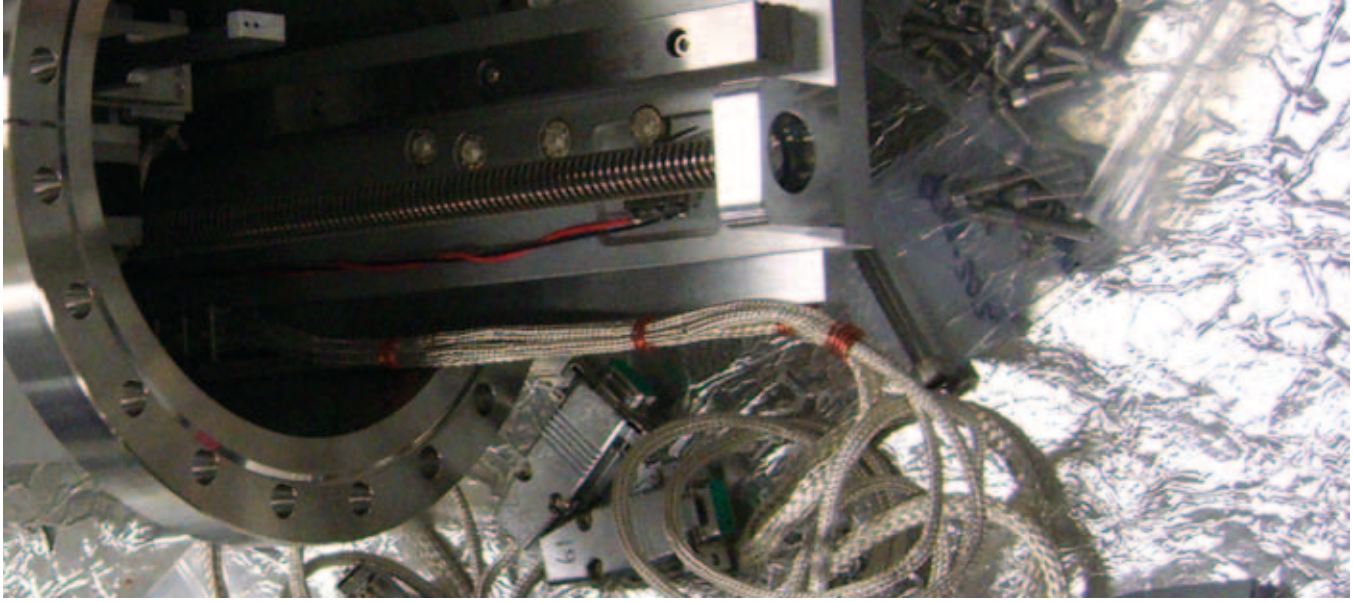
HIGH HARMONIC GENERATION (HHG)

A combination of a lens and an axicon, which provide a Bessel-Gaussian beam, can be used to improve the generation of a few harmonic orders in a semi-infinite Ar gas cell. Improved macroscopic phase-matching is achieved for harmonics in the cut-off region compared to a Gaussian beam because of the new dispersion term, giving better control of the spectrum and the coherence. We have monitored the changes in the HHG spectrum as a function of lens-axion distance and show that the spectrum can be tuned to some degree using this variable (Figure 1).

We have demonstrated the importance of the phase-matching effect on the HHG signal from aligned molecules. The alignment of molecules can be achieved by the interaction of the molecules with a short, relatively weak pulse to create a rotational wave packet. This wave packet rephases after the pulse is finished and the molecules are strongly aligned periodically at intervals separated by their fundamental rotational period. To observe the alignment dependence of HHG, a second delayed higher intensity laser pulse is used to generate HHG at different time intervals when the molecules undergo a rapid change in their alignment. By varying the delay of this pulse, the HHG emission intensity for different magnitudes and angles of alignment can be detected and used to study the rotational molecular dynamics. The phase-matched HHG spectrum shows a clear imprint of the rotational Raman coherence and can be used to study molecular dynamics. Two molecular gases, N_2 and O_2, where the ground state has σ– symmetry in the case of N_2 and π–symmetry in the case of O_2, are used in this study (Figure 2). This study opens up a new technique for studying the coherence dynamics of the ground states of molecules.

The experimental results indicate that the modulation of the intensity of the low-order harmonics (< H33, fig 3d–f) and that of the higher-order harmonics (H33-H35, fig 3b,c) are out of phase at time T ≈ 8.4 ps in the case of N_2. It has been shown that ionization and also recombination in the HHG process are stronger for the HOMO-1 state relative to the HOMO state when the molecules are aligned perpendicular to the laser field. Our results show that electrons from the HOMO state make a contribution to the generation of harmonics with low order (< H33, fig 3, 3d-f) while electrons from the HOMO-1 state make a stronger contribution to the high harmonic orders (H33-H35, Figure 3b,c). At the magic angle ($\theta \approx 54.7^0$), only an isotropic response is measured. This leads to no change in the refractive index, i.e., there is no modulation of the harmonic intensity (Figure 3a – squares)

To enhance the dynamic range of the CCD detector, especially for coherent diffractive imaging (CDI) with a multiple harmonic source, an x/y-beam-stop is required for the acquisition of short-exposure, low-resolution and long-exposure, high-resolution diffraction images. The design of this beam-stop involves the acquisition of



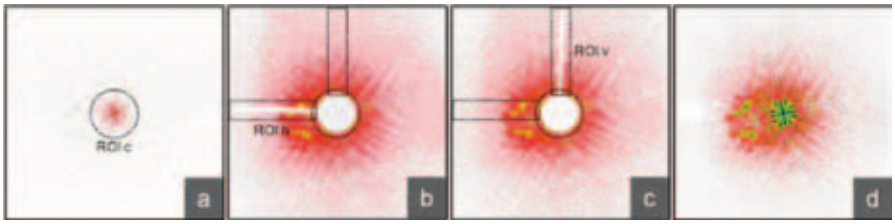


Figure 4. High-dynamic range diffraction images: an image (a) of low-angle and two images (b and c) of high-angle diffraction information are acquired and stitched together to form one single image (d).

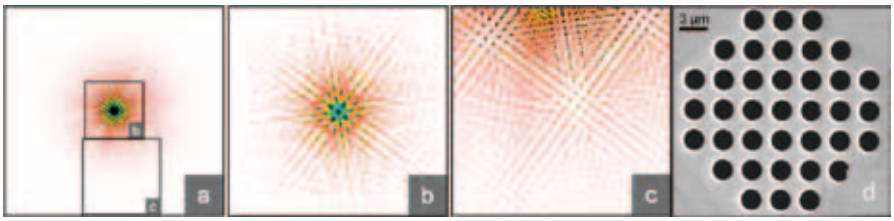


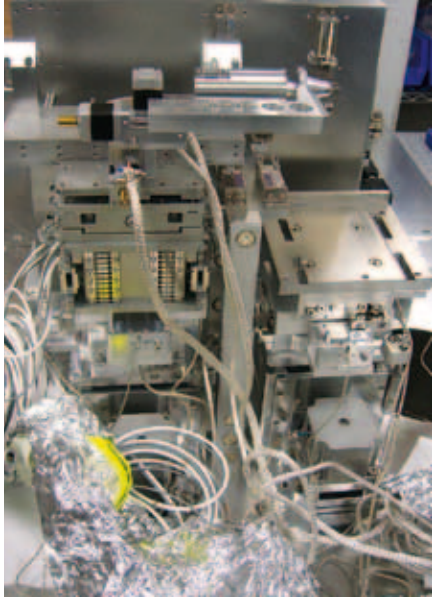
Figure 5: Perfect version of the diffraction image: full diffraction pattern (a); and zoom into low-resolution and high-resolution regions (b and c), scanning electron microscopy image of the sample (d).

a number of different diffraction images that complement each other and need to be combined. We have reviewed this stitching process (Figure 4) in which the combination of the images is achieved by means of applying Gaussian coefficient functions to chosen regions with diffraction speckles.

The high angle diffraction patterns are given in Figure 5. We note that the reconstruction of this diffraction pattern based on a multiple-order harmonic beam has yielded a value of 100 nm (full width at half maximum) for the resolution and is consistent with the simulated value of 100 nm based on the Sparrow criterion. A Fresnel transform has been employed in this case as the far-field condition did not hold in this experiment.

SUPER-RESOLUTION OPTICAL MICROSCOPY:

In conjunction with high resolution X-ray imaging, we are also interested in the rapidly developing field of "super-resolution" *optical* microscopy. These methods are potentially capable of providing resolution comparable to that achievable by the X-ray imaging methods of interest to the Centre, but using optical methods on samples prepared using standard protocols, thereby providing complementary information. Within the past few years, methods including structured illumination microscopy (SIM), scanning



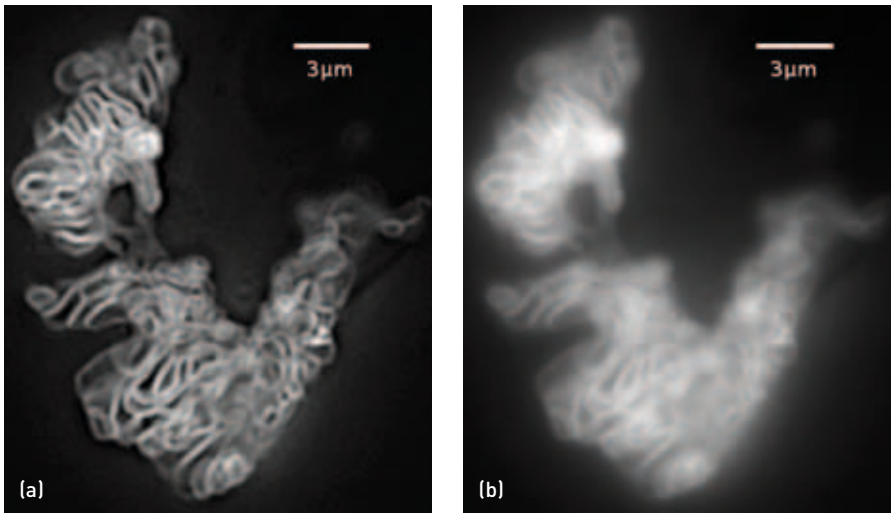
near field optical microscopy (SNOM), stimulated emission depletion (STED) microscopy, photoactivated localisation microscopy (PALM) and stochastic optical reconstruction microscopy (STORM), have been developed by various groups around the world. The laws of diffraction are not being broken – rather "tricks" are implemented to try to circumvent these fundamental laws of physics.

We have been active in establishing several of these techniques in association with the Biological Sciences Program. In particular, we have recently concentrated on structured illumination microscopy. In this method, a fluorophore is photoexcited by a laser in a wide-field microscope format; however, a pattern is first imposed on the optical excitation beam using an optical transmission grating. This pattern essentially mixes with the high frequency information reported by the fluorescence of the sample and the high-frequency information is converted into a lower-frequency Moiré pattern, which an ordinary microscope and sensitive CCD camera can image. Then, through computational methods, similar in some ways to the approach taken in coherent diffractive imaging, the high-frequency, and therefore higher spatial resolution, features of the image are recovered through image reconstruction software. This provides approximately twice the optical resolution of conventional fluorescence microscopy. This is a very attractive feature in the investigation of biological samples, but SIM also has other advantages over some of the other super-resolution methods, such as acquisition speed and applicability to conventional fluorophores and existing sample preparation methods.

We have constructed a structured illumination microscope based on available lasers, presently operating with excitation at 408 and 488 nm – but this can be adapted. This is currently one of just two SIM systems in Australia. An example of the improvement in optical resolution achieved using our system compared to wide-field microscopy is shown in Figure 5. These images are (a) SIM and (b) wide-field fluorescence microscopy of green fluorescence protein-labelled mitochondria in fixed COS7 cells provided by Mike Ryan's group at Latrobe.

Other super-resolution techniques are also currently under development within our group, including STED and SNOM. CXS has also been instrumental in initiating a State-wide consortium, called the Victorian NanoImaging Consortium (VNIC) in an attempt to bring together as many parties as possible who are interested in the various super-resolution optical microscopy approaches and their applications. Through this initiative we have hosted a super-resolution microscopy workshop at Latrobe University and identified a very large level of interest through many institutions, and we hope this will help coordinate future instrument development, purchases and usage.

Figure caption: (a) Structured illumination microscopy image compared to (b) wide-field microscopy image of GFP-labelled mitochondria in fixed COS7 cells.



SHORT WAVELENGTH LASER SOURCE PROGRAM CASE STUDY

Because of the high ionization energy and small cross section of the helium atom radiation with much shorter wavelengths can be generated and the optimal gas pressure is typically much higher than in the case of an argon gas atom [1]. Under these conditions, the harmonic emission from helium has a significantly short coherence length. The optimal interaction length, the focus position and the intensity of the fundamental beam, which are related to the plasma formation and the Gouy phase shift, have to be studied in more detail in order to balance the harmonic generation process with the re-absorption. Effectively, we show that a harmonic beam with 4 to 6 intense harmonic orders around ~ 9 nm is obtained [2]. Thus, this source is a potential source for time-resolved spectroscopy, such as femtosecond photoelectron spectroscopy, in the extreme ultraviolet and soft x-ray region [3], and for multiple-wavelength CDI with high spatial resolution [4], where a few harmonic orders of short wavelength or a dominant photon energy are required and any optics in the harmonic beam path is undesirable.

1. L. Van Dao, S. Teichmann, J. Davis, and P. Hannaford, J. Appl. Phys. 104, 023105 (2008)
2. S. Teichmann, P. Hannaford, L.V. Dao, App. Phys. Lett. 94, 171111 (2009)
3. M. Bauer, J. Phys. D: Appl. Phys. 38, R253 (2005)
4. B. Chen, R. D. Dilanian, S. Teichmann, B. Abbey, A. G. Peele, G. J. Williams, P. Hannaford, L. Van Dao, H. M. Quiney, and K. A. Nugent, Phys. Rev. A 79, 023809 (2009)

STRUCTURE DETERMINATION METHODS PROGRAM

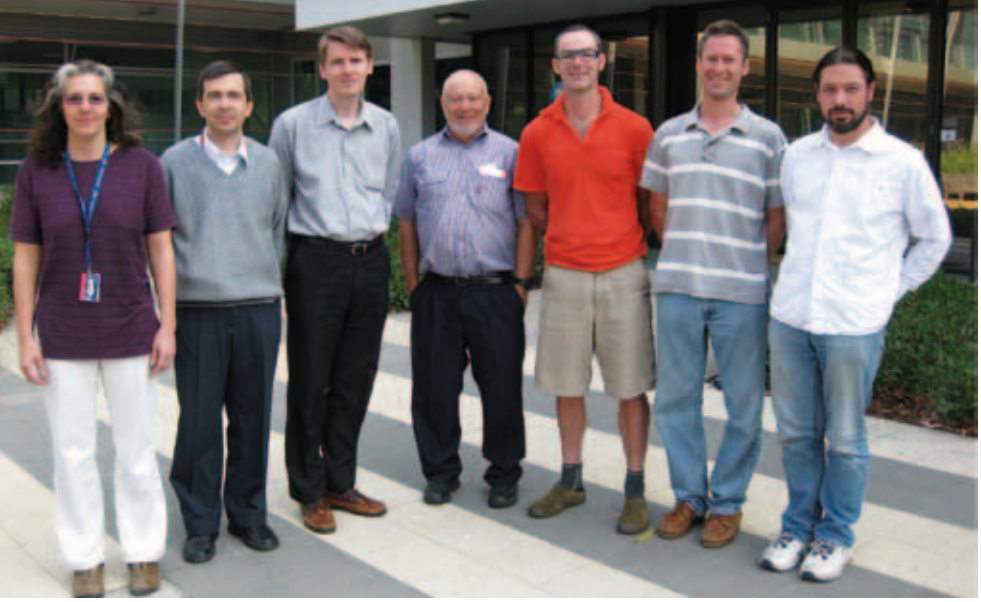
The Structure Determination Methods Program (SDP) consists of CSIRO researchers working broadly within the fields of X-ray and electron crystallography in collaboration with other CXS Centre members. Its main aim is to develop novel experimental techniques and data analysis methods for extracting structural information from 2D crystals and 3D nanocrystals, especially relating to the determination of the structure of the pharmaceutically very important class of proteins known as integral membrane proteins. This Program brings with it internationally recognised expertise in the preparation, purification, crystallization and handling of these samples.

The ongoing study of Purple Membrane, a naturally occurring 2D crystal of the membrane protein Bacteriorhodopsin, serves as a useful test case because there is high-resolution structural information available from 3D X-ray crystallography and 2D cryo-electron microscopy that can be used for comparison. Collaboration under CXS centre has helped link into expertise in developing and applying computer programs for deconvoluting data for diffraction from 2D crystal powders and led to alternative ways to explore the use of 2D crystal samples in the context of different X-ray diffraction techniques.

Development has begun of novel experimental and related theoretical methods for the preparation and analysis of powder samples for integral membrane proteins. These techniques include preparation of and data collection from various 2D crystal powders, a little explored line of approach. They offer the exciting possibility of providing alternative and easier paths to the X-ray structure determination of this very important class of proteins that have mostly resisted efforts based on conventional 3D single-crystal methods.

On the CSIRO Molecular & Health Technologies (CMHT) side, work has progressed on the preparation of a number of different types of powder samples of integral membrane proteins consisting of preferentially and randomly oriented 2D crystal layers.

Work at CSIRO Materials Science and Engineering (CMSE) has been continuing on the development of analytical methods for structure determination using X-ray diffraction with two-dimensional (2D) protein crystals in powder samples. The research can broadly be divided into three areas. The first is concerned with fitting 2D powder diffraction data using a non-empirical approach based on a physical model of the scattering process. The second and third areas are closely linked: phase retrieval and refinement, and structure determination. While these are separate problems, they are generally best treated together. Structure determination in the 2D crystal powder diffraction context amounts to reconstruction of a 2D projection map of the electron density in the crystal. This can be viewed as a technique between coherent diffractive imaging and 3D crystallography aimed at high-resolution 3D structure determination. The advantage of the technique being developed here is that it does not require 3D crystals, nor does it require 2D crystals of the size needed for structure determination by electron diffraction.



The Structure Determination Methods Program team

ACHIEVEMENTS

NEW METHODS OF STRUCTURE DETERMINATION

Phasing low resolution bR data for structure imaging using solvent flattening and flipping using small increments in resolution required for phase improvement and obtaining higher resolution images. Initial trials indicate that the solutions are unstable, so protocols are being developed for phase combination using methods developed for 3D protein crystallography.

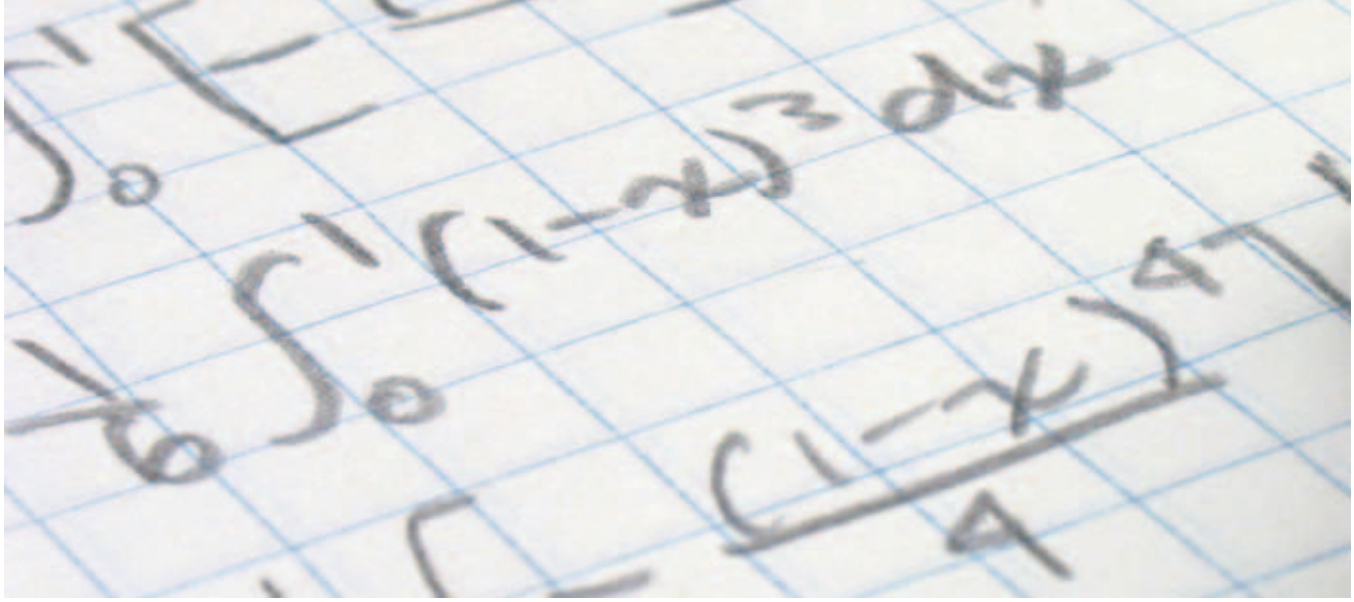
Work has progressed on structure determination methods, particularly on adapting the solvent flattening method of phase refinement to 2D powder diffraction data. A stepwise "one data point at a time" iterative scheme has been implemented and reconstructions performed from previously acquired synchrotron data. The algorithm also incorporates a strategy to resolve exactly overlapping non-equivalent reflections by imposing constraints that ensure consistency with experimental data while allowing other parameters to evolve within the solvent flattening scheme. It is considered that the robustness of the algorithm, especially with respect to sensitivity to the initial low-resolution guess for the electron density, needs to be improved by incorporating a figure-of-merit weighting scheme for unknown phases and possibly by combining solvent flattening with a maximum entropy method. A paper providing a physical model for fitting 2D protein crystal powder diffraction data is in a late stage of preparation for Acta Crystallographica A.

MEMBRANE PROTEINS

G-Protein Couple Receptors are difficult proteins to express and purify in large enough amounts for crystallization trials. Currently we are expressing both Butyrate and Dopamine receptors in our laboratory.

Butyrate receptors have been cloned into baculovirus vectors and large scale virus has been produce at a high titre. Small scale protein expressions have been carried out in several cell lines (Sf9, Sf21 and HighFives) and have shown to optimally express in Sf9 cell lines. Solubilisation of one receptor has been optimized using FOS-choline and we are currently in the process of testing its functionality and setting up the purification protocol. These proteins, once purified will be used to set up 2D crystallisation trails.

The long form of Dopamine receptor has been expressed and purified and has entered 2D crystallisation trials, 2D crystals are being characterized by EM. Tiny 2D crystals in the order of 1µm in size have been seen under the TEM, but not in abundances. These conditions need to be optimized in order to increase the number of crystals present in the sample and to carry out test studies.



THEORY AND MODELLING PROGRAM

The Theory and Modelling Program (TMP) is responsible for developing the theoretical and computational physics needed to support the experimental programs in CXS. Our interests currently involve (i) the solution of inverse problems (ii) the characterization of partial spatial and temporal coherence in short wavelength light sources (iii) the relativistic formulation of molecular electronic structure and quantum electrodynamics (iv) the dynamical description of non-linear interactions between molecules and strong coherent fields (v) coherent energy transfer processes in biomolecules, (vi) the design of efficient computational algorithms and (vii) structural analysis and molecular characterization using powder diffraction techniques.

The Theory and Modelling Program collaborates closely with the other programs in the Centre, especially in identifying fruitful directions for the experimental programs to pursue, and by supporting these activities with theoretical and computational tools. The key aims of TMP involve the development of:

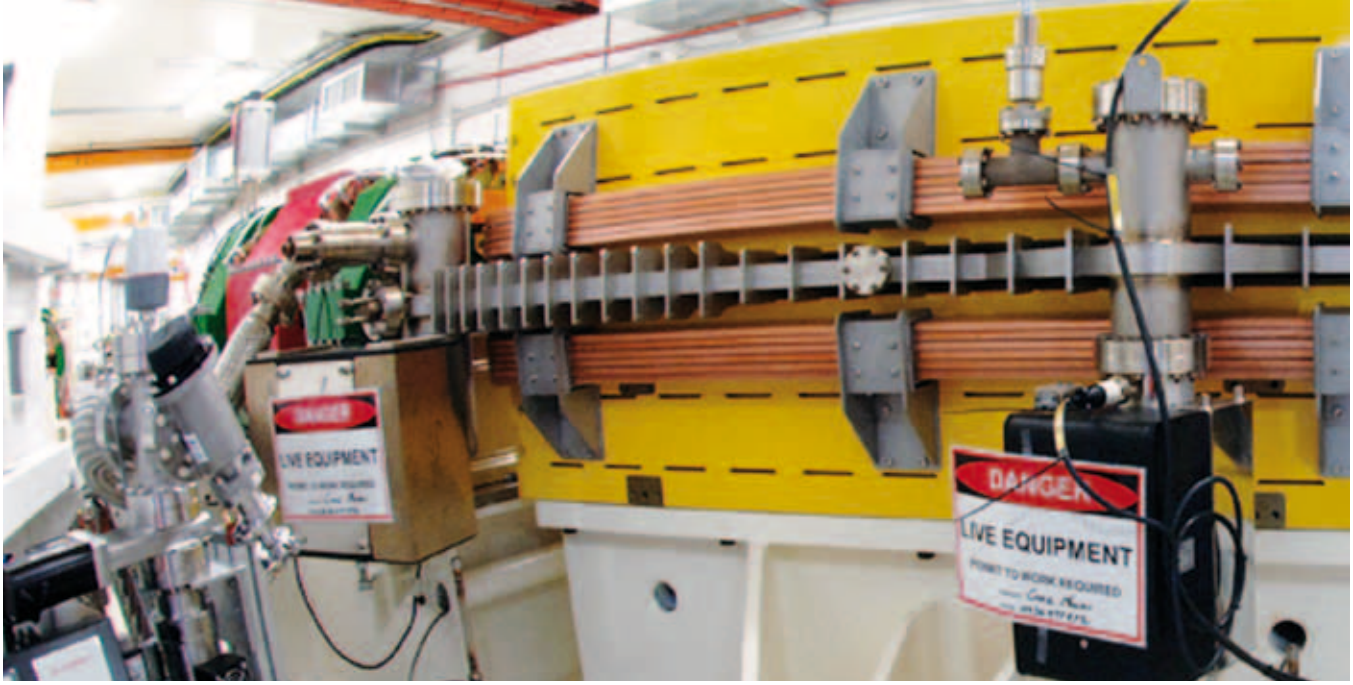
- Image reconstruction algorithms for diffraction data obtained using sources exhibiting partial spatial or temporal coherence.
- Quantum electrodynamical models of high-harmonic generation and above threshold ionization in atomic systems using visible and infra-red light sources.
- Models of the interaction of molecules with strong-field high-frequency X-ray free-electron laser (XFEL) sources and high brightness coherent electron sources.
- Non-interferometric phase recovery techniques in photon echo spectroscopy.

ACHIEVEMENTS

The Theory and Modelling Program (TMP) collaborates closely with the physics-based experimental activities in CXS: the Experimental Methods Program (EMP), the Short Wavelength Laser Source Program (SWLP), the Ultra-Cold Plasma Source Program (UCP). In the second half of 2009, largely as an outcome of the CXS Retreat at Beechworth, new collaborations were also initiated with the Australian Attosecond Sciences Facility (AASF) at Griffith University, the Biological Sciences Program (BSP) at La Trobe and the Structure Determination Methods (SDM) Program within the CSIRO. Consequently, the TMP can identify one or more collaborations with every other active CXS research program. Many of these collaborations are recorded in their reports, and we describe our contributions to them here.

IMAGING ALGORITHMS FOR PARTIALLY COHERENT SOURCES

Our formulation of diffractive imaging algorithms within a representation in which modal expansions play the leading role was realised, and further refined, by the experimental efforts of the members of EMP and SWLP. Initially proposed as a means of reducing the effects of partial spatial coherence on coherent diffractive imaging using synchrotron radiation sources, the scope of this approach was extended to include the spectral structure of the output from an HHG source and, most recently, the spectral structure of a complete synchrotron harmonic in diffractive imaging applications. Moreover, it was also demonstrated that a modal representation of the mutual optical intensity of a synchrotron source may be used to recover its spatial coherence properties directly from experimental data. Two PhD students within CXS, Lachlan Whitehead (EMP) and Sam Flewett (EMP), have developed this approach into a set of powerful tools for imaging applications in which the source falls short of the ideal case in which it possesses complete spatial and temporal The use of HHG sources for imaging using modal expansions was developed by post-doctoral researcher Bo Chen (EMP)



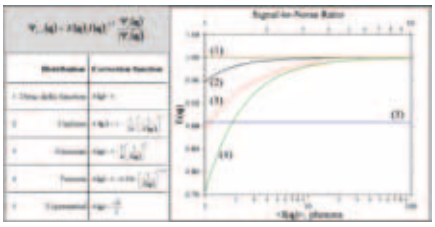


Figure 1: Analytical representation of the correction function for a statistically regularized amplitude constraint.

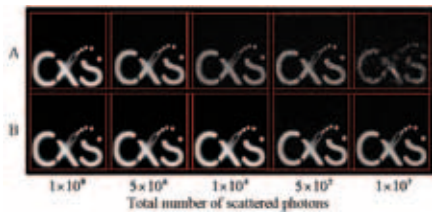


Figure 2: Reconstructions from the noisy data. (A) Reconstruction without statistical correction. (B) Reconstruction with statistical correction.

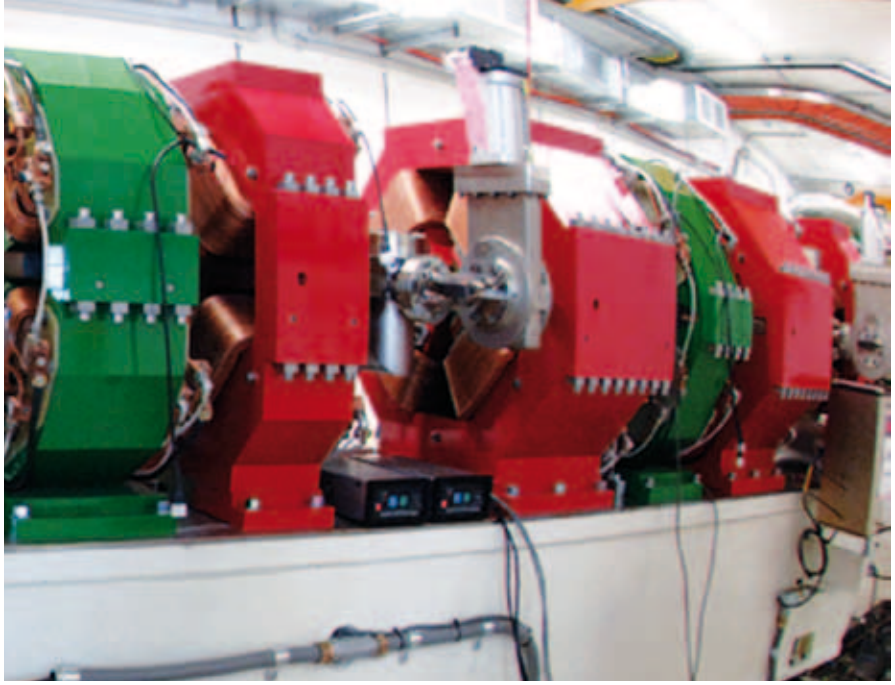
and PhD student Sven Teichmann (SWLP), in collaboration with senior members of CXS. The resolution of the handedness of optical vortices with the controlled use of cylindrical phase curvature was achieved, using experimental data, in a collaboration with Clare Henderson (EMP), a PhD student.

Another aspect of diffractive imaging in which the experimental conditions fall short of ideal behaviour concerns the influence of measurement noise on the quality of reconstructions. A collaboration with EMP and led by Ruben Dilanian, resulted in the development of a statistically- based method to handle experimental diffraction data, including the effects of measurement noise. The formulation introduces a statistical correction factor, denoted E(**q**) in Figure 1, which adjusts the estimate of the coherent wavefield amplitude that is employed as a constraint in iterative imaging algorithms. The effect of this prescription is to suppress the estimated amplitude if the signal-to-noise ratio is small, and otherwise to preserve the conventional estimate, $I^{½}$(**q**). The precise details of the correction factor depends on the statistical character of the measurement errors, and in practice an empirical scheme was developed, based on Poisson and Gaussian models.

The efficacy of this approach is demonstrated in Figure 2, in which the effects of Poisson-distributed measurement errors on the quality of image reconstructions are displayed for simulated images in which the total number of scattered photons varies from 105 to 108. Results using conventional algorithms are displayed in Row A of Figure 2, while results obtained using the statistically regulated scheme appear in Row B. The gradual degradation of the image in Row A is apparent, as the signal-to-noise ratio of the diffraction data corresponding to the largest scattered angle approaches unity. The regulated results in Row B show almost no degradation, even for the simulation corresponding to 105 scattered photons. This represents a typical practical limit in the number of photons that need to be scattered in order that sufficient information exists to obtain an image with a resolution close to the theoretical diffraction limit. The use of the statistical regulator brings clear benefits in image reconstruction quality for negligible additional computational cost.

STRUCTURE DETERMINATION OF MOLECULES USING FREE-ELECTRON LASERS

An unexpected insight into the use of free-electron X-ray lasers for molecular structure determination by diffractive imaging was obtained from the development of coherent mode expansions of partially coherent light sources described earlier. It has generally been assumed that a free-electron X-ray laser source would possess full spatial coherence but, as become apparent recently, such sources are described at their host facilities at Hamburg and Stanford as being "neither free, nor lasers". Even on the assumption of high spatial coherence of a single frequency component of such a source, their high brightness leads to a large number of competing electrodynamical processes in any electronic target, such as a molecule, drafted to serve as a scattering target. The electronic structure of a molecule



undergoes profound changes during an encounter with a five femtosecond pulse from an XFEL, even if the nuclear framework does not distort significantly during that period. Even if the illumination on such a target is fully coherent and perfectly monochromatic, the radiation scattered from it behaves as if it is a partially-coherent secondary source, because of the rapid evolution of the electron density throughout its interaction with the pulse. This led us to adapt the physical principles embodied in the expansion of partially coherent sources in modal basis sets to the description of the interacting molecular density as a set of electronic modes. This was reported at the SRI Satellite Workshop hosted by CXS in October 2009, and since been developed, with the participation of graduate students Evan Curwood (EMP) and Rebecca Ryan (EMP), into a working algorithm to recover molecular structures from diffraction data using X-ray free-electron laser sources, including the effects of damage to the electronic structure. This development represents, in our view, the removal of a significant obstacle along our journey towards the primary research goals of CXS.

ULTRA-COLD ATOM IMAGING AND COHERENT ELECTRON DIFFRACTION

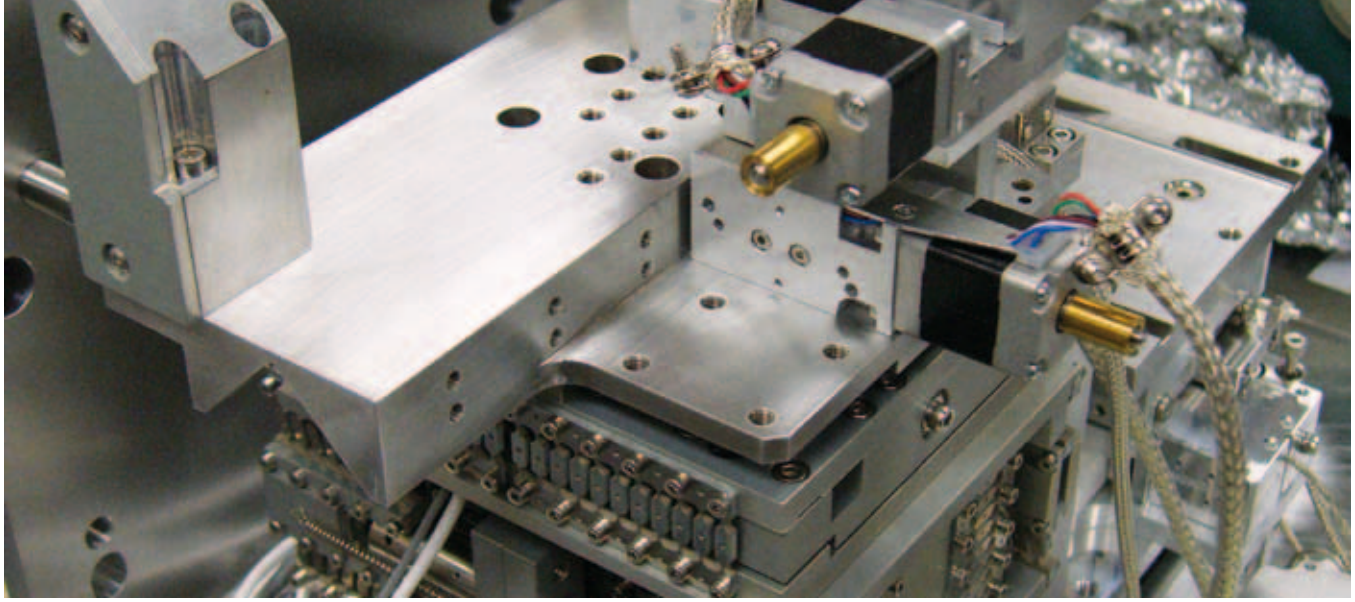
A non-iterative phase retrieval algorithm developed by TMP, based on functional analysis, was adopted by UCP in order to image cold atom clouds from a single optical measurement. The development of this technique provides a good example of how regular interactions between the groups can fortuitously lead to surprising solutions to problems. This project sprang out of student report by Sebastian Saliba, in which it became clear that the standard techniques were deficient. This has since been developed and published as a routine methodology within UCP for imaging the cold-atom clouds that are to be used as targets in their ultra-cold plasma research. Our contribution to this project will now focus on the problem of extracting structural information from scattering data obtained using their coherent electron source and nano-scale electronic targets. Many of the techniques already developed for X-ray diffraction imaging can be utilized in these studies, including the use of optical mode expansions to accommodate partial coherence of the electron probe incident on the target.

FOURIER TRANSFORM SPECTROSCOPY

The collaboration with Dr Jeff Davis (Swinburne) continued to develop phase retrieval techniques for Fourier transform spectroscopy, and the use of this non-interferometric technique in understanding energy transfer dynamics within chromophores. This work was supported by an ARC Discovery Project, which formed a partnership involving members of SWLP, TMP, EMP and a Japanese researcher. The method was considerably refined throughout the year, and benefited from the close interaction of Dr Davis with a leading group at U.C. Berkeley during his extended visit to the laboratory of Prof. G. R. Fleming. It was demonstrated that the phase retrieval approach is, with a small number of well-characterized exceptions, able to recover the same dynamical information that is obtained using interferometry. The great advantage of our new approach, which combines local expertise in imaging and ultrafast spectroscopy, is that we are also able to recover this information in two-colour four-wave mixing experiments, greatly extending our ability to interrogate the dynamics of light-harvesting complexes and quantum dots.

MOLECULAR PHYSICS AND QUANTUM CHEMISTRY

Our long-standing and fruitful collaboration was continued with the University of Perugia in the development of high-performance algorithms in relativistic density functional theory. These will feed into CXS programs through the development of 'real-time' methods for modelling the time-evolution of molecular systems subjected the light from fourth-generation XFEL sources, and the modelling the optical properties of scattering targets containing heavy elements.



CASE STUDY

While CXS is dedicated to the development of new methods in the structure determination of membrane proteins, it would be unwise simply to discard the possibilities offered by existing methods, suitably refined and extended. Membrane proteins do not, as discussed elsewhere in this report, generally form large crystals suitable for conventional protein crystallography. It is possible, however, to obtain nano-crystalline samples of high purity that might form the basis of studies using powder diffraction. The number of membrane protein structures that have been solved using this approach is small, and the method of solution requires very careful use of all of the available diffraction data and the incorporation of a considerable amount of a priori structural information in the solution algorithm.

In a collaboration involving the SDM at CSIRO at Parkville and Monash and the BSP at La Trobe University, Ruben Dilanian demonstrated that the powder diffraction method can be applied to the determination of the structure of bacteriorhodopsin, our prototype membrane protein molecule for which the structure is known to high accuracy by independent methods. A critical component of his analysis concerns the initial fit to the experimental data, Figure 3(a) which must be corrected for background errors and signal from the solvent. The anisotropic line-shape profiles must also be preserved in this process so that information from near-coincident reflections may be resolved, and the relative contributions from fully-overlapping reflections represented accurately.

This advanced refinement of protein structure determination by powder diffraction and the world-leading expertise within CXS, our CSIRO partners and our international collaborators in the purification, preparation and handling of these samples, may well offer a viable route to achieve our primary research goals. Certainly, the successful demonstration of this approach using experimental data, Figure 3(b,c) indicates that we should be alert to all possibilities to achieve our goals.

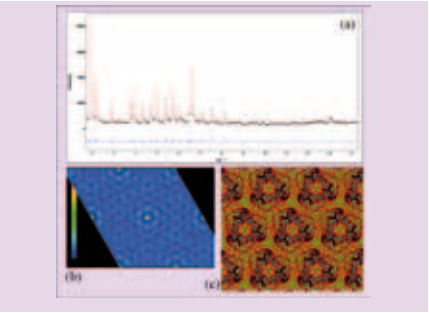
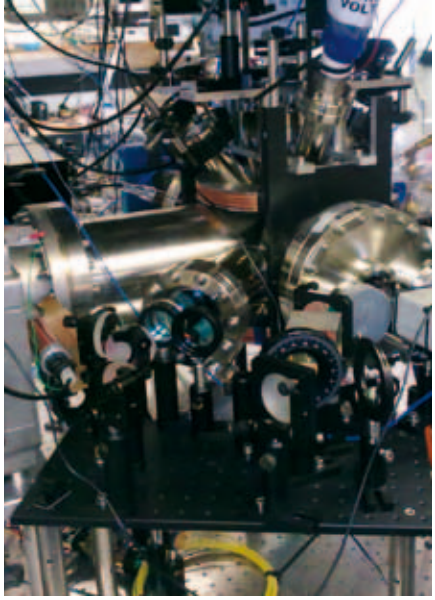


Figure 3: Structure of bacteriorhodopsin from powder diffraction data. (a) Pattern fitting using Le Bail analysis. (b) Patterson Map at 4 Å resolution. (c) Electron density at 7 Å resolution.

Ultra Cold electron source.



ULTRA-COLD PLASMA SOURCE PROGRAM

The Ultra-Cold Plasma Source Program (UCP), formed within CXS in 2007, is developing an ultra-bright, coherent source of electrons for imaging of biologically relevant targets. By applying technical developments taken from the ultracold atom community, and the theoretical algorithms developed in the TMP program, we will enable a new approach to electron imaging. The enhanced probe-molecule interaction strength that a coherent electron source offers, combined with an improvement of four orders of magnitude in brightness over existing electron sources, will enable high-resolution imaging of biological targets with atomic scale resolution.

The crux of the UCP source, the basis of the dramatic enhancement in brightness that it promises, is the origin of the electrons: they will be extracted from ultracold atoms, just a few millionths of a degree above absolute zero. The brightest conventional electron sources start with hot material, by blasting a target with a high-energy laser pulse. The hot electrons then expand like steam from a kettle, and are equally difficult to tame and control. Electrons extracted from ultracold atoms can be accelerated and focused with unprecedented resolution. The comparison is like that of a conventional light bulb and a laser: we need laser-like coherence and brightness to image molecular structure with atomic resolution.

The UCP team has strong expertise with ultracold atom technology, with conventional optical imaging, and with electron optics. They are collaborating with the world-leading research group in this area, at the University of Eindhoven in The Netherlands. The project is strongly connected with the Centre's TMP program. We have jointly published work based on the Centre's imaging approaches for applications in characterising the cold atom cloud. We are now collaborating with the TMP group to employ their expertise on partially coherent x-ray sources for modeling our now-operational electron source. The theoretical formalism of partial coherence has not previously been applied to electron imaging, but recent development of new sources has made partial coherence highly relevant. Our modeling will be used to design the imaging component of our system, firstly to enable verification that the electron source is indeed coherent and bright, and secondly to enable imaging applications. In the longer term, collaboration with TMP will be essential to unravel electron-molecule interactions so that target structural information can be separated from the complexity of the diffraction data. The ultimate goal, the high-impact demonstration of electron diffraction from molecules, will require close liaison with the Biological Sciences Program, to determine the optimum biological targets and the appropriate sample

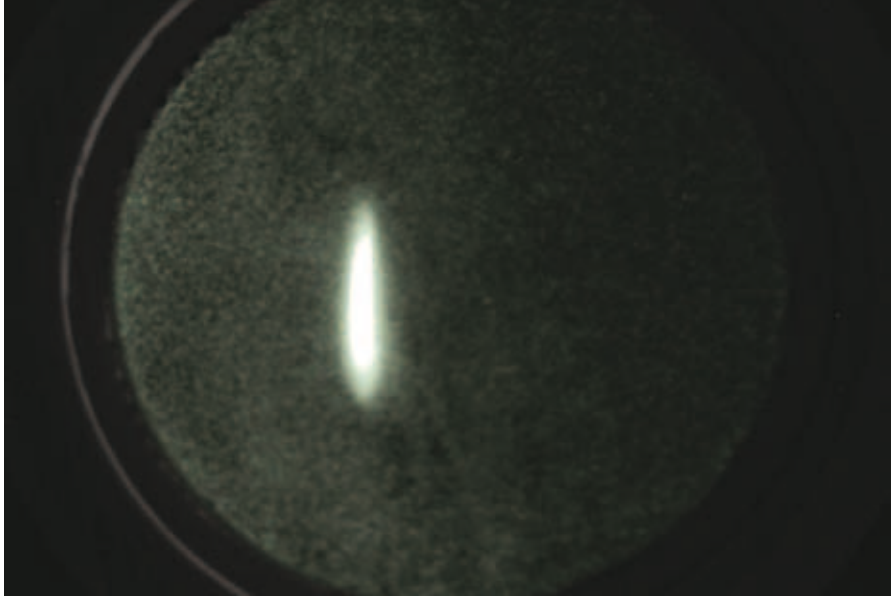


Fig. 1: Ultracold electron bunch illuminating phosphor screen.

preparation strategies. Our initial collaboration with BSP has established two-dimensional crystals of bacteriorhodopsin as a promising target for the first experiments. Such inter-program collaborations, the envy of our colleagues at Eindhoven, are simply not available to other groups around the world and will allow the UCP team to rapidly achieve high-impact results across disciplines.

ACHIEVEMENTS

THE ULTRA-COLD PLASMA SOURCE PROGRAM (UCP): PROGRESS IN 2009

The group has made substantial progress during 2009, in particular successfully demonstrating its novel slow atom source, cooling and trapping of the slow atoms, photoionisation of the cold atom cloud, and production of electron bunches (Fig. 1).

We developed a novel source for the slow atoms, beginning with a highly efficient effusive oven, followed by a Zeeman slower using a tapered helix solenoid to produce a precisely shaped magnetic field (Fig. 2). The source generates a large flux of slow atoms which dramatically enhances our ability to create high charge electron bunches (Fig. 3). *Rev. Sci. Instrum.* **81** 013105 (2010).

The atoms are trapped between counter-propagating lasers in a combination mirror/electrode system (Fig. 4). Once a large, high-density cloud of cold atoms has been formed, they are ionized by an intense nanosecond pulse of laser light at precisely the energy needed to separate the electrons, which are accelerated by the electric field established between the mirror electrodes. The electrons are detected on a phosphor screen CCD imaging system (Fig. 1).

Lasers are a critical component of the ultracold electron source, in particular the frequency tunable narrow linewidth diode lasers used to slow atoms along the Zeeman coil, cool atoms in the magneto-optic trap, image the cold atoms, and to excite the atoms prior to the photoionisation laser flash. We have investigated two performance metrics for external cavity diode lasers, establishing critical factors affecting laser linewidth and mode stability. *Appl. Opt.* **48** p6961, 2009; *Appl. Opt.* **48** p6692, 2009.

The qualities of the electron bunch depend on the distribution of cold atoms. In collaboration with the TMP group, we developed a new approach to imaging cold atom clouds, based on coherent diffractive imaging (CDI) concepts. The method is important across cold atom research areas, such as for Bose-Einstein Condensation experiments, because it allows for the fist time a method to extract both the amplitude and phase of an atomic cloud, using only non-interferometric intensity images. *Optics Express* **18** p1586 (2010).

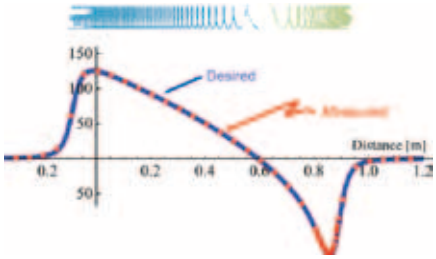


Fig. 2: Atoms are slowed from 350 m/s to a few tens of m/s using a novel Zeeman slower. The slower uses a tapered helix solenoid (top) which produces a precisely shaped magnetic field (below). Rev. Sci. Instrum. 81 013105 (2010).

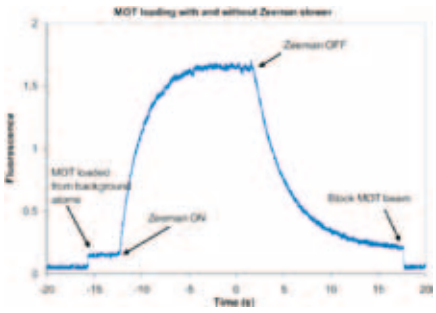


Fig. 3: Demonstration of enhanced cold atom production using Zeeman slower source.

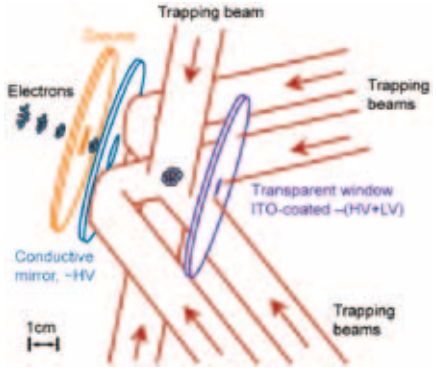


Fig. 4: Combination mirror/electrode system, to cool and trap atoms, and accelerate electrons.

Finally, again in collaboration with the TMP group, we are developing a computational simulation of partially coherent electron imaging, using Fresnel wave propagation in combination with a Gaussian-Schell model for partial coherence. Figure 5 shows calculated electron and x-ray diffraction patterns for a two-dimensional crystal of bacteriorhodopsin molecules, and recovered electron density distributions, for plane wave illumination.

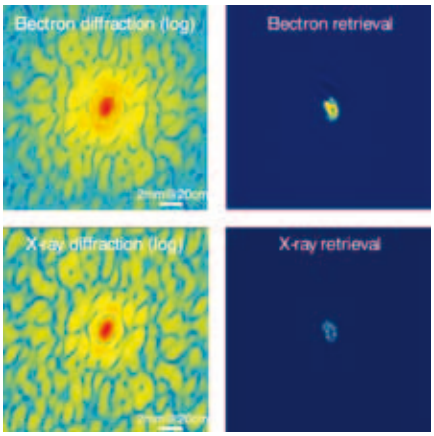


Fig. 5: Calculated electron and x-ray diffraction patterns (left) and object retrievals (right), for plane wave illumination of two-dimensional bacterio¬rhodopsin crystals. Established atomic form factors are used for both x-ray and electron diffraction.

ULTRA-COLD PLASMA SOURCE PROGRAM CASE STUDY

THE ULTRA-COLD PLASMA SOURCE PROGRAM (UCP): CASE STUDY

In 2009, the UCP Program achieved its primary goal of producing cold electrons by cooling and trapping atoms and then photoionising those atoms to release the electrons. One step towards that goal was a reliable, robust, efficient source of very slow atoms. At room temperature, free neutral atoms such as those in air move at speeds of several hundred metres per second (over 1000 km/hr). We use lasers to slow our atoms down to speeds of a few metres per second, in the first instance using lasers and a carefully shaped magnetic field. The method led to the award of a Nobel prize to Bill Phillips in 1997. We used the method of Phillips, but our magnetic field was produced with a novel electromagnetic solenoid consisting of just one winding of hollow wire (actually refrigerator copper tubing). The winding has a variable pitch (see figure 2), closely spaced where we need a strong field and widely spaced where the field must be weak. PhD student Simon Bell calculated the winding spacing using a detailed model formulated in Mathematica®. When constructed and tested, the agreement between prediction and model was extremely precise, and more importantly, the slower worked brilliantly: we increased our flux of slow atoms by nearly a hundred-fold. The large number of atoms that we can obtain will allow us to create high density cold atom clouds and high brightness electron bunches for biological imaging. *Rev. Sci. Instrum.* **81** 013105 (2010).

STUDENTS LIFE @CXS

STUDENTS LIFE @ CXS

JEFF YEOMAN, BIOLOGICAL SCIENCE PROGRAM

LA TROBE UNIVERSITY

As part of the CXS I am carrying out my PhD studies in Leann Tilley's lab within the Biological Sciences Program. My project has been characterising the inner membrane complex of the Malaria parasite, *Plasmodium falciparum* using fluorescence microscopy. As well as presenting my own work at conferences throughout the past year, being part of the CXS in 2009 has given me the opportunity to attend a number of workshops. One highlight was the CXS retreat in Beechworth. It was good to be involved in discussions and to give feedback on how each program was going at an important time for the centre. I was also a presenter at the 'Talking Backwards' workshops where I had to research and present a seminar explaining structure determination. The exposure CXS has given me to the various techniques outside my area of expertise has been interesting and valuable to my development as a scientist.

Jeff Yeoman preparing samples.

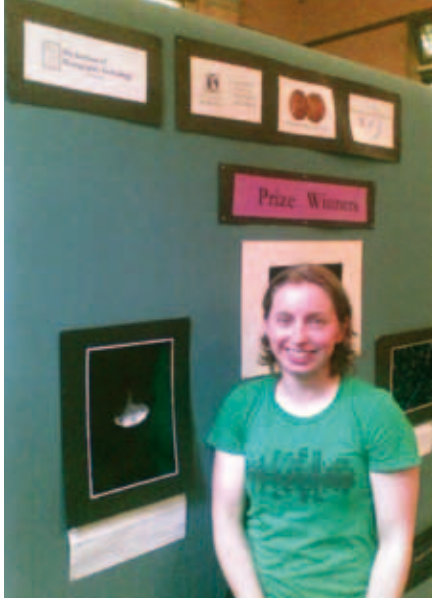
Sebastian and friends enjoying CXS retreat presentations in the sun.

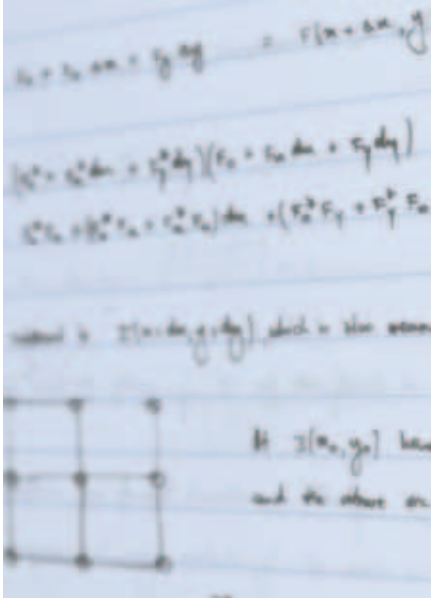
SEBASTIAN SALIBA, ULTRA-COLD PLASMA SOURCE PROGRAM

UNIVERSITY OF MELBOURNE

My 2009 was a solid year in the Ultra Cold Plasma Source Program. It's great being involved in a well-resourced group both financially and intellectually. As a member of CXS I had the opportunity to present my work at the International Conference on Laser Spectroscopy in Japan during June, as well as having access to workshops such as Talking Backwards, where physicist David Vine presented an excellent talk on *Understanding protein structure*s that I found particularly beneficial, and the Beechworth retreat which I've reported on previously. It's also great to be part of a group that is concerned with student advocacy and interests, such as the intellectual property seminar and forum, and the postgraduate-postdoctoral workshop being organised for 2010. My PhD progress has benefited greatly from having direct access to other CXS members' expertise, as well as collaborating with international visitors such as Jolanda van der Ven when she was on sabbatical with the UCP group in September. Somehow with everything that's going on in the CXS I still found time to have two papers published!

Clare Henderson and the award winning photo at the Under the CoverSlip Scientific photography competition.





CLARE HENDERSON, EXPERIMENTAL METHODS PROGRAM

UNIVERSITY OF MELBOURNE

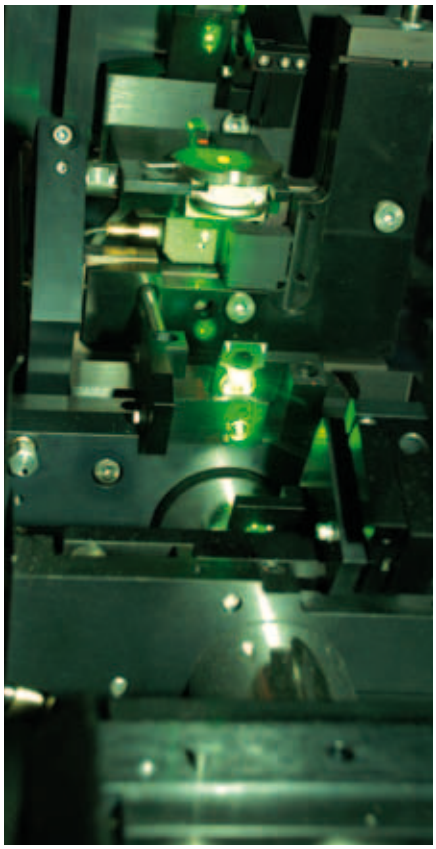
My PhD research has been on the phase retrieval of optical vortices. An optical vortex is a light beam, which has a spiralling phase. They can appear spontaneously in any light field, and cause hindrances to the many phase retrieval algorithms developed by the Experimental Methods Program.

Using the CXS optical laboratory to create and photograph optical vortices, I tested new phase retrieval methods. 2009 saw the results published, and one of my movies of phase retrieval on a vortex was chosen as the cover for Optics Express for that issue.

The success of 2009 continued for me when I was awarded 2nd prize in the "Under the Coverslip" scientific photography competition, held for post-graduate students of The University of Melbourne. One day in the lab, quite by chance, I knocked a lens causing the vortex to fold in on itself. Liking the image, I photographed it, not realising at the time that it in fact shows an interesting optical effect that only a vortex can produce – a split fringe – making it a useful optical experiment.

My photograph was the only non-biologically related image in the competition, and differed from the others because it is not of a sample per se, but of light interfering with itself – its three dimensional appearance being an illusion. Being a member of the CXS has given me a good foundation for communicating physics concepts to scientists with a biological background – which came in handy when asked to give an impromptu speech and explanation of the photograph at the awards night.

FRIEND OR FOE



One of the important goals of a Centre of Excellence is to ensure that its members have access to state-of-the-art scientific facilities with a performance that is second to none. CXS is all about the application of X-ray techniques to problems in the biosciences and we wanted to ensure that we were able to provide access to the best resources possible.

As such, as part of the Experimental Methods Program under the leadership of Andrew Peele, we commenced negotiations for the acquisition of a state of the art interferometrically controlled experimental endstation specifically designed to enable our work in Fresnel coherent diffraction imaging. We have dubbed this instrument the FREsnel Imaging END station, or FRIEND.

The facility was commissioned via the Californian based company Xradia run by Wenbing Yun, an ex-synchrotron scientist with an excellent reputation that was also shared by Xradia. For our work, we have particularly stringent demands on the satbiloty of the system – it must hold the sample in the same place for hours to within a few nanometres.

With the design underway, we needed a place for it to be located. CXS had developed an excellent relationship with the National Synchrotron Radiation Research Centre (NSRRC) in Taiwan and we had negotiated an agreement that we locate the facility there, signed a Memorandum of Understanding to underpin the agreement and successfuly acquired a grant from the ARC to develop this collaboration. There were some problems with the choice, including the facts that the source was second generation and so did not have as great a coherent flux as we would have liked, and the floor had some vibration problems. However we were confident that these issues could be manage, the NSRRC were showing themselves to be excellent partners and contributors to the program and the beamline wold operate in the biologically important water window region of the X-ray spectrum.

Shortly after the MOU had been signed, to considerable fanfare, we were approached by the Advanced Photon Source and asked if we would like to locate FRIEND at the 2-ID-B line. There were pros and cons. The pros were that the APS is a world-leading third-generation synchrotron source with whom we had been working for many years, and the floor was very stable with the result that the technical issues were likely to be more tractable. The cons were that we would no longer have access to the water window at this location and, importantly, that we would be reneging on an agreement with our valued collaborators at the NSRRC. After considerable debate, it was agreed that we had an obligation to follow the course that would bring most benefit to CXS members and that this was the one offered by the APS. I therefore wrote a very sheepish letter to the Director of the NSRRC, Professor Keng Liang, explaining our decision. Keng accepted with very good grace – he had every right to be angry with us.

FRIEND TIMELINE

FRIEND CONCEIVED

JUNE 2005

2006

DESIGN STAGE

BUILD COMMENCES

FEB 2007

JUNE 2007

MOU WITH TAIWAN

AGREEMENT WITH APS

JAN 2008

2008

PARTNER USER PROPOSAL

LIEF TO UPGRADE SCANNING MICROSCOPY

MID 2008

2009

TROUBLE SHOOTING

COMPLETE UPGRADE & OPERATIONAL

2010

2011

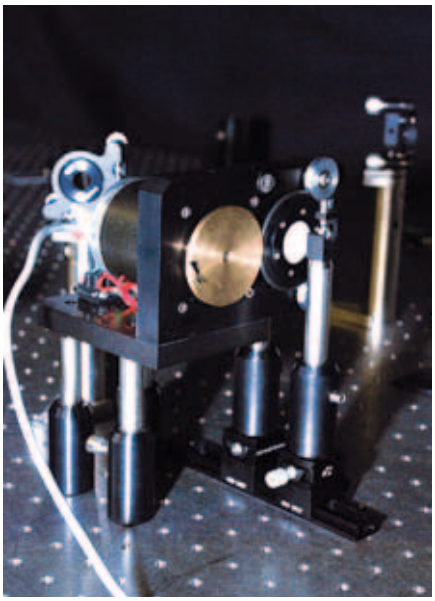
BUILD LIEF COLLABORATION FOR SCANNING TRANSMISSION X-RAY MICROSCOPY

ORGANISE MOVE TO AUSTRALIA

2012

2013

OPERATING AT AUSTRALIAN SYNCHROTRON



Access to the APS was, with the closure of the Australian Synchrotron Research Program (ASRP), an issue. However we were successful in being awarded a Partner User Proposal (PUP) giving us guaranteed access to the APS for a period and the Australian Synchrotron, the organisation that inherited the responsibilities of the ASRP, agreed to fund our travel to the facility for commissioning and operation. In return, we agreed to enable access to the facility to other Australian users. The PUP agreement also required us to provide access to other APS users from around the world.

With the agreements and funding in place, we now sought to get the machine to operate to the required specifications. This has turned out to be an amount of work that we simply did not anticipate. The requirements to keep the sample in place with the required precision are enormous and, it has to be said, have turned out to be initially beyond the capabilities of the supplier. The testing, trouble-shooting and re-design tasks have been enormous. We owe Andrew Peele and Garth Williams a particular debt of gratitude for the work they have put into getting all of this sorted out. In 2008, Garth calculated that his average speed, 24 hours a day 7 days a week, was in excess of 20 km per hour due to the number of times he crossed the Pacific in this trouble shooting process. Qantas loved him! Garth seemed to thrive, though he did get increasingly grumpy.

CXS needs to play a community leadership role. FRIEND has, with some additional investment, the capacity to be a very flexible X-ray microscopy device. We therefore led, at the beginning of 2008, a collaboration that successfully sought funding from the ARC LIEF program to enable FRIEND to ultimately be brought back to the Australian Synchrotron. This collaboration consists of a number of CXS members but also other parts of Monash University, The University of Sydney, The University of Newcastle, The University of South Australia and the Australian Synchrotron. The agreement also sees the Australian Synchrotron fund a post-doctoral fellow to work on external users with the facility.

2009 saw the teething problems finally ironed out. This has put us about one year behind schedule but we are now able to solidly move forward on opening up the facility to other users and to commence the upgrade process. We have paid a sum to the AS for the development of the branchline at which FRIEND will be located and are now in detailed negotiations for the next stage in the upgrade.

It has been a difficult birthing process and technological development is hard. However, while our FRIEND was looking more like a foe for a while, we seem to have managed to make-up. We are now well on track and fully anticipate excellent science to come from FRIEND through 2010 and beyond.

CXS MANAGEMENT & GOVERNANCE

CXS MANAGEMENT & GOVERNANCE

CXS is a collaborative research program between the University of Melbourne, La Trobe University, Monash University, Swinburne University of Technology and CSIRO, funded under the Australian Research Council (ARC) Centre of Excellence program and the Victorian Government's Science, Technology and Innovation (STI) Initiative.

As Lead Administering node, the University of Melbourne manages the grants and distributes funds in accordance with the signed agreements. These agreements cover CXS management, collaboration and intellectual property arrangements.

All collaborating organisations are represented within CXS boards. Commercial expertise is represented on the CXS Intellectual Property Committee and Sub Committee. A Scientific Advisory Board and a General Advisory Board have been established and meet annually.

CENTRE MANAGEMENT

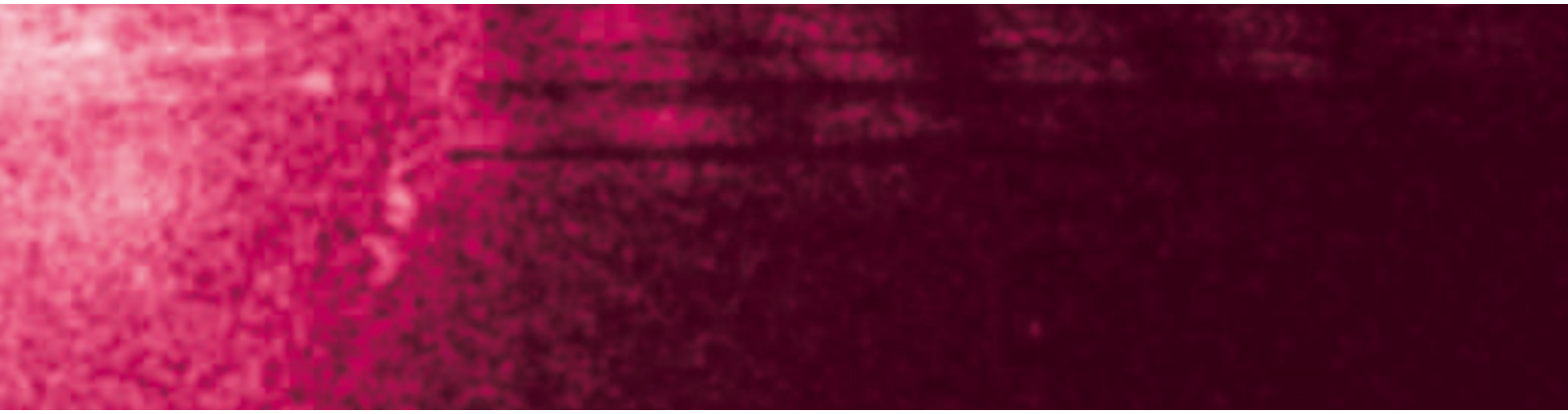
The CXS Management team and its Executive Committee are responsible for administration as it pertains to centre policy, performance, financial matters, research output, research training and professional education of members, partnerships, national and international liaison, commercialisation and outreach.

The management team is:

PROFESSOR KEITH NUGENT
Director of Research

PROFESSOR LEANN TILLEY
Deputy Director of Research

MS TANIA SMITH
Chief Operating Officer



EXECUTIVE COMMITTEE

During 2009, the administration of CXS was overseen by the Executive Committee, which comprises:

MS ROSSLYN BALL
Executive Officer to Committee

DR CHRIS HALL
Detector and Beamline Development Group Member

PROFESSOR KEITH NUGENT
Research Director

ASSOCIATE PROFESSOR ANDREW PEELE
Experimental Methods Group Leader

DR HARRY QUINEY
Theory and Modelling Group Leader

ASSOCIATE PROFESSOR MIKE RYAN
Biological Sciences Group Leader

ASSOCIATE PROFESSOR ROBERT SCHOLTEN
Ultra Cold Plasma Source Program Group Leader

MS TANIA SMITH
CXS Chief of Operations

ASSOCIATE PROFESSOR TREVOR SMITH
Short Wavelength Laser Source Group Member

PROFESSOR LEANN TILLEY
Deputy Research Director

PROFESSOR LAP VAN DAO
Short Wavelength Laser Source Group Leader

PROFESSOR JOSE VARGHESE
Structure Determination Methods Co-Group Leader

PROFESSOR STEVE WILKINS
Structure Determination Methods Group Leader

ADVISORY BOARD

The CXS Advisory Board met in September 2009 as part of the CXS Beechworth Retreat. The meeting focussed on the recommendations of the ARC review, CXS achievements, industry and community outreach and intellectual property.

CXS would like to thanks Ken Ghiggino, Anita Hill and Steven Langford for their contribution to this years meeting.

PROFESSOR TIM BROWN
Deputy Vice Chancellor (Research)
La Trobe University

PROFESSOR EDWINA CORNISH
Deputy Vice Chancellor (Research)
Monash University, or nominee

DR CAL DRUMMOND
CSIRO

PROFESSOR ANDREW FLITMAN
Pro Vice-Chancellor (Research) Swinburne University of Technology, or nominee

PROFESSOR JOHN HELLIWELL
Professor of Structural Chemistry
University of Manchester

DAVID KRENUS
CEO
Cyclotek

DR STEPHEN LANE
Chief Science Officer
NSF Centre for Biophotonic, Science & Technology, UC Davis

PROFESSOR PETER RATHJEN (CHAIR)
Deputy Vice Chancellor (Research)
University of Melbourne

PROFESSOR BONNIE WALLACE
Professor of Crystallography
Birkbeck College

BRUCE WHAN
Chairman of INNOVIC (Victorian Innovation Centre Ltd) & Director Swinburne Knowledge

SCIENTIFIC ADVISORY BOARD

The Scientific Advisory Board members are:

PROFESSOR JOHN HELLIWELL (CHAIR)
Professor of Structural Chemistry
University of Manchester

DR STEPHEN LANE
Chief Science Officer
NSF Centre for Biophotonic, Science & Technology, UC Davis

PROFESSOR KEITH NUGENT
CXS Director of Research
University of Melbourne

PROFESSOR LEANN TILLEY
CXS Deputy Director of Research
La Trobe University

PROFESSOR BONNIE WALLACE
Professor of Crystallography
Birkbeck College

PROFESSIONAL STAFF

ROSSLYN BALL
PA to Director & Administrator,
University of Melbourne

JAMES GIBBONS
Finance Officer, Monash University

NORMA HAYES
Administrator, Monash University

FABIENNE PERANI
PA to Deputy Director & Administrator,
La Trobe University

TATIANA TCHERNOVA
Administrator, Swinburne University

RESEARCH TEAMS

ATTOSECOND SCIENCE PROGRAM

ASSOCIATE PROFESSOR DAVE KIELPINSKI
Program Leader, Griffith University

ASSOCIATE PROFESSOR ROBERT SANG
Research Fellow, Griffith University

ADAM PALMER
Research Assistant, Griffith University

MALCOLM KELSON
Technical Officer, Griffith University

BIOLOGICAL SCIENCES PROGRAM

ABHISHEK AWASTHI
MSc Student, La Trobe University

TIM BROWN
Research Assistant, La Trobe University

SAMANTHA DEED
Research Assistant, La Trobe University

DR MATT DIXON
Research Fellow, La Trobe University

DR JACQUI GULBIS
Structural Biology Division, WEHI

DR ERIC HANSSEN
Research Fellow, La Trobe University

DR NICK KLONIS
Associate Researcher, La Trobe University

LYNN LIANG
PhD Student, La Trobe University

DR ALEX MAIER
Research Fellow, La Trobe University

DR PAUL MCMILLAN
Research Fellow, La Trobe University

VED MOOGA
MSc Student, La Trobe University

LAURA OSELLAME
PhD Student, La Trobe University

ASSOCIATE PROFESSOR MIKE RYAN
Program Leader, La Trobe University

DR DIANA STOJANOVSKI
Research Fellow, La Trobe University

PROFESSOR LEANN TILLEY
CXS Deputy Director, La Trobe University

JEFF YEOMAN
PhD Student, La Trobe University

DETECTOR AND BEAMLINE DEVELOPMENT PROGRAM

ANDY BERRY
Engineer, Monash University

DR WILFRED FULLAGER
Research Fellow, Monash University

DR CHRIS HALL
Research Fellow, Monash University

DR GEORGE JUNG
Research Fellow, Monash University

PROFESSOR ROB LEWIS
Program Leader, Monash University

EXPERIMENTAL METHODS PROGRAM

MAC BA LUU
MSc Student, La Trobe University

DR BENEDICTA ARHATARI
Research Fellow, La Trobe University

NOR AZAH ABDUL AZIZ
PhD Student, University of Melbourne

DR EUGENIU BALAUR
Research Fellow, La Trobe University

GUIDO CADENAZZI
PhD Student, University of Melbourne

DR BO CHEN
Research Fellow, University of Melbourne

JESSE CLARK
PhD Student, La Trobe University

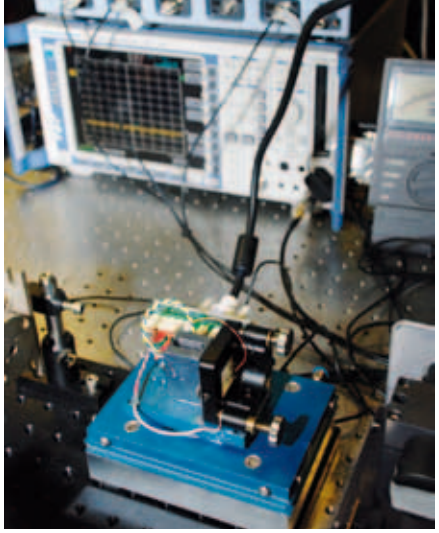
EVAN CURWOOD
PhD Student, University of Melbourne

CHANDNI DOSHI
PhD Student, La Trobe University

SAMUEL FLEWETT
PhD Student, University of Melbourne

KEVIN HANNAH
PhD Student, La Trobe University

CLARE HENDERSON
PhD Student, University of Melbourne



MAC BA LUU
MSc Student, La Trobe University

ASSOCIATE PROFESSOR ANDREI NIKULIN
Research Fellow, Monash University

DR ROBERT NORMAN
Research Fellow, La Trobe University

PROFESSOR KEITH NUGENT
CXS Director, University of Melbourne

ISAAC PETERSON
Honours Student, University of Melbourne

ASSOCIATE PROFESSOR ANDREW PEELE
Program Leader, La Trobe University

DR MARK PFEIFER
Research Fellow, La Trobe University

THANH BAO PHAM
PhD Student, La Trobe University

COREY PUTKUNZ
PhD Student, La Trobe University

REBECCA RYAN
MSc Student, University of Melbourne

DR CHANH TRAN
Research Fellow, La Trobe University

ANGELA TORRANCE
Honours Student, University of Melbourne

DR DAVID VINE
Research Fellow, University of Melbourne

KAUSHAL VORA
Research Fellow, La Trobe University

LACHLAN WHITEHEAD
PhD Student, La Trobe University

DR GARTH WILLIAMS
Research Fellow, University of Melbourne

SHORT WAVELENGTH LASER SOURCE PROGRAM

EVERLYN CANNON
PhD Student, Swinburne University

DR JEFFREY DAVIS
Research Associate, Swinburne University

BA KHONG DINH
PhD Student, Swinburne University

PROFESSOR PETER HANNAFORD
CAOUS, Swinburne University

DR LIISA HIRVONEN
Research Fellow, University of Melbourne

DR LACHLAN MCKIMMIE
University of Melbourne

BEN MORRISON
PhD Student, University of Melbourne

ASSOCIATE PROFESSOR TREVOR SMITH
Chemistry, University of Melbourne

SVEN TEICHMANN
PhD Student, Swinburne University

PROFESSOR LAP VAN DAO
Program Leader, Swinburne University

DR CHUNYU ZHANG
Research Fellow, Swinburne University

STRUCTURE DETERMINATION METHODS PROGRAM

DR MATTEO ALTISSIMO
CSIRO – Clayton

DR CONNIE DARMANIN
CSIRO – Parkville

PROFESSOR CAL DRUMMOND
Membrane Chemistry, CSIRO – ParkvilleDR DACHAO GAO

CSIRO – Clayton

DR TIM GUREYEV
CSIRO – Clayton

DR STEVE HOMOLYA
CSIRO – Clayton

LYNN LIANG
PhD Student, CSIRO – Parkville

DR PETER LYNCH
CSIRO – Clayton

DR SHERRY MAYO
CSIRO – Clayton

DR DAMIAN E. MYERS
University of Melbourne

DR YAKOV NESTERETS
CSIRO – Clayton

DAVID PARRY
CSIRO – Clayton

DR ANDRE POGANY
CSIRO – Clayton

DR ANDREW STEVENSON
CSIRO – Clayton

DR VICTOR STRELTSOV
CSIRO – Clayton

PROFESSOR JOSE VARGHESE
Group Leader, CSIRO – Parkville

PROFESSOR STEVE WILKINS
Program Leader, CSIRO – Clayton

DR JANELLE WILLIAMS
CSIRO – Parkville

THEORY AND MODELLING PROGRAM

DR RUBEN DILANIAN
Research Fellow, University of Melbourne

DR OLENA PONOMARENKO
Research Fellow, University of Melbourne

DR HARRY QUINEY
Program Leader, University of Melbourne

ULTRA-COLD PLASMA SOURCE PROGRAM

SIMON BELL
PhD Student, University of Melbourne

MARTIJN JASPERSE
Honours Student, University of Melbourne

DR MARK JUNKER
Research Fellow, University of Melbourne

ANDREW MCCULLOCH
PhD Student, University of Melbourne

LIAM MCGUINESS
Honours Student, University of Melbourne

SEBASTIAN SALIBA
PhD Student, University of Melbourne

ASSOCIATE PROFESSOR ROB SCHOLTEN
Program Leader, University of Melbourne

DAVID SHELUDKO
PhD Student, University of Melbourne

MEMBER DEPARTURES

The following members departed CXS in 2009:

MICHAEL BAKER
PhD Student, La Trobe University

DR JENNY CARMICHAEL
Research Fellow, La Trobe University

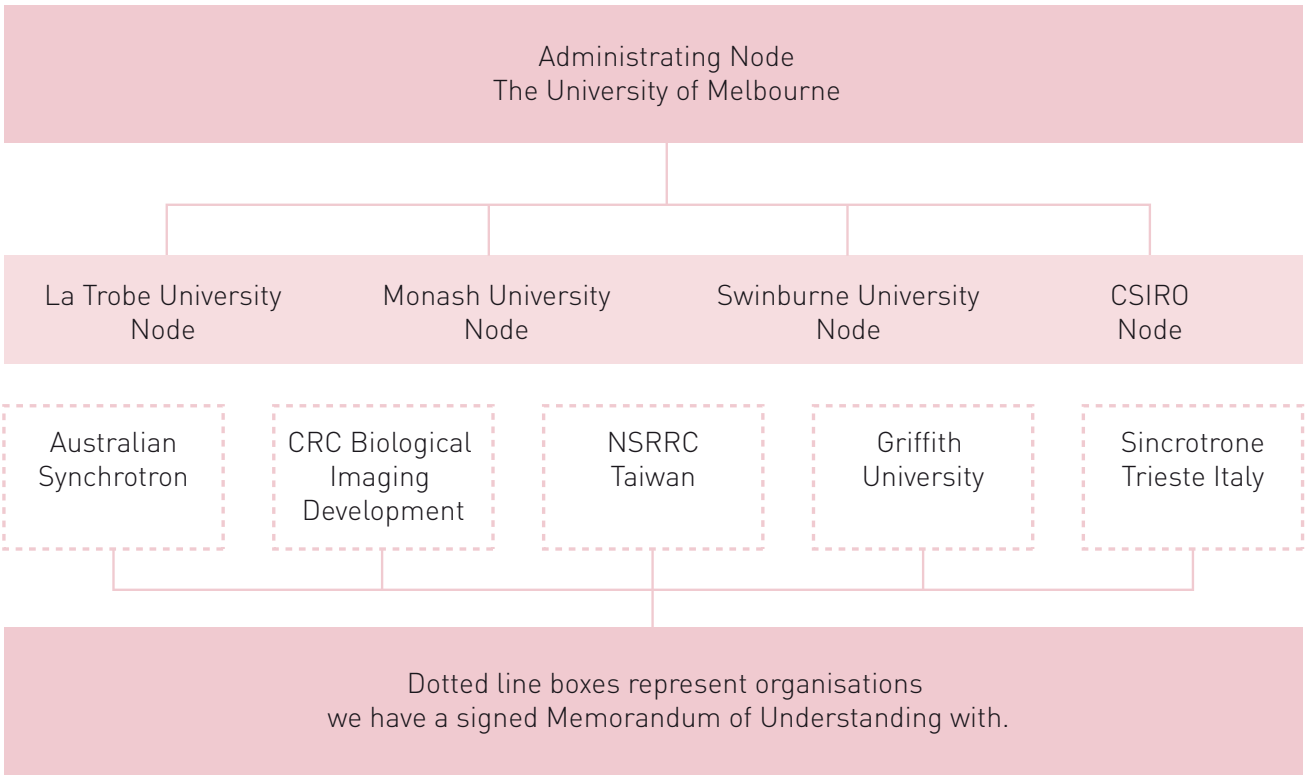
STEFANIA CASTELLETTO
Research Fellow, University of Melbourne

LAHIRU GANGODA
MSc Student, La Trobe University

DR MARK PFEIFER
Research Fellow, La Trobe University

DR GARTH WILLIAMS
Research Fellow, University of Melbourne

ORGANISATIONAL CHART AS OF JUNE 2009



PRESENTATIONS, CONFERENCES & LABORATORY VISITS

DR BENEDICTA AHATARI
- Poster Presentation – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009
- Poster Presentation – Australasian Corrosion Association Conference, Coffs Harbour, Australia, November 2009

BO CHEN
- Poster Presentation – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009
- Speaker – 18th AIP National Congress, Adelaide, Australia, December 2009

JESSE CLARK
- Poster Presentation – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009
- Visited – Advanced Photon Source, Argonne National Laboratory, Chicago, USA, December 2009

EVAN CURWOOD
- Visited – Advanced Photon Source, Argonne National Laboratory, Chicago, USA, December 2009

DR JEFFERY DAVIS
- Speaker – 18th AIP National Congress, Adelaide, Australia, December 2009

DR ROUBEN DILANIAN
- Attended – Crystal, Barossa Valley, Australia, April 2009
- Invited Speaker – SRI Satellite Workshop, University of Melbourne, Australia, October 2009
- Attended – CXS Beechworth Retreat, Australia, October 2009

MATTHEW DIXON
- Invited Speaker – Malaria in Melbourne Symposium, Australia, October 2009

SAMUEL FLEWETT
- Poster Presentation – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009

DR WILFRED FULLAGAR
- Invited Speaker – Monash Chemistry, Monash University, March 2009
- Speaker – Occasion of Bill Thomlinson, Monash Centre for Synchrotron Science, Australia, April 2009
- Speaker – IP show and Tell Forum, University of Melbourne, August 2009
- Speaker – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009

DR JACQUI GULBIS
- Attended – MPSI, United Kingdom, March 2009

DR CHRIS HALL
- Attended – ISRP, University of Melbourne, Australia, September 2009
- Invited Speaker – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009

PROFESSOR PETER HANNAFORD
- Speaker – 18th AIP National Congress, Adelaide, Australia, December 2009

KEVIN HANNAH
- Poster Presentation – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009

DR MARK JUNKER
- Attended – Quantum Frontiers Symposium, Brisbane, Australia, April 2009
- Visited – University of Queensland, Australia, April 2009

DR NICK KLONIS
- Invited Speaker – Live Cell Imaging Workshop, Melbouorne, Australia, November 2009

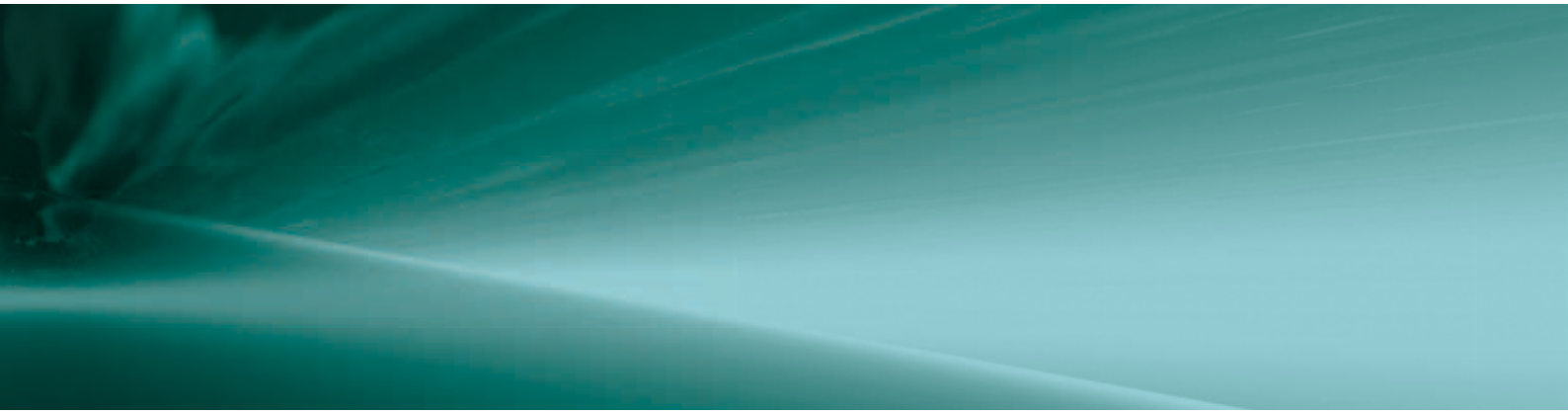
PROFESSOR ROB LEWIS
- Attended – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009

DR MAC LUU
- Poster Presentation – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009

LACHLAN MCKIMMIE
- Speaker – 5th Asian Photochemistry Conference, Beijing, China, November 2009

DR PAUL MCMILLAN
- Invited Speaker – Malaria in Melbourne Symposium, Australia, October 2009

PROFESSOR KEITH NUGENT
- Invited Speaker – Advanced Photon source Users Week, Chicago, USA, May 2009



- Plenary Speaker – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009
- Visited – Advanced Photon Source, Argonne National Laboratory, Chicago, USA, December 2009
- Speaker – 18th AIP National Congress, Adelaide, Australia, December 2009

ASSOCIATE PROFESSOR ANDREW PEELE

- Invited Speaker – 1st Workshop on FEL Science, Jeju, South Korea, February 2009
- Invited Speaker – Joint conference of the Asian Crystallographic Association and Chinese Crystallography Society, Beijing, China, October 2009
- Visited – Advanced Photon Source, Argonne National Laboratory, Chicago, USA, December 2009

DR MARK PFEIFER

- Poster Presentation – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009

DR OLENA POMOMARENKO

- Attended – CXS Beechworth Retreat, Australia, October 2009

COREY PUTKUNZ

- Poster Presentation – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009
- Visited – Sring – 8, Japan, November 2009
- Visited – Advanced Photon Source, Argonne National Laboratory, Chicago, USA, December 2009

DR HARRY QUINEY

- Invited Speaker – Atomic and Laser Physics Seminar, Brisbane, Australia, January 2009
- Invited Speaker – Swinburne Optical Laser Laboratory Seminar, Melbourne, Australia, February 2009
- Invited Speaker – Workshop on Coherent Intense X-rays in Physics and Bilogoy, Jeju Island, Korea, February 2009
- Invited Speaker – SRI Satellite Workshop, University of Melbourne, Australia, October 2009
- Invited Speaker – CXS Beechworth Retreat, Australia, October 2009
- Invited Speaker – Australian Synchrotron Asia-Oceania Forum, Melbourne, Australia, December 2009
- Speaker – 18th AIP National Congress, Adelaide, Australia, December 2009

ASSOCIATE PROFESSOR MIKE RYAN

- Invited Speaker – Monash University, Melbourne, Australia, May 2009
- Invited Speaker – University of New South Wales, Australia, May 2009
- Invited Speaker – Gordon Conference on Molecular and Cellular Bioenergetics, Hew Hampshire, USA, June 2009
- Invited Speaker – University of Cologne, Germany, June 2009
- Invited Speaker – University of Gottingen, Germany, June 2009
- Invited Speaker – conference on Mitochondrial Assembly and Dynamics in Health and Disease, Phoenix, USA, July 2009
- Invited Guest – Saitama Medical Centre Seminar, Tokyo, Japan, November 2009
- Invited Guest – Nagoya university Seminar, Nagoya, Japan, November 2009
- Plenary Speaker – 51st Annual Meeting of Japan Society for Inherited Metabolic Disease, Tokyo, Japan, November 2009

REBECCA RYAN

- Poster Presentation – Developments in Coherent X-ray Methods Workshop, Melbourne, Australia, October 2009

ASSOCIATE PROFESSOR ROB SCHOLTEN

- Visited – Advanced Photon Source, Argonne National Laboratory, Chicago, USA, December 2009

TANIA SMITH

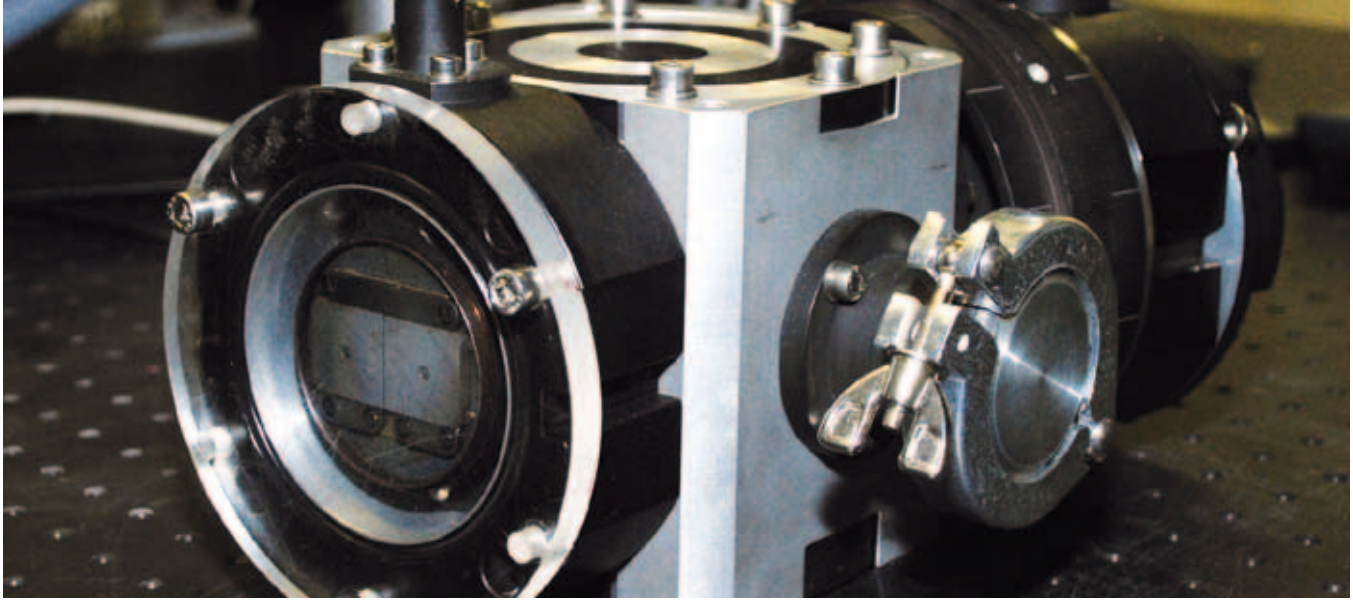
- Invited Speaker – Science Teachers Association of Victoria Conference, Melbourne, Australia, November 2009

ASSOCIATE PROFESSOR TREVOR SMITH

- Attended – Methods and Applications of Fluorescence Conference (MAF11), Budapest, Hungary, September 2009
- Speaker – 5th Asian Photochemistry Conference, Beijing, China, November 2009
- Attended – UTS Opening of the OMX facility, Sydney Australia, November 2009

SVEN TEICHMANN

- Speaker – 18th AIP National Congress, Adelaide, Australia, December 2009



PROFESSOR LEANN TILLEY

- Invited Speaker – Asia-Pacific Congress on Electron tomography, Brisbane, Australia, January 2009
- Invited Speaker – Cell Biology of Malaria: Understanding Infection, Targeting Interventions, Maryland, USA, May 2009
- Invited Speaker – Malaria Scholars Program Seminar, Atlanta, USA, June 2009
- Invited Speaker – Institute of Urban and Global Health, New York, USA, June 2009
- Attended – CXS Beechworth Retreat, Australia, October 2009
- Invited Speaker – Light in Life Sciences Conference, Melbourne, Australia, November 2009

DR CHANH TRAN

- Poster Presentation – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009
- Invited Speaker – 11th International Symposium on Radiation Physics, Melbourne, Australia, September 2009
- Visited – Australian Synchrotron, Melbourne, Australia, November 2009

PROFESSOR LAP VAN DAO

- Attended – Monash Centre for Synchrotron Science Seminar, Melbourne, Australia, September 2009
- Speaker – School of Physics, University of New South Wales, Australia, October 2009
- Speaker – 18th AIP National Congress, Adelaide, Australia, December 2009

DR DAVID VINE

- Speaker – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009
- Visited – Advanced Photon Source, Argonne National Laboratory, Chicago, USA, September 2009
- Visited – Advanced Photon Source, Argonne National Laboratory, Chicago, USA, December 2009

DR GARTH WILLIAMS

- Attended – LCLS Research Seminar, California, USA, August 2009
- Invited Speaker – International Conference on Synchrotron Radiation Instrumentation (SRI09), Melbourne, Australia, September 2009
- Invited Speaker – Developments in Coherent X-ray Methods Workshop, Melbourne, Australia, October 2009
- Visited – Advanced Photon Source, Argonne National Laboratory, Chicago, USA, December 2009

DR CHUNYU ZHANG

- Speaker – 18th AIP National Congress, Adelaide, Australia, December 2009

AWARDS & HONOURS

Clare Henderson's award winning image "Twisted Light" – a vortex captured with photography.

CXS recognised a number of its members for their work in 2009. We extend our congratulations to each of them for their efforts and awards in the following honours:

- Michael Baker was awarded best poster presentation at the Lorne Protein Conference in Lorne, Victoria, Australia, February 2009
- CXS was awarded a Knowledge Transfer Award from the University of Melbourne for its outreach program Growing Tall Poppies: An Authentic Science Experience for Year 10 Students, July 2009
- Santa Maria College, in collaboration with CXS, was awarded a Victorian Impact Grant Award of $50,000 for its outreach program Growing Tall Poppies: An Authentic Science Experience for Year 10 Students, by the National Australia Bank, Australian Council of Educational Research and the Federation of Young Australians, October 2009
- Santa Maria College, in collaboration with CXS, was awarded the Victorian State Finalist Award of $50,000 for its outreach program Growing Tall Poppies: An Authentic Science Experience for Year 10 Students, by the National Australia Bank, November 2009
- The following presentation was awarded the best oral presentation by a senior investigator the the meeting of Trauma Melbourne 2009: Myers, D.E., Ryan, C.G., Kirkham, R., Paterson, D., Moorhead, G., Dunn, P.A., Siddons, D.P., de Jonge, M.D., Howard, D., De Geronimo, G., Altissimo, M., O'Brien, T.J., Jones, N.C., Stevenson, A.W., Mayo, S., Wilkins, S., High-definition mapping of trace metal elements in the hippocampus in a model of closed-head traumatic brain injury. http://www.vni.com.au/news/id/181)]

SCHOLARSHIPS & STUDENTSHIPS

We would like to congratulate the following students for their successful applications in 2009:

ABHISHEK AWASTHI
CXS Summer Scholarship, Biological Sciences Program, La Trobe University

EVELYN CANNON
PhD Scholarship, Swinburne University of Technology

MEGAN DEARNLEY
CXS Summer Scholarship, Biological Sciences Program, La Trobe University.

MINH TAM NGUYEN
CXS Internship, Experimental Methods Program, La Trobe University

NGOC THANH NGUYEN
CXS Summer Scholarship, Biological Sciences Program, La Trobe University

LUKE FORMOSA
CXS Summer Scholarship, Biological Sciences Program, La Trobe University

RESEARCH TRAINING & PROFESSIONAL EDUCATION

The Centre met all of its recruitment and professional education targets for 2009, and has exceeded expectations in the areas of Postgraduate Recruitment and Presentations to Schools and/or Teaching Communities. An increase in CXS member awareness was also a focus in 2009 with presentations in intellectual property and career development.

Growing Tall Poppies Program Students from Santa Maria College.

CXS RETREAT AT BEECHWORTH

The CXS 4th Annual Workshop was held at The Pines Convention Centre at the La Trobe at Beechworth Campus, from 13th – 15th September, 2009.

Sixty-three CXS members travelled north to the historic town of Beechworth, stopping en route to taste the wines at nearby wineries or to stock up on smelly cheeses at the Milawa Cheese Factory. The retreat location was the heritage-listed former Beechworth Lunatic Asylum. Most of the original buildings on this 11 hectare site remain, however the rooms have been refurbished as conference rooms and lodge or hotel-style accommodation suites. The beautiful setting and the chance to escape from the normal daily routine provided the perfect environment to discuss the future of our innovative enterprise. Perhaps the ghosts of past residents helped to channel our discourses on the application of coherent x-ray science and other high level imaging approaches to solving biological problems.

The Retreat kicked off with Strategic Discussions by the CXS Executive Committee expertly facilitated by two members of the international Advisory Board members: Professor Bonnie Wallace and Professor Steve Lane. This group considered ideas for revising and fine-tuning the scientific mission, undertook a critical analysis of our strengths and weaknesses and started planning for life after the CXS, as well as tackling the weighty issue of budget allocations.

The retreat aimed to discuss and develop the Strategic Plan for the recently renewed CXS for the period through to the end of 2013. Discussions leading to concrete strategies concentrated on four key scientific areas and were lead by senior CXS members: Imaging at the Atomic Level (Jose Varghese), X-ray Sciences (Andrew Peele), Laser Sciences (Harry Quiney), and Optical Imaging Methods (Trevor Smith & Mike Ryan).

The mission of the CXS is to be the world leader in the application of coherent X-ray diffraction to the imaging of biological structures. A major area of discussion was whether we should extend our scope to high-resolution imaging using photons with a range of wavelengths. It was agreed that CXS will pursue the development of high-resolution optical microscopy as part of its leadership role in the development of interdisciplinary science in Victoria. CXS will seek additional funding to make it possible to achieve this new aim as well as achieving its core aims in X-ray imaging. To recognize these developments we will adopt a new by-line for our logo: "CXS: An interdisciplinary collaboration for high-resolution bio-imaging".

The retreat was enlivened by the enthusiastic participation of members on 'snowballing' exercises. Discussion groups were lead by senior CXS research personnel (Garth Williams, Benedicta Arhatari, Mark Junker, Diana Stojanovski, David Vine, Liisa Hirvonen and Jeff Davis). The groups rotated between the different conveners and covered areas such as future workshops; promotion of the careers of CXS members; recruitment of talented new students;

improving grant outcomes; CXS visibility & outreach objectives; and working together on high impact cross-disciplinary scientific problems. The recommendations of the snowballers were collated and reported back to the collective group.

The Retreat was a great opportunity for CXS members from different disciplines and institutions to interact in a relaxed atmosphere. The ideas that were generated have been discussed further by the Executive Committee and we are currently implementing some of the excellent suggestions. Keith and Leann thank everyone for their time and effort; the commitment to excellence through collaboration that was evident at the Retreat is critical to the success of cross-disciplinary research efforts such as the CXS.

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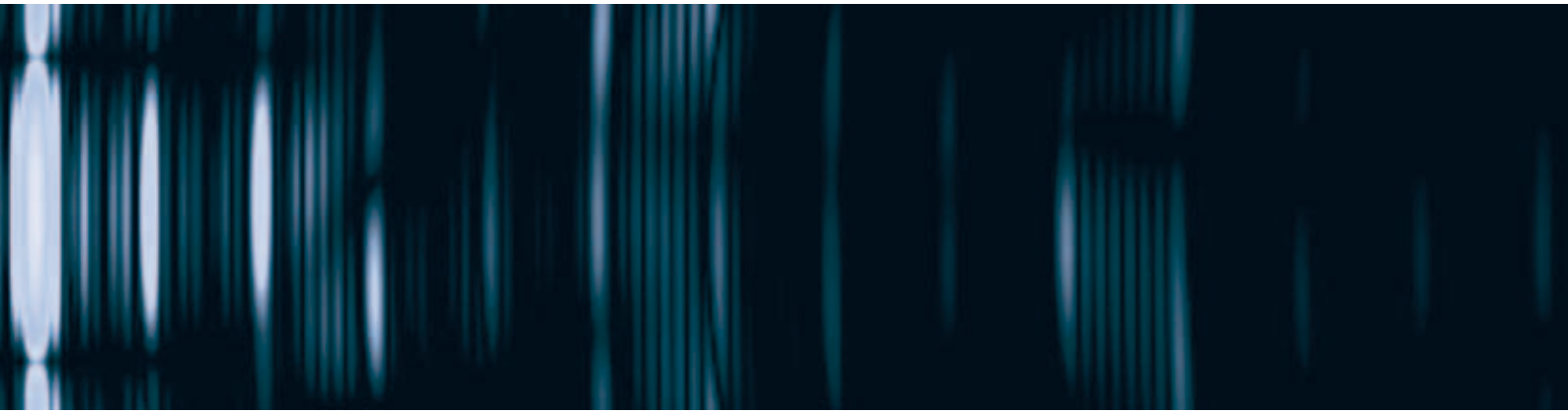

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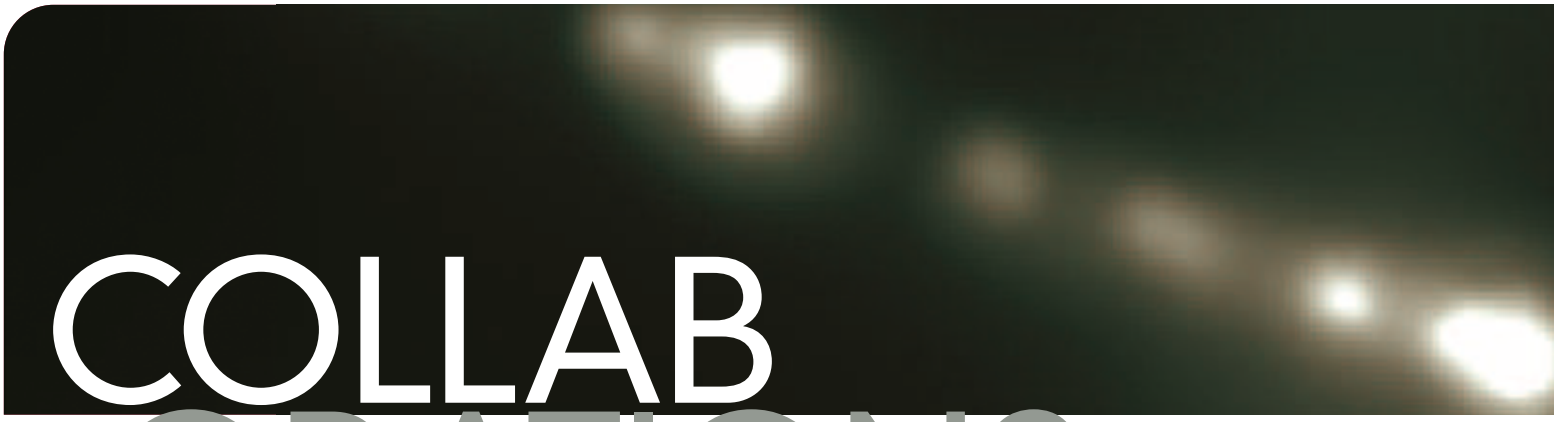


COLLAB -ORATIONS

A number of ongoing collaborations continue to develop with the following groups:

CENTRE FOR QUANTUM DYNAMICS, GRIFFITH UNIVERSITY, QUEENSLAND
Developing a number of projects with CXS.

ELECTRICAL AND ELECTRONIC ENGINEERING, UNIVERSITY OF MELBOURNE
Collaboration on bionic eye experiments.

MELBOURNE SCHOOL OF DENTISTRY
Collaboration to prepare and mount dental sample for CDI tomography experiment.

GRIFFITH UNIVERSITY
Collaboration between the Kielpinski Attosecond laser physics group and CXS Theory and Modelling Program and Short Wavelength Laser Source Program.

COCHLEAR IMPLANT
Benedicta Arhatari is collaborating with Graeme Clark on the tomography imaging of the first cochlear implant.

UNIVERSITY OF CALIFORNIA BERKELEY
Collaboration between Dr Jeffrey Davis of the Short Wavelength Laser Source Program and Professor Fleming investigating 4-wave mixing experiments involving biomolecules involved in photosynthesis.

EUROPEAN LIGHT SOURCE (ESRF)
The Structure Determinations Program is collaborating with Dr Irena Margiolaki on the powder diffraction beamline.

CRC BIOMEDICAL IMAGING DEVELOPMENT
Collaboration to develop interaction with the Experimental Methods Program and CXS.

AUSTRALIAN SYNCHROTRON
CXS continues it collaborate as part of the Beamline Advisory Panel for the development of the branch line at the soft X-ray beamline at the Australian Synchrotron and the development of the FRIEND detector project.

SCIENTIFIC LINKAGES

CXS is pleased to announce the signing of a Memorandum of Understanding with:

Australian Synchrotron

Australian Synchrotron

國家同步輻射研究中心
National Synchrotron Radiation Research Center

National Synchrotron Radiation Research Center of Taiwan

elettra

ELETTRA

CRC BID Biomedical Imaging Development

CRC for Biomedical Imaging Development

Center for BIOPHOTONICS Science & Technology

The Centre for Biophotonics Science and Technology

COMMERCIAL-ISATION

Professor Keith Nugent continued to head the development team of Iatia Ltd. Using their globally patented QPI technology, Iatia has continued to expand into life sciences, nanotechnology, ophthalmology and defence markets, with customers including GE Healthcare, Columbia University, Oxford University, the Federal Bureau of Investigations (FBI) and the Australian Defence Force.

The Ultra-Cold Plasma Source Program developed the MOGlab's range of external cavity diode laser (ECDL) controllers. Each MOG unit provides everything needed to run an ECDL and lock it to an atomic transition. Marketing material has been produced and a targeting marketing strategy was developed in 2008. All revenue derived from this activity will be the property of The University of Melbourne and one student inventor. There were been 50 sales in 2008 and there is no license agreements to date.

Dr Chanh Tran obtained an Australian Provisional Patent, "Imaging Method and apparatus", No. 2008901157.

CXS and Melbourne Ventures have produced a DVD on the commercialisation of IP.

OUTREACH

As part of the CXS Outreach Program a number of key initiatives took place in 2009; expanding on current activities and implementing a number of new ones.

As well as the two feature projects – Growing Tall Poppies and the CXS Film Project, the following activities took place:

- Associate Professor Mike Ryan gave a talk on Stem Cells to students at the St Helena Secondary College
- Matt Dixon did a presentation on Malaria for a class of year 9 students from Pascoe Vale Girls Secondary College.
- Professor Leann Tilley took part in an interview featured in the research video "Infinite Possibilities Through Research" produced by La Trobe University.
- Dr Chris Hall delivered a lecture series on the physics of X-ray imaging for the Department of Medical Imaging and Radiation Science at Monash University.
- CXS sponsored the Light in Life Sciences Conference in 2009.
- Sven Teichmann of the short Wavelength Laser Source Program was interviewed for a Swinburne University of Technology video on research activities.
- The Ultracold Plasma Source Program posted the Dancing Magneto Optical Trap footage on Youtube for public access, http://www.youtube.com/watch?v=qtWpaxxVkDA

St Catherine's School students from Left: Sharon Lee, Luciana Darling, Emma Clark, Georgina Edwards, Amelia Hamer, Natalie Ng.

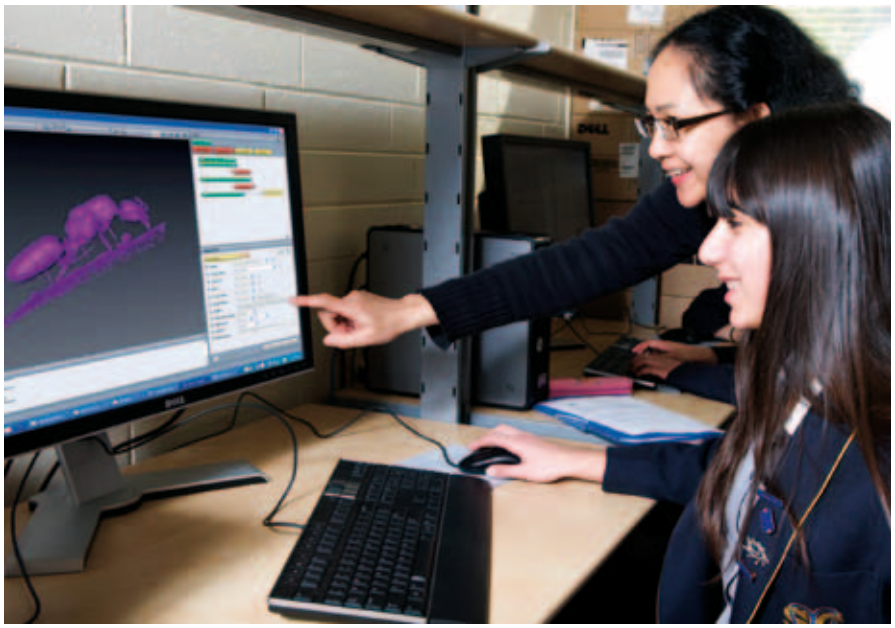
CXS hosted the St Catherine's School in their AKORN Educational Service Project; Finding a Cure for Malaria. Six year 10 students were selected to participate in the Science Students @ Work Program. The girls chosen were Emma Clark, Luciana Darling, Georgina Edwards, Sharon Lee, Natalie Ng and Amelia Hamer. The girls visited each of the CXS partner institutions and the Australian Synchrotron over a four day period, and completed some extensive research based on the topic of finding a cure for malaria. The students then presented their findings to an audience of their peers, CXS members, friends and family. Since this time Aquinas College in Ringwood have also taken part in the Science Students in Schools project hosted by the CXS La Trobe University node.

GROWING TALL POPPIES PROJECT

The *Growing Tall Poppies Program* is a partnership between CXS and Santa Maria College to provide an authentic science experience to high school students. This partnership was awarded the inaugural Victorian State Impact Award from the new Schools First grant program supported by the National Australia Bank. The winning of this award was a remarkable achievement and led to considerable media coverage for the program and therefore also for CXS. We are delighted to report that the principal driver of the project, Dr Eroia Barone-Nugent, was identified by the Herald-Sun was one of "ten Victorians who inspired us".

School enrollment numbers indicates that girls are seriously under-represented in physics and are more inclined to study the biological sciences, as its applicability is transparent. The interdisciplinary nature of CXS is an ideal vehicle to show that physics is relevant and important to society in general and biology in particular. This program immerses a small number of highly motivated Year 10 students into a CXS activity for one week. Year 10 girls are targeted because this is the time at which students are making important decisions concerning their further study of science. The *Growing Tall Poppies Program* is an opportunity to showcase the importance and relevance of the integrated sciences in the modern world and encouraging girls to continue with the physical sciences.

The teacher partner, Dr Eroia Barone-Nugent, from Santa Maria College has developed the program over the last two years and has utilised AKORN Educational Services to facilitate the program. She is committed to providing opportunities for students in science and in promoting the physical sciences in schools. The curriculum that she has developed, underpins the program, and has clear, achievable and authentic outcomes for students making this a unique outreach program. The curriculum structure considers the needs of both students and the scientists they work with. Students from diverse schools have investigated projects such as: *Malaria – is there a cure?* (St Catherine's with a number of CXS programs) which was an overview of the activities of CXS, *How do plants see?* (Padua College worked with the Short Wavelength Laser Program



through Evelyn Cannon) which investigated the photosynthetic plant molecules using lasers, *Jurassic Park in Miniature* (Santa Maria College worked with the Experimental Methods Program through Corey Putkunz and Benedicta Arhatari) that took a 3D Tomographic image of an ant in amber and concluded that recreating dinosaurs from amber insects is remote.

Each project gave students authentic hands on experience in which they collected first hand data and also allowed them to set their own questions and make hypothesis that they could test, or perhaps leave for a subsequent group of students. Most student groups toured the Australian Synchrotron giving them experience of the cutting edge technology. The first *Growing Tall Poppies: and authentic science experience for teachers* was conducted in November in the Experimental Methods Program. The teachers built on the work of students and further investigated the structure of a 10 million year old spider in amber. The teachers recorded and analysed first hand data and produced learning activities for students to use when they return to school.

As part of the program a web page has been constructed linked to the CXS web page and the students' and teachers' work is published there to create an overall story of what CXS is doing and to build students' confidence and awareness of the importance of communicating ideas, information and experiences further making this a unique experience for students and teachers to share their experiences.

WORKSHOPS

CXS conducted or sponsored the following interdisciplinary workshops in 2009:

- Talking Backwards: Physicists and Biologists explain each others fields workshop, Melbourne Australia, 18 May 2009
- Post Graduate Careers Forum 2009, Melbourne Australia, 10 June 2009
- IP @ CXS 2009, Melbourne Australia, 28 July 2009
- IP Show and Tell forum 2009, Melbourne Australia, 18 August 2009
- Super Resolution Microscopy Workshop, Melbourne Australia, 25 August 2009
- CXS Beechworth Retreat, Beechworth, Victoria Australia, 14–15 September 2009
- Developments in Coherent X-ray Methods: An SRI2009 Satellite Workshop, Melbourne Australia, 2–4 October 2009
- Light in Life Sciences Conference, Melbourne Australia, 24–27 November 2009

CXS FILM PROJECT

As part of the CXS Outreach Program at La Trobe University, a group of year 10 students from a number of local schools have produced a series of short documentary videos, which communicate the relevance and importance of cutting edge research carried out by CXS scientists.

One of these videos, which will be entered into the 2010 Australian Museum Eureka Science Prize Awards, highlights the history and basics of X-rays, their current applications in medicine and other areas.

For both the students and mentors, the journey has been a very exciting and challenging one. After delving into the research world of CXS scientists, the students were exposed to the world of filmmakers. They worked in groups to plan the content of the video, create a storyboard and write a script.

A highlight of the process was when the students were able to hire costumes and re-enact the story behind the discovery of the X-rays. This is where students used their creativity in different areas including filming, directing, lighting, editing and even incorporating some light humour into the finished product.

The students input in this video ensured that the content is both informative and most of all engaging for their high school peers. Hopefully, the video will be a useful resource in the science classroom and will inspire other students to produce similar video clips to highlight exciting science research.

This project has had many successful outcomes that meet the requirements of the CXS community awareness initiatives and the Department of Education and Early Childhood Development's (DEECD) recent blue print for enhancement of science engagement in secondary schools.

Bryon Filming.

MEDIA COMMENTARIES

The following articles relating to CXS were published or appeared in 2009:

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- *ARC Centres of Excellence refunded,* R & D info, News Alerts, February 2009
- *Network Travel Award Profiles,* ARC/NHMRC Research Network for Parasitology Newsletter, Page 5, Issue 25, February 2009
- *Extended funding boost for University of Melbourne led ARC Centres for Excellence,* University of Melbourne News, http://uninews.unimelb.edu.au/view.php?articleID=5689, 25 February 2009
- *Funding boost for University of Melbourne led ARC Centres for Excellence,* MUSSE Newsletter, http://blogs.unimelb.edu.au/musse/?p=550, 18 March 2009
- *Photosynthesis comes into the light,* Swinburne Magazine, Issue 5, page 8, March 2009
- *Photosynthesis comes into the light,* Science Alert, http://www.sciencealert.com.au/features/20093003-18972.html, 30, March 2009
- *X-ray Imaging:* A beautiful friend, La Trobe Bulletin, http://www.latrobe.edu.au/bulletin/2009/winter/research3.html, April 2009
- *ARC Centre of Excellence for Coherent X-ray Science,* News School of Engineering and Mathematical Sciences, La Trobe University, http://www.latrobe.edu.au/sems/news/details.php?ID=173, April 2009
- Professor Leann Tilley and Associate Professor Andrew Peele radio interview with Robin Williams, ABC Science Show, May 2009
- *Unveiling Cellular Bioenergetics' Secrets,* Genetic Engineering & Bioltechnology News, Vol 29, no. 7, April 2009
- Professor Leann Tilley filmed interview for the La Trobe University research documentary *"Infinite Possibilities through Research".* http://deimos3.apple.com/WebObjects/Core.woa/Browse/latrobe.edu.au.2757756627
- *Students trace "Amber" the 10 million year old ant,* La Trobe University News Vol, 21. No. 39, 19 October 2009
- *Santa Maria College – the science behind $100K, Victorian Schools First State Award Recipient Announced,* Schools First Media Release, www.schoolsfirst.edu.au/docs/state-award_-vic_231009.pdf, 23, October 2009
- *Encouraging girls in physics: Program wins $100,000 award,* Advancement Office News System, University of Melbourne, http://cms.unimelb.edu.au/?a=171036, October 2009
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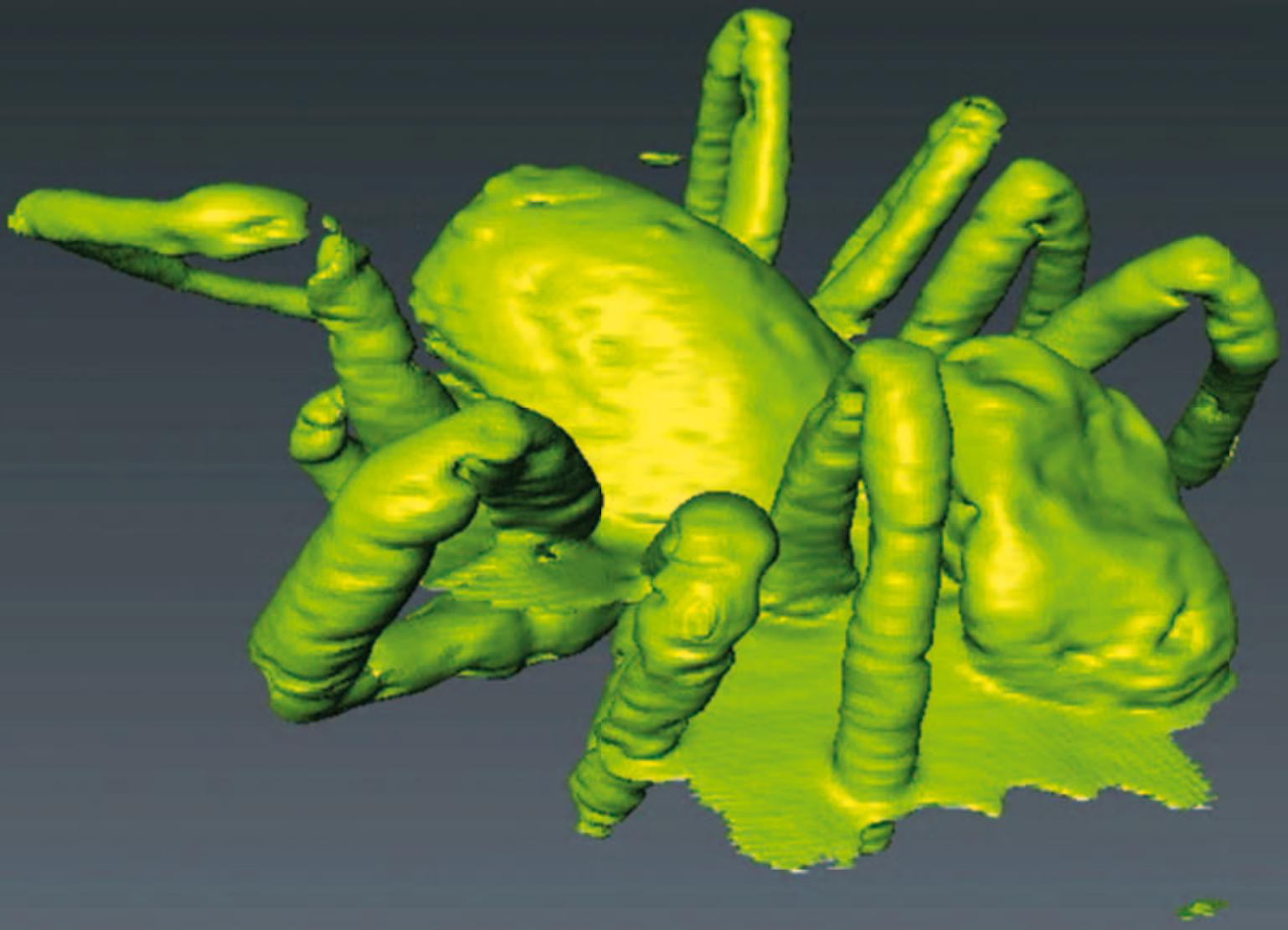
- *Dr Eroia Barone-Nugent encourages girls and science,* Herald Sun, http://blogs.news.com.au/heraldsun/robynriley/index.php/heraldsun/comments/dr_eroia_barone_nugent_encourages_girls_and_science, November 2009
- *Standing tall for science,* The Age Education Resource Centre, Rewarding partnerships, page 2, Monday, 30 November 2009
- *Blood Wars: Malaria Research in Australia,* The Economist, November 2009
- *Canberra College wins $750K – Schools First national Impact award winner,* Australian Council of State School Organisations, Vol 3, 44, 1 December 2009
- *Most of Australian Synchrotron Advisory Board Resigns,* Science Insider, http://news.sciencemag.org/scienceinsider/2009/12/most-of-austral.html, 10, December 2009

PUBLICATIONS



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BOOK CHAPTERS

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2009 COVERS


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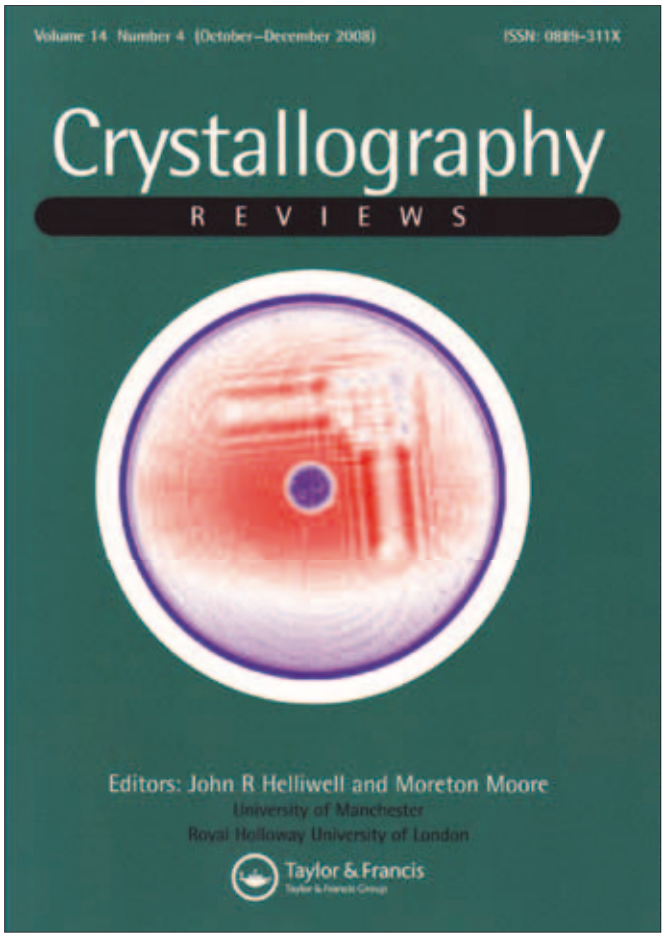
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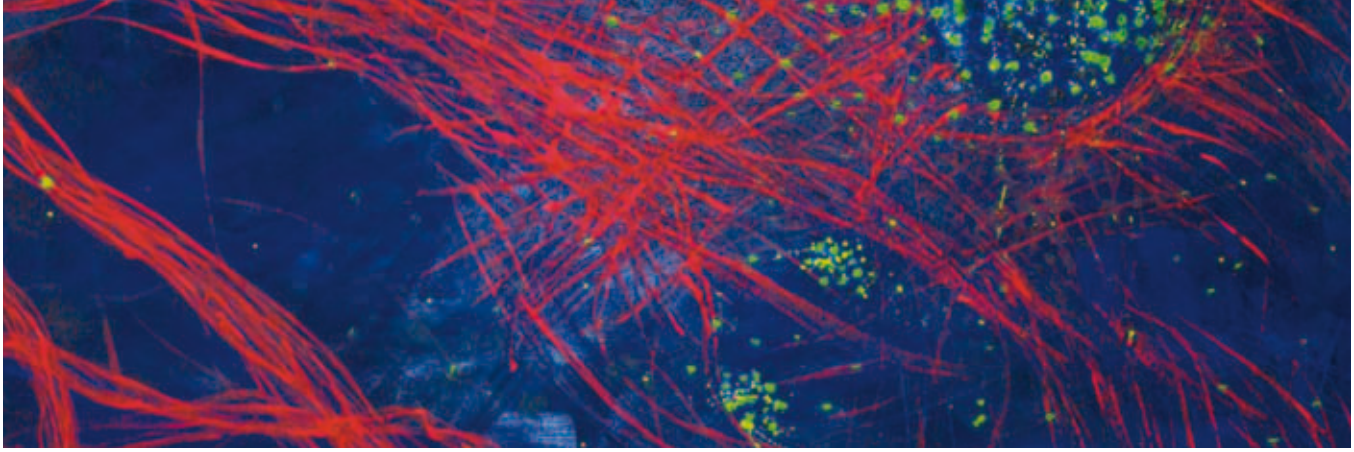

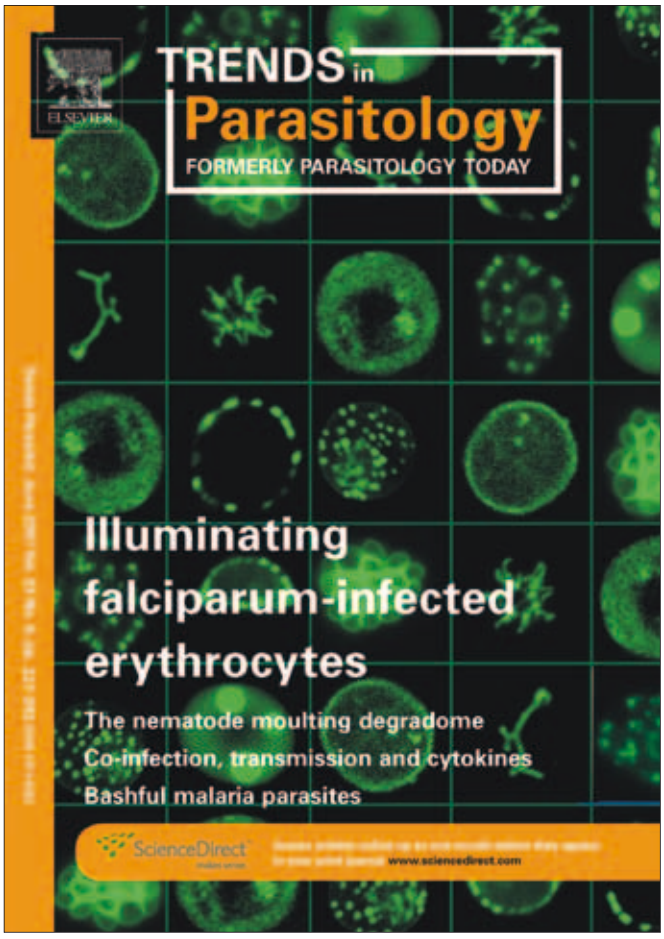
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International Synchrotron Access Program	$31,400
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Discovery Project: Development and application of new materials for high speed, high efficiency radiation detectors	$449,000
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LIEF: Versatile scanning x-ray microscopy facility at the Australian Synchrotron	$1,280,000
Linkage: Increasing the efficacy of laboratory x-ray sources for imaging	$191,500
NHMRC	
Equipment Grant: Automated stage fluorescence microscope for quantitative cellular imaging	$36,675
Detecting breast cancer in the absence of histopathological evidence of invasive disease, using scattered X-ray	$153,000
Optimisation of Synchrotron MRT for cancer treatment	$600,000
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Schools First Victorian Impact Grant	$50,000
Schools First State Finalist Award Grant	$50,000
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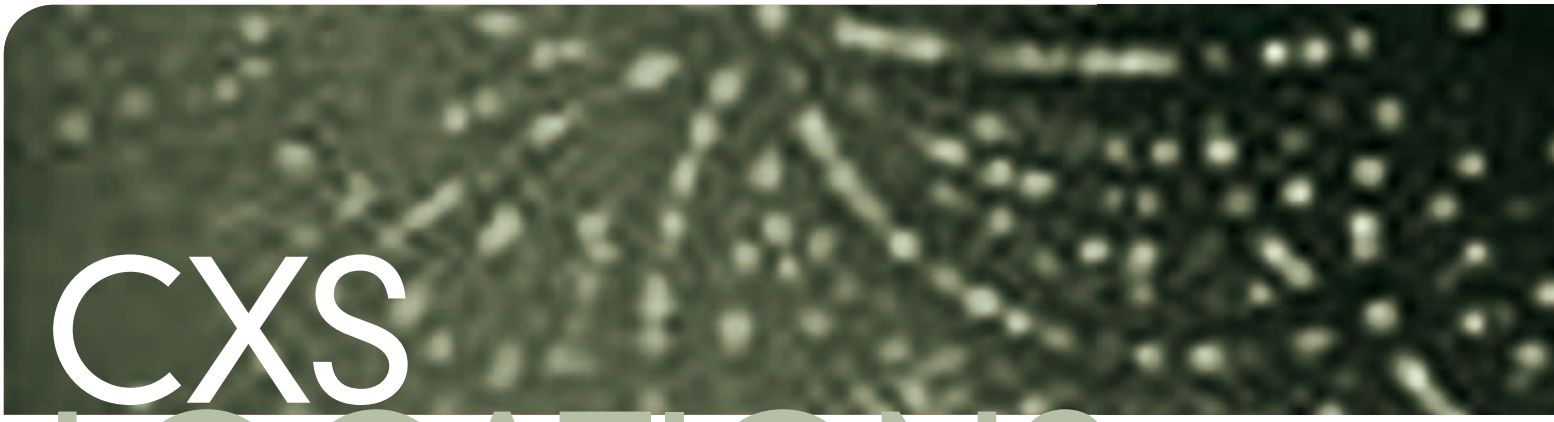

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The Theory and Modelling Program

The Ultra-Cold Plasma Source Program

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The Biological Sciences Program

The Experimental Methods Program (also at University of Melbourne)

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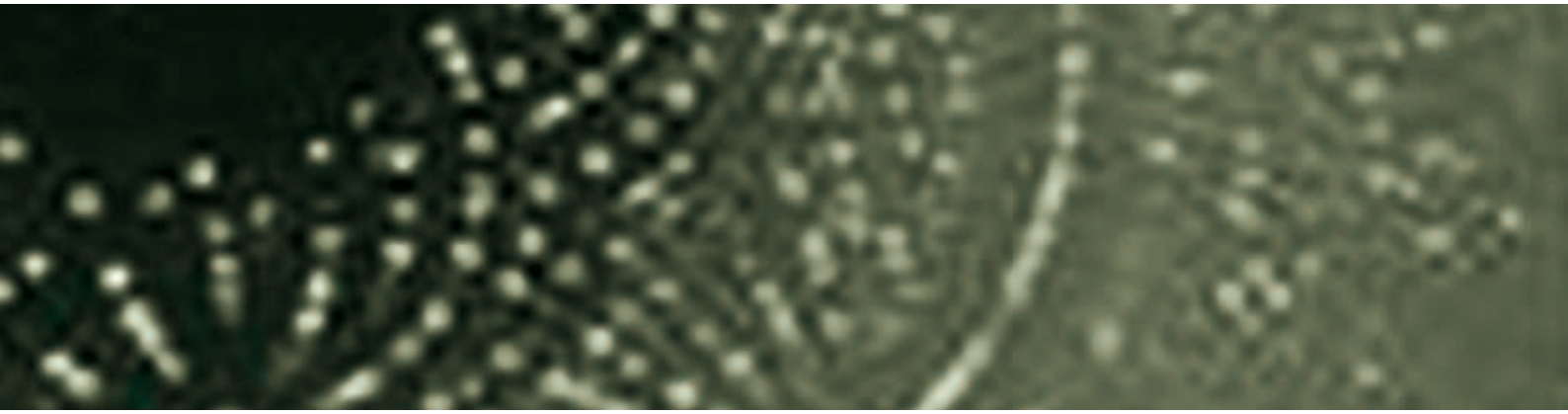

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FINANCIAL STATEMENT

CXS FINANCIAL REPORT JANUARY – DECEMBER 2009

	2009 REPORTING PERIOD ($)		2010 REPORTING PERIOD (ESTIMATED) ($)	
Carry Forward	$2,661,634		$ 2,715,056	
Other Funds	$1,800,000	ARC Income	$2,000,000	ARC Income
	$188,318	ARC Indexation	$160,350	ARC Indexation
	$740,000	Node Contribution	$750,000	Node Contribution
	$200,000	ARC Federation Fellow Support	$200,000	ARC Federation Fellow Support
Total Income	**$5,589,952**		**$5,825,406**	
Expenditure	$1,893,044	Salaries	$2,097,095	Salaries
	$320,737	Equipment	$983,500	Equipment
	$256,183	Travel, Accommodation and Conference	$368,800	Travel, Accommodation and Conference
	$194,707	Materials, Provisions and Services	$255,100	Materials, Provisions and Services
	$124,410	Scholarships	$89,293	Scholarships
	$85,815	Marketing, Outreach & Sponsorship	$75,000	Marketing, Outreach & Sponsorship
	$2,874,896		**$3,868,788**	
Balance	**$2,715,056**		**$1,956,618**	

IN-KIND REPORT JANUARY – DECEMBER 2009

University of Melbourne	$1,773,241
La Trobe University	$1,760,386
Monash University	$532,977
Swinburne University of Technology	$434,204
Griffith University	$189,945
CSIRO	$260,794
Total	**$4,951,547**

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