

2012 ANNUAL REPORT

ARC CENTRE OF EXCELLENCE FOR
COHERENT X-RAY SCIENCE



CXS

ARC Centre of Excellence for
COHERENT X-RAY SCIENCE

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Cover Image: *Plasmodium falciparum* goes bananas.

P. falciparum gametocytes adopt a banana shape as they prepare for transmission to mosquitoes and sexual reproduction. The elongated shape helps gametocytes passage through small slits in the spleen so they can survive in the circulation. Rendered cryo X-ray tomograms showing the parasite (blue) and the host red blood cell (red) overlaid with fluorescence images of the tubulin cytoskeleton (green).

Image datasets generated by Eric Hanssen and Megan Dearnley.

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, Griffith University 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 and the National Australia Bank.

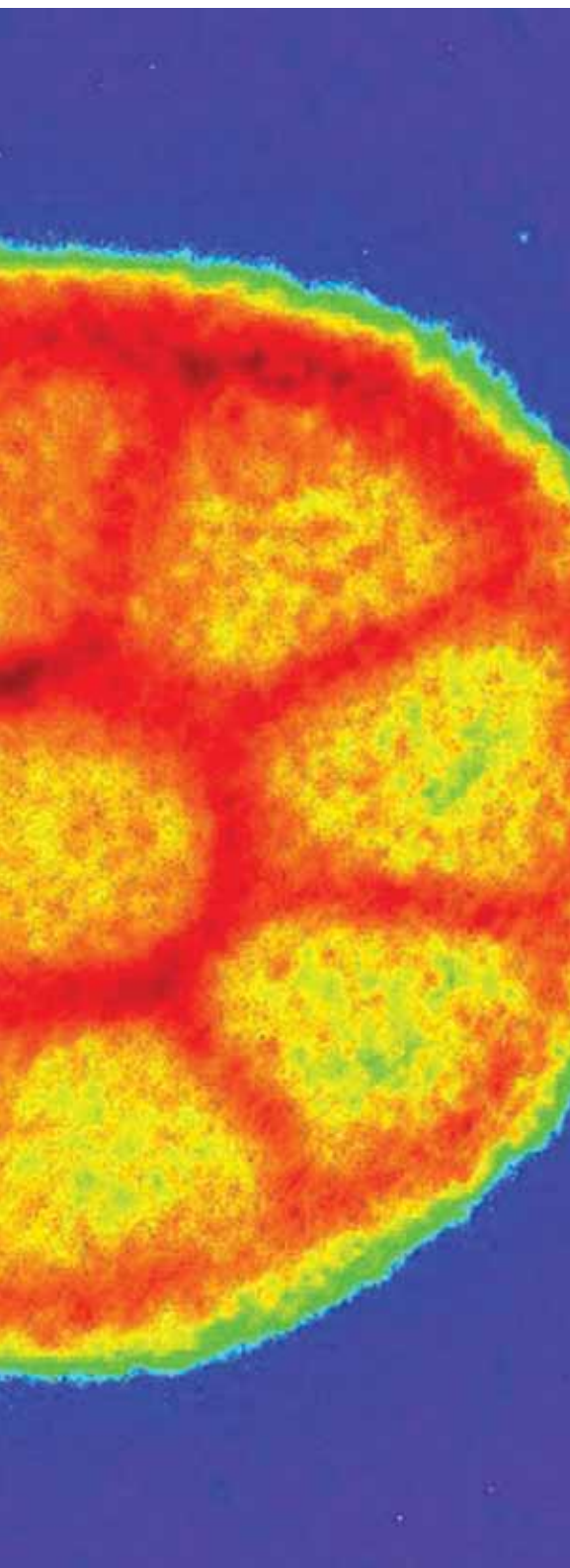
CXS would like to thank the following people for their support: Professor Terry Price for permission to use Professor Vassilios Sarafis' obituary; the School of Physics at the University of Melbourne; Tania Smith, Rosslyn Ball, Kathy Palmer and Nicole Anderson from University of Melbourne; Fabienne Perani of La Trobe University; Tatiana Tchernova of Swinburne University of Technology and Elena Saj of Griffith University.

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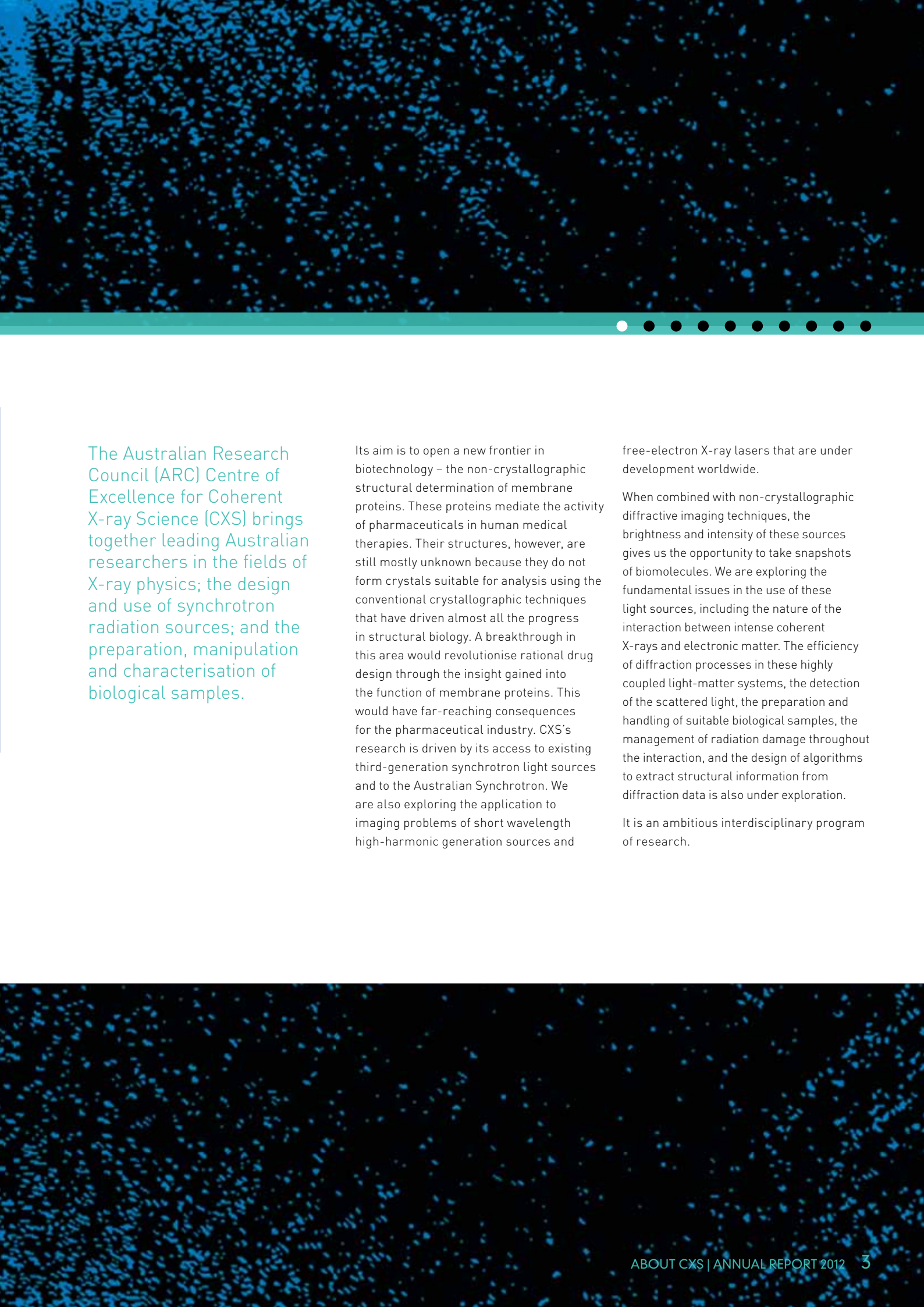


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ABOUT CXS

MISSION STATEMENT

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



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.

DIRECTOR'S REPORT

2012 has been another great year for the ARC Centre of Excellence for Coherent X-ray Science. We continue to develop and diversify and our science continues to be outstanding. As I discuss in more detail below, my time has been rather fractured with commitments to a major sustainability program at the University of Melbourne for the first half of the year and a nominal 20% commitment to the Australian Synchrotron for the entire year. While this has been demanding, the leadership of CXS has been in very safe hands with Assistant Director Harry Quiney, Deputy Director Leann Tilley and Chief Operating Officer Tania Smith.

In addition to our significant scientific achievements outlined below, we have some non-scientific achievements to be proud of as well. During the reporting period, Tania was invited by the ARC to convene the inaugural meeting of COOs for all Centres of Excellence across Australia. This is a terrific acknowledgement of our reputation as one of the best run Centres of Excellence in the country, and of Tania's contributions to the cohesive operation and management of a diverse and challenging organisation. Efficient and nimble management is critical to a successful Centre of Excellence, and Tania has continued to demonstrate the ability to remain agile and flexible in her leadership.

I am also delighted with the continued success of the Growing Tall Poppies program. This initiative continues to attract national attention and we were all thrilled to see its Director, Dr Eroia Barone-Nugent, recognised as a finalist in the high school teacher section of the Eureka Prizes this year. As the premier research structures supported by the Australian Research Council, Centres of Excellence are expected to take their outreach activities very seriously and I believe our highly outcome-focussed approach makes it safe to claim that we do it better and more effectively than most – and perhaps any other centre.

It is pleasing to note that a number of CXS members have been individually recognised for their achievements. These include: Victor Streltsov, who was awarded a fellowship by the Japanese Society for the Promotion of Science; Ben Norton, under David Kielpinski, who achieved second place in the Canon Extreme Imaging Competition with publicity via Cosmos and National Geographic; and Ved Mooga, who was awarded a poster prize by the Melbourne Protein Group.

As part of our continuing development, we welcome a new team into CXS this year as part of the Biological Science Program, led by Associate Professor Martin Scanlon and

based at Monash University, is developing extremely well.

2013 sees the conclusion of the current funding round and we are now deeply engaged in planning our next round of research. The relationships and collaborative links that characterise CXS are enormously valuable. We believe they establish the basis for a further world-leading research program. It is my view that, in particular, our work on the application of X-ray free electron lasers to structural biology is putting us in an excellent position to spearhead our national engagement in this new scientific frontier. The work of University of Melbourne alumnus and CXS Partner Investigator, Professor Henry Chapman, and his team continues to demolish potential barriers and continues to give a great deal of confidence that this important new approach to biomolecular structural determination is going to be profoundly important. While I believe this area will remain the keystone, the other projects that are emerging as our discussions progress are also tremendously exciting.

The scientific goals for CXS are of course deeply integrated with the development of the Australian Synchrotron and it is important for us and for the nation that the Synchrotron continues to thrive and grow. An important part of ensuring the continuation of the Synchrotron has been fulfilling a need for appropriate expertise. Since 2011, CXS resources have been heavily drawn upon in this regard, with Andrew Peele taking on the full-time role of Head of Science and the role of Director being filled by me on a part-time basis. The year 2011 was very much a period of laying groundwork with the Australian Synchrotron. Andrew has done a wonderful job at helping improve communication and structures internally and I concentrated on making sure that broader external understanding and perception of the synchrotron were accurate; that the Australian Synchrotron



is recognised as a well-managed and highly productive facility that is delivering great science for Australia. With the perceptions sorted out and proven via a clear analysis of the performance, we were in a position to make the case for ongoing funding. It was a bit of a roller-coaster ride but by the middle of the year it was clear that we were going to secure a budget of \$100M over four years from a range of stakeholders. This is a tight budget for the facility but will secure the operation for the next four years and allow us to develop an ongoing base of funding and hopefully to develop the capital program, including the construction of more beamlines. I am delighted that ANSTO has stepped up to be the operator of the facility. I think the Australian Synchrotron has found its natural home with ANSTO and I am very confident about its future.

CXS can be proud of the role its members have played in this latest chapter of the development of the Australian Synchrotron. I believe it is indicative of the esteem in which we are collectively held and I feel we have stepped up to play a national leadership role, regardless of any potential negative effect on our own scientific output. It has been tremendously important to have taken this on, and CXS – as well the research outputs it will deliver over the years to come – will most certainly be a beneficiary. The development of the soft X-ray imaging branch-line is just one important example.

CXS continues to make major scientific contributions. We have lead a major collaboration in the development of high-resolution soft X-ray imaging and we have, over the last seven years, developed a wide range of novel approaches and brought them to the point where they can be reliably applied. While we did experience some technical challenges with the development of our facility at the Advanced Photon Source, it has now been brought back to Australia and we are in the process of installing

it at the branch line at the Australian Synchrotron. We hope that this will be an important scientific resource for the future of Australia. We have also undertaken a major project in the development of the NADIA (Novel Algorithms for Diffraction Imaging Applications) software package that is to be made available to the international community. Additionally, the centre can boast some noteworthy publications, with an article by Leann Tilley and colleagues highlighted on the cover of *Trends in Parasitology*; and a high profile paper by Corey Putkunz's team published in *Physical Review Letters* and reported as a highlight in the *Asia Pacific Physics Newsletter*.

We were also delighted that Brian Abbey and colleagues were the first Australian team to gain access to the Linac Coherent Light Source X-ray free electron laser at the SLAC laboratory in Stanford. The results from this experiment are extremely exciting and we hope to announce their publication in next year's report.

CXS members have continued to play a role in the public eye. Andrew Peele was interviewed by the Canberra Times on the 3 June 2012, while Robert Sang and Dave Kielinski appeared on the program Scope on Channel 10 on 9 February 2012. Robert Sang undertook the Queensland branch of the Australian Institute of Physics Annual Youth Tour with lectures across Queensland.

We hosted Dr Felix Frank from Imperial College London, Adjunct Assistant Professor Jacob Taylor from the Joint Quantum Institute at the University of Maryland USA, Professor Ron Steer from the University of Saskatchewan Canada, Dr Paul Janssen and Professor Jamie White from Juiata College, USA as visitors over the year and we welcomed new members Dr Andrew Martin and T'Mir Julius to the Theory and Modelling Program, Luke Formosa, Chen Xie, Coralie Millet, Associate Professor Martin Scanlon,

Dr Martin Williams and Dr Biswaranjan Mohanty to the Biological Sciences Program, Rory Spiers and Richard Taylor to the Ultracold Plasma Source Program, Aidan Jessen to the Attosecond Science Program, and Dr Ashish Tripathi to the Experimental Methods Program.

As you may know, I have accepted a position as Deputy Vice-Chancellor and Deputy President (Research) at La Trobe University. The reasons for my decision to accept this position are complex and I step down from my leadership of CXS with considerable regret. While I will continue to be an active member of CXS, my role as its leader for the best part of eight years has been a tremendous privilege. I am delighted, however, to be able to move to a senior position with La Trobe University as it has been an exemplary partner institution and I believe it appropriate for it to become the home of our Experimental Methods Program for 2013. CXS is in safe hands as Leann Tilley steps up to the Director's role.

PROFESSOR KEITH NUGENT
DIRECTOR

ASSISTANT DIRECTOR'S REPORT

The scientific achievements made by CXS during 2012 have been comprehensively reviewed by Keith Nugent and I can only reiterate what a splendid year it has been in terms of the research and outreach of the Centre. It has been a privilege to serve as the CXS Assistant Director during this year, which has involved conducting the program reviews, chairing the Executive Committee and overseeing the smooth running of the Centre in its period of rapid transition.

These tasks have been made simpler and more enjoyable by the professionalism of the administrative team of CXS and by the efficient processes that are in place to keep the Centre moving. It is the case that other Centres look to CXS for how to achieve these tasks efficiently and much of the credit for this must be given to Tania Smith for devising these processes and implementing them so successfully.

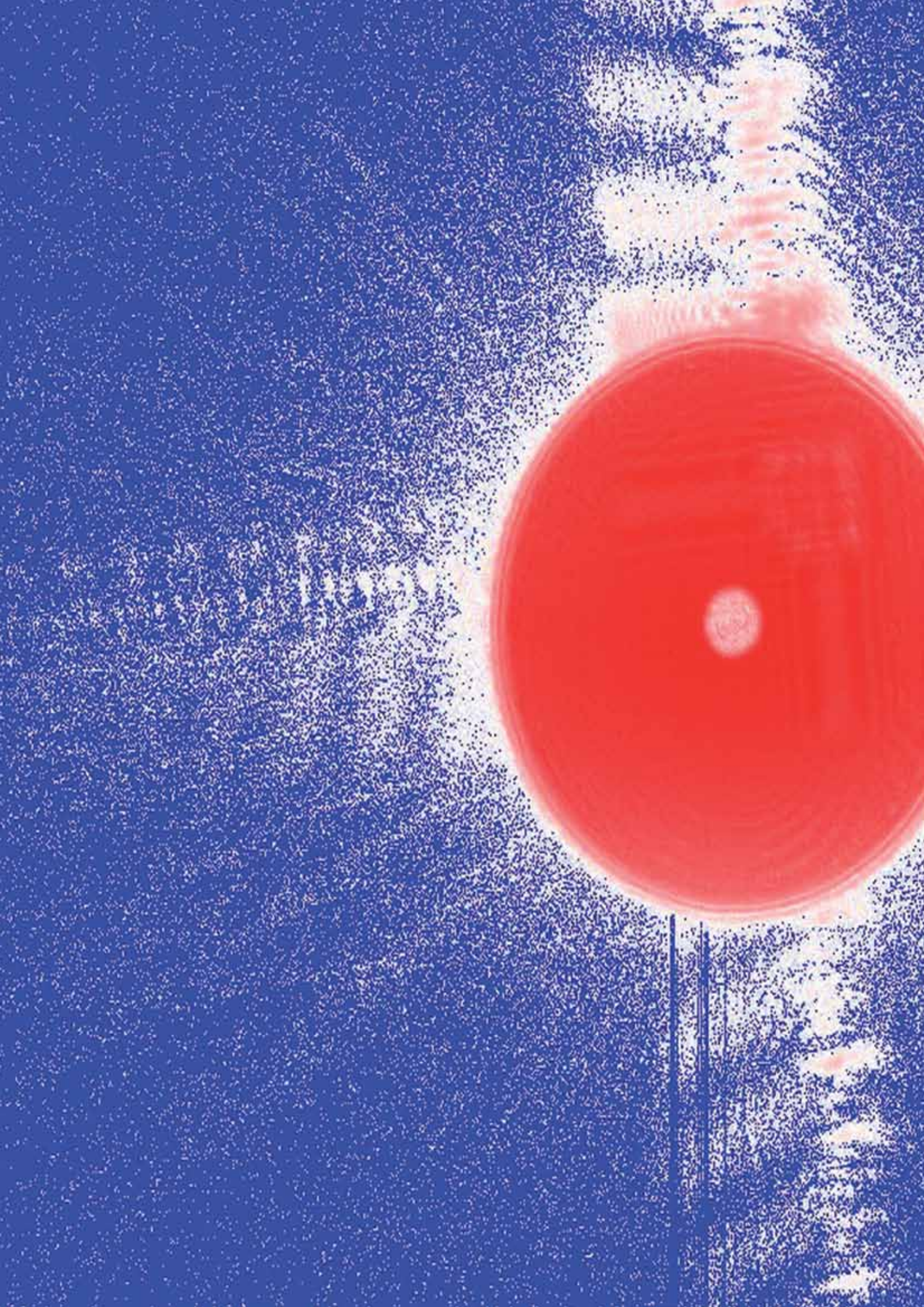
I had the opportunity to travel to Europe three times in 2012, each time visiting the Centre for Free-Electron Laser Science in Hamburg. The very high regard for the work of CXS was evident in these visits and at the international scientific meetings that I attended on my travels. There is no doubt that CXS is seen as a significant presence in the field of biomolecular imaging and in the design and conduct of interdisciplinary programs involving physics and biology.

Having had the opportunity to walk a short distance in the shoes of our Director this year, it did drive home to me what a magnificent achievement the success CXS has been and how much of that is due to his vision and leadership. It has been an honour to serve as the Assistant Director and to gain some insights into what it takes to assemble a large and seemingly inhomogeneous group of researchers towards a common purpose. While I understand some of the reasons that Keith has taken on the considerable challenges of university leadership, it is certainly the case that I will greatly miss his regular company at The University of Melbourne and his wise counsel on a broad spectrum of issues. We will strive to carry on the good work of CXS

into its final year and it is certainly the case that we will be in excellent hands under Leann Tilley's Directorship.



HARRY QUINEY
ASSISTANT DIRECTOR



RESEARCH PROGRAMS

ATTOSECOND SCIENCES PROGRAM

The Attosecond Science Program, which joined 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 only one of its type in Australia and is therefore uniquely utilised for attosecond science investigations. The facility is directed by Professor Kielbinski, who has also been leader of the CXS Attosecond Science Program since January 2010. The heart of the facility is a laser source providing 6 fs, 300 μ J, phase-stabilised 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 Modeling 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 Modeling 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 back-action on molecular diffraction imaging, a key step in realising CXS goals in biomolecular structure determination. Modelling of back-action during the long X-ray pulses 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 a 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. To 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. It is anticipated that XUV pulses of duration <500 as and peak intensities of 100 GW/

cm², 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. These studies will be extended 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 this group and end-users will prove essential in realising the promise of attosecond science and new methods will be rapidly taken up worldwide. The group has already generated XUV radiation at wavelengths as short as 30 nm by focusing the AASF laser through an argon gas jet and is 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 evaluation of the full dynamic structure factor of chemical and biological samples under X-ray irradiation for detailed comparisons with back-action models.

2. To investigate the effects of atomic structure on strong-field interactions through quantum control of the ultracold metastable neon atoms currently generated in our laboratory.

High-order harmonic generation (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 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.

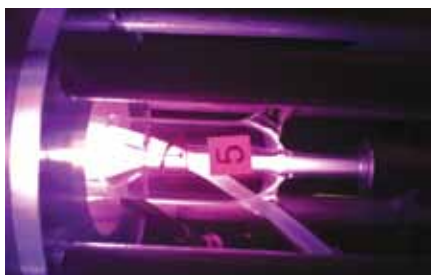
The single-atom dipole response to a strong IR field is a crucial input for optimisation of HHG sources. A recent experiment has shown that interference between the dipole amplitudes of different atomic species in a mixture of gases can boost HHG by over three orders of magnitude. However, the standard theory of HHG is inadequate for describing atomic structure effects and numerical predictions of the HHG spectrum vary by a factor of two, 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 as well as a more conventional finite difference approach. Current experimentation examines ionisation of atomic hydrogen with few-cycle laser pulses, and we are now working with the CXS Theory and Modelling Group to interpret the results. Because the hydrogen atom is so simple, subsequent HHG studies in hydrogen will be an excellent benchmark for HHG modelling.



The attosecond pulse source. An intense laser comes in from the left and creates a plasma in the vacuum chamber (purple glow at centre). The excited plasma emits extreme ultraviolet light in a single burst with attosecond pulse duration.

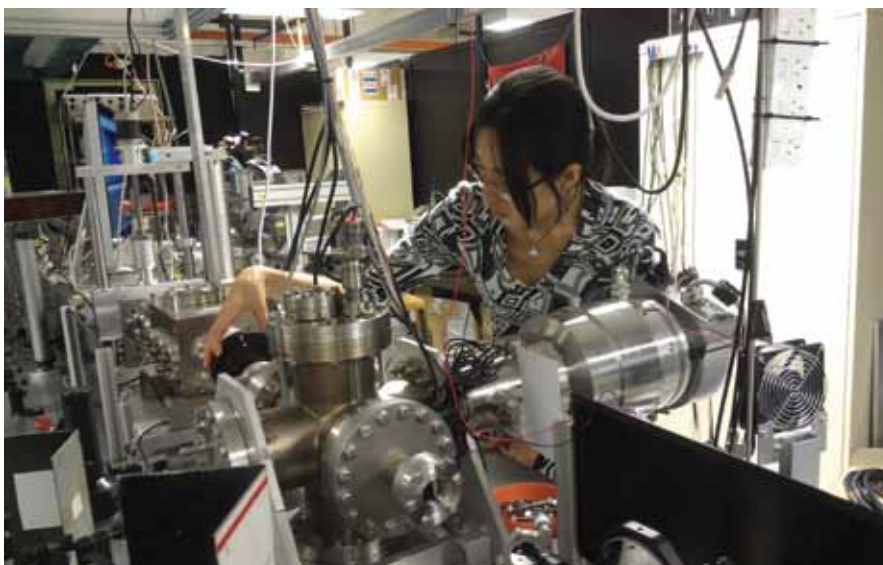
HYDROGEN EXPERIMENT

The Attosecond Science Program designed and built a new time-of-flight spectrometer to provide higher resolution in measuring the energy of photons and electrons from strong-field ionisation. The spectrometer was modelled in detail with regard to vacuum and magnetic field considerations, including numerical simulations of electron trajectories over the energy range of interest. The spectrometer was calibrated by observing the electron spectra from atomic H at 25 fs laser pulse duration. These spectra exhibit well-known regular peaks at energies separated by the laser photon energy. By observing the times at which the electrons in each peak arrived at the detector, it was possible to determine the relationship between electron time of flight and electron energy. Preliminary electron spectra from atomic H at 5.5 fs pulse duration were measured.



Top: Hydrogen gas is electrically excited to form a plasma in a glass tube. The hydrogen molecules break apart, giving us a source of hydrogen atoms, the simplest of all atoms.

Figure 1, right: Xiaohong Han, a CXS postdoctoral research fellow, adjusts the attosecond pulse generation apparatus.



The new spectrometer was additionally used to measure the H^+ and H_2^+ ions generated in photoionisation of a combined molecular beam containing both H and H_2 . Since the mass ratio of these ions is known exactly, these measurements provided an alternative, independent calibration of the spectrometer. By comparing with measurements that contained H_2 alone, it was possible to obtain a new and independent calibration of the proportion of H in the molecular beam.

With the new spectrometer, the team measured the yield of H^+ and H_2^+ under photoionisation by few-cycle pulses. From this data, the total ionisation probabilities for H and H_2 as a function of intensity over a wide range have been extracted. These measurements serve as a probe of effects beyond the standard 'ADK' theory of ionisation. Preliminary analysis reveals close agreement with full time-dependent Schrödinger equation simulations and significant disagreement with the ADK theory.

The program team designed and fabricated an optical phase plate for transforming our Gaussian laser focus to a near-flat-top intensity profile. Future experiments can use this device to sample constant-intensity dynamics, avoiding the averaging of signal over intensity that currently obscures comparison with theory.

ISOLATED ATTOSECOND PULSE GENERATION

Our efforts to generate attosecond XUV pulses have now shifted to the demonstration of 'attosecond streaking'. This technique uses a combination of XUV

and infrared (IR) few-cycle laser pulses to realise a direct measurement of the laser electric field during the few-cycle pulse, similar to visualising a voltage waveform on an oscilloscope. Attosecond streaking is a key technique for measuring the electronic dynamics of materials, by using the XUV pulse as a trigger for the dynamics, which are then read out by the IR laser. It is also used to measure the duration of isolated attosecond pulses. Only six laboratories in the world currently have access to this technique.

The CXS Attosecond Science Program designed and largely constructed the complex beamline to be used for attosecond streaking. At the heart of the beamline is a 'split mirror' that generates precisely controllable time delays between the XUV and IR pulses. The time delay can be varied over tens of femtoseconds, but must remain stable to tens of attoseconds over the measurement time of about 10 minutes the pulses ionise a gas jet and the resulting electron energy spectra are detected in an electron spectrometer. At the time of writing this report, these parts of the are being fabricated and are due for completion in, 2013.

The beamline also includes a dedicated XUV generation setup and diagnostic XUV spectrometer, optimised for the 95 eV XUV photon energy that is most widely used in the field. The generation of XUV power was verified at 95 eV using few-cycle pulses in a Ne gas cell, with the detector being our previous commercial XUV spectrometer. The new diagnostic XUV spectrometer has now been constructed and tested with these 95 eV photons.

CASE STUDY: ATTOSECOND PULSES

Creating attosecond XUV pulses requires extremely fine control of intense laser pulses. The laser pulses ionise gas, generating plasma, and the laser field drives the electrons in the plasma to high energy. The energy is then emitted in a single burst of XUV light that lasts a much shorter time than the period of the driving laser. Even with the state-of-the-art laser at the CXS Griffith node, the attosecond pulses are generally quite faint. In order to do useful experiments with attosecond pulses, we have to make the pulses as bright as possible by optimising the XUV power generated in our high-harmonic gas cell. The length of the gas cell, the pressure of gas, and the intensity of the laser all play a role in this process. Xiaohong Han, a postdoctoral research fellow, and Amna Zahid, a PhD student, have been systematically testing many gas cell configurations and laser beam focusing conditions to get the brightest attosecond pulses possible (Figure 1).



Biological Science Program at Monash University

BIOLOGICAL SCIENCES PROGRAM

The Biological Sciences Program (BSP) involves research groups from La Trobe University, University of Melbourne and Monash University.

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 cells and cellular compartments. Members of this program also interact with members of the Structure Determination Methods program and the Theory and Modelling program to optimise techniques to determine the structures of membrane proteins and other components of biological interest. BSP Members are also working with members of the Attosecond Science program and the Short Wavelength Laser Source program to develop non-linear spectroscopic methods to investigate the mechanisms of electron transport to understanding the structure and dynamics of oxidative protein folding.

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

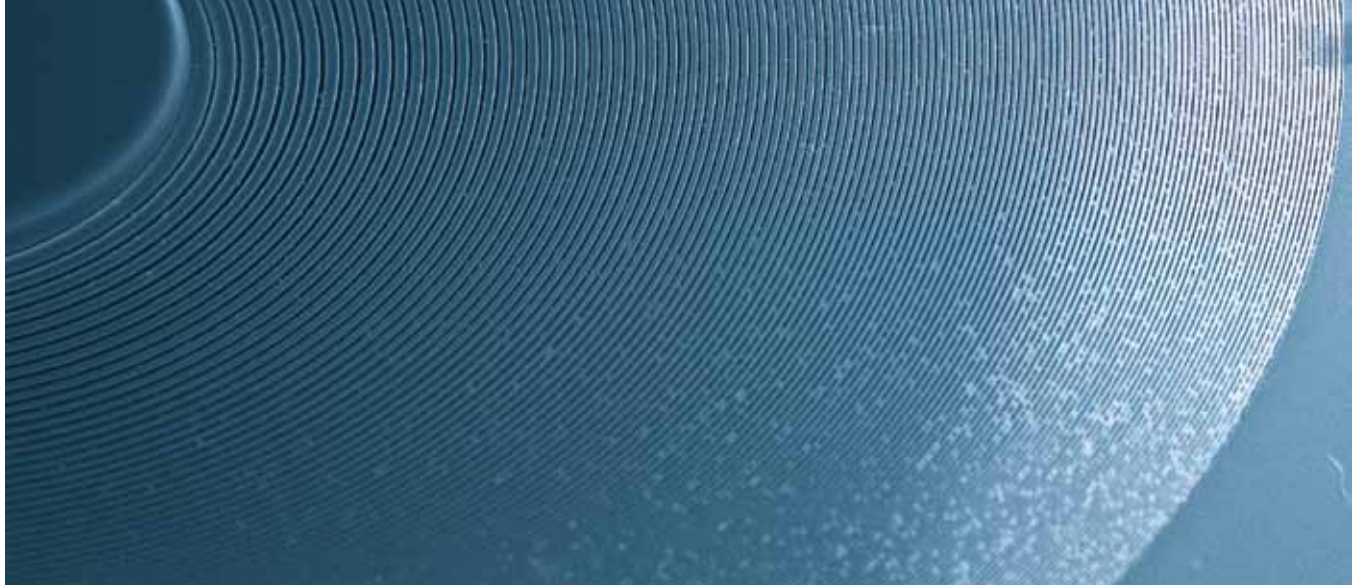
MALARIA AND REMODELLING OF THE RED BLOOD CELL

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 nucleus 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, organisation 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 combat the serious problem of malaria.

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 disease. In addition, efforts to activate the machinery involved in mitochondrial permeabilisation can act as anti-cancer agents. Work is being undertaken within CXS 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 in progress to provide insights into the structure of mitochondrial membrane proteins and their complexes.

PROTEIN-SMALL MOLECULE INTERACTIONS FOR DRUG DESIGN

This project is focused on understanding the interaction of proteins with small molecules. The information gained will be used to better understand how drugs work and to design new drugs that target proteins that cause disease. A family of bacterial proteins that are catalysts of oxidative protein folding have been shown to be important in virulence, antibiotic sensitivity and infection. Consequently, these proteins are potentially targets for the development of an entirely new class of antibiotics. Structure determination of these proteins using the coherent X-ray imaging methods is underway. Members of this research group are also working with members of the Attosecond Science Program and the Short Wavelength Laser Source Program to develop non-linear spectroscopic methods that will enable them

to investigate the mechanisms of electron transport in this system. Understanding the structure and dynamics of the oxidative protein folding system will provide us with key information for the design of potent and specific antibiotics. This group has the following goals:

- Prepare and optimise cellular samples for use as test-beds for X-ray coherent diffraction imaging and for other pioneering imaging techniques.
- 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.
- Undertake studies on protein dynamics using conventional and non-linear spectroscopic methods.

ACHIEVEMENTS

NEW INSIGHTS INTO IMAGING THE MALARIA PARASITE

The human malaria parasite *Plasmodium falciparum* is responsible for the deaths of up 800,000 people annually. The parasites have a complex life cycle within the human host consisting of both asexual and sexual stages. Work in the Tilley lab focuses on using multi-modal imaging techniques to investigate the basic biology of the parasites with a view to better understanding the pathology of the disease.

During the asexual stages, which are the symptomatic stage of infection, the parasite modifies its host cell to enable the

trafficking of virulence factors important to the pathology of the disease. In order to do this, the parasite generates a number of membranous structures in the host cell, collectively known as the exomembrane system. The Biological Sciences Program has investigated the genesis and maturation of each of the exomembrane system components, and has identified the temporal generation of the components. The role of the exomembrane system in the trafficking of the major virulence factor, *Plasmodium falciparum* Erythrocyte Membrane Protein-1 (PfEMP1) has also been investigated. This identified a number of novel compartments that are involved in PfEMP1 trafficking on the parasite periphery and in membrane cisternae called Maurer's Clefts.

The parasites' sexual stages undergo a series of remarkable morphological changes as they develop into mature forms capable of sexual reproduction within the mosquito. Indeed, *P. falciparum* is named after the crescent of falciform shape observed in these mature sexual stages. The elongation to this crescent shape has been shown to arise from cisternal membrane compartments associated with microtubules. We investigated the origin, organisation and composition of the cisternal compartments across the different stages of sexual development. This identified that they are analogous to the inner membrane complex involved in host cell invasion in asexual stages.

The projects outlined above have utilised a number of imaging techniques including light microscopy, electron microscopy, electron tomography and cry-electron microscopy. These studies have been aided by the installation of a 3D Structured

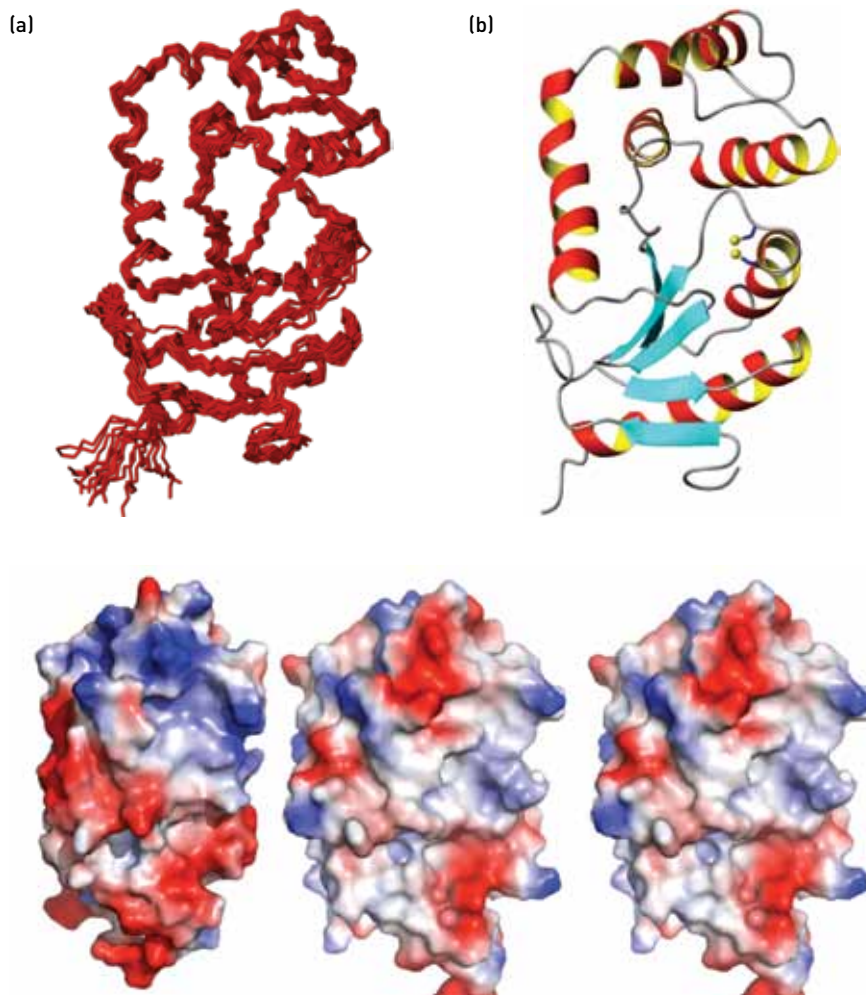


Figure 2. (a) Ensemble of NMR solution structures and (b) conformer closest to the mean of oxidised NmDsbA2, showing α -helical domain (upper half of protein structure) inserted into thioredoxin-like domain.

In comparison to the other two NmDsbA enzymes in *Neisseria*, NmDsbA2 resembles NmDsbA3 more than NmDsbA1. It is also closer to NmDsbA3 in terms of its relatively open peptide-binding groove, which is hydrophobic in NmDsbA3 but acidic in NmDsbA1. In contrast, the substrate specificity of NmDsbA1 and NmDsbA2 are similar and distinct from that of NmDsbA3

Electrostatic surface potential of (a) NmDsbA1; (b) NmDsbA2 and (c) NmDsbA3 showing the hydrophobic groove, distribution of positive (blue) and negative charges (red).

Illumination Microscope (3D-SIM) at the Bio21 Institute (purchased following a successful ARC LIEF grant application led by Professor. Tilley). 3D-SIM is a super-resolution optical microscopy technique that provides eight-fold increased volume resolution over standard fluorescent microscopes.

IMPORTANCE OF DISULFIDES IN SMALL TIM CHAPERONES

The small TIM family of chaperones sort hydrophobic precursor proteins in the intermembrane space. In our previous structural analysis (Webb et al. Mol Cell 2006; Baker et al., MBC 2009) it was found that every small TIM contains two disulfide bonds. The most N-terminal cysteine residue of this motif has also been shown to be involved in protein biogenesis. Recently however, we found that no individual cysteine residue is required for the function of Tim9 or Tim10 but some defective assembly induces proteolytic clearance from mitochondria through a specific degradation machinery. In collaboration with Diana Stojanovski,

members of the Ryan lab delineated a clearance mechanism for the mutant proteins and their unassembled wild-type partner protein within mitochondria. This work was published in the Journal of Molecular Biology.

NEW STRUCTURES TO UNDERSTAND ENZYME DYNAMICS AND UNCOVER NOVEL ANTIBIOTICS

The Biological Sciences Program team is studying protein oxidation pathways in *Neisseria meningitidis* and *N. gonorrhoeae*, two obligate human pathogens and causative agents of fatal meningitis and sexually transmitted gonorrhoea, respectively. These oxidation pathways are essential for bacterial virulence. We are seeking to clarify structural and functional aspects of the enzymes involved in protein oxidation (called Dsb) in efforts to design novel, narrow spectrum inhibitors of their activity. A key aspect of the work is to develop a structural understanding of the substrate specificity that is observed in the system. We have

previously reported structures of two of the three DsbA enzymes that are expressed in *N. meningitidis*. The third, NmDsbA2 has proven refractory to X-ray crystallography.

STRUCTURE OF NMDSBA2

The team has recently solved the solution structure of one of three disulfide bond-forming enzymes found in *N. meningitidis*, NmDsbA2, using biomolecular NMR. The solution structure of NmDsbA2 conforms to the typical DsbA topology, consisting of an α -helical domain inserted into a thioredoxin-like fold (Figure 2).



CASE STUDY: IMPROVING IMAGE ANALYSIS

Electron tomography produces highly magnified 3D image volumes useful for investigating the structure and function of cellular components. Image quality is degraded by multiple scattering events and quantum noise, which depend on the angle at which individual tilt projections are collected. In collaboration with Harry Quiney (Theory and Modelling Program) members of the Tilley group have developed an algorithm that can be applied to electron tomography data to improve the image quality by filtering multiple scattering events and quantum noise from individual tilt projections. After applying the filter, PhD student Mauro Maiorca was able to demonstrate a quantitative improvement in image quality in the final reconstructed volume for both plastic embedded and cryo-stabilised samples of malaria parasite-infected erythrocytes. This work has been published in the *Journal of Structural Biology*.

Application of filtering techniques to poor contrast electron microscopy data. A fixed section of a malaria infected red blood cell stained with uranyl acetate was subjected to electron tomography. Conventional imaging is shown in (A) while filtering was applied in (B).

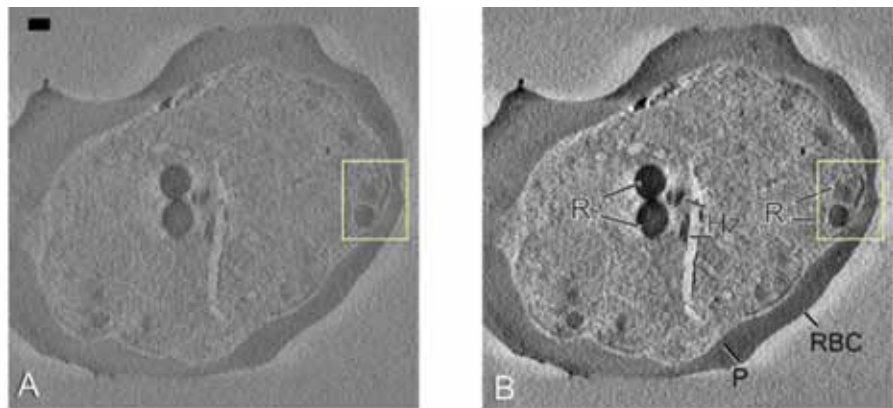
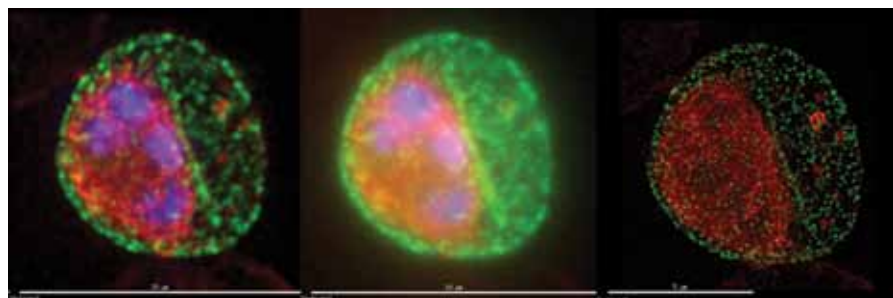


Fig. 5. Application of pre-NAO filtering to poor contrast EM data. A fixed section of a *P. falciparum*-infected erythrocyte was subjected to a staining with uranyl acetate alone. A tilt series was collected and tomograms were constructed without (A and C) and with (B and D) pre-NAO filtering. Scale bar: 300 nm. Parameters: $\lambda_c = \lambda_s = \lambda_d = 30$.

Improved imaging of malaria





EXPERIMENTAL METHODS PROGRAM

The Experimental Methods Program (EMP) develops imaging methods using coherent and partially coherent light sources. The research profile of EMP includes design of experimental systems; sample handling and nanofabrication techniques; tomographic imaging of three-dimensional objects; detailed characterisation of radiation sources; and the development of novel imaging methodologies using diffraction data.

The EMP group has members based at La Trobe University and University of Melbourne. Through its broad spectrum of members and activities, the EMP has 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 the Theory and Modelling Program, which analyses imaging data obtained from biological samples. EMP and BSP researchers regularly work together to develop methods for imaging and specimen preparation. To further facilitate the mutual translation of physics and biology, the BSP team attends EMP experiments at various overseas facilities. This has led to the exploration of access to other imaging techniques and facilities around the world.
- **Theory and Modelling Program (TMP)** – TMP and EMP regularly cross fertilise. EMP provides experimental data to which TMP can apply new methods of analysis, 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.

- **UltraCold Plasma Source Program (UCP)** – the UCP was formed within CXS to exploit techniques developed by EMP and TMP in order to demonstrate imaging using a bright coherent source of high-energy electrons. With membership based at the University of Melbourne, UCP and EMP have a high degree of interaction.
- **Structure Determination Methods Program (SDMP)** – the SDMP is an EMP partner in an effort aimed at understanding electronic and structural damage to biomolecules induced by femtosecond X-ray free electron laser pulses. Experimental tests of damage models developed by the TMP are an important step toward determining bio-molecular structures from diffraction experiments.

ACHIEVEMENTS

In 2012 the EMP continued an intensive program of experiments using our laboratory facilities and synchrotron light sources around the world. Together with other CXS groups, we also undertook groundbreaking studies of the interaction of matter with intense laser pulses produced by the world's first hard X-ray Free Electron Laser (X-FEL). This work marks major progress towards the key goal of CXS to open a new frontier in biotechnology through the non-crystallographic structural determination of membrane proteins.

This year has seen our long investment in developing novel ultra-high resolution X-ray imaging based on coherent diffraction culminate in the implementation of a versatile X-ray imaging facility at the Australian Synchrotron with a dedicated

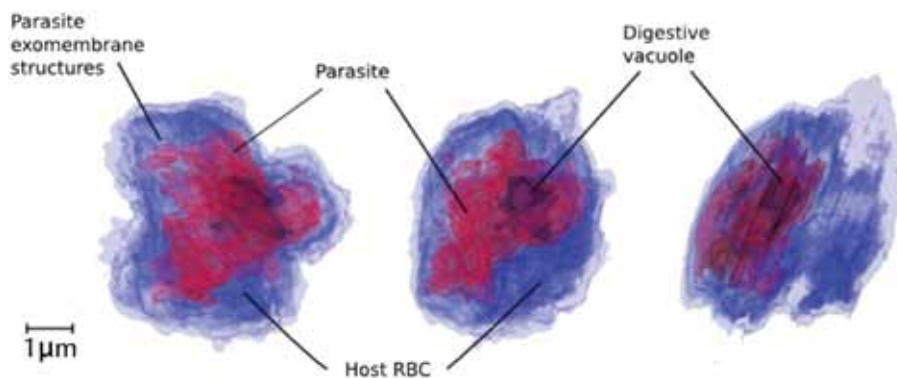


Figure 3. 3D visualisation of the tomographic reconstruction of a set of phase images obtained by ptychographic coherent diffractive imaging of a red blood cell infected with the malaria parasite at the trophozoite life-cycle stage. The cell (blue) is shown at two orthogonal angles with the parasite (red) and the parasites' digestive vacuole (grey) identified by analysis of the complex refractive index of the sample that is obtained directly from the tomograms.

branch beamline. This facility will provide a lasting foundation for coherent X-ray science research and will address the growing need to explore the structure and properties of materials and biological systems at the nanoscale.

In addition to our stated program goals the EMP continued to explore new methods in imaging and coherence. Some of the key results achieved in 2011 include:

- Dramatic demonstrations that the conditions produced by highly focused X-FEL beams induce electrodynamic changes in molecular nanocrystals that manifest in unexpected changes to high-resolution diffraction patterns and the observation of a new transient phase of crystalline C_{60} .
- Quantitative three-dimensional imaging of whole eukaryotic cells that provide insight into the progression of disease. Various developments in coherent diffractive imaging were combined to enable sensitive, dose efficient imaging.
- Detailed study of the effects of partial coherence in image formation leading to significant improvement in image quality and reliability with greatly reduced measurement time.

PARTIALLY COHERENT DIFFRACTIVE IMAGING

The wave properties of light lead to interference, but certain conditions of coherence must be met for these interference effects to be exploited in coherent diffractive imaging (CDI). CDI is a powerful imaging technique that recovers an object from its diffraction pattern by computational methods.

It has experienced rapid growth due to the availability of highly coherent synchrotron radiation X-ray sources, and more recently, X-ray free electron lasers. We know from our earlier work, however, that such light sources are generally not perfectly coherent, which can result in reconstructions that suffer from artefacts or fail completely. This motivated our past efforts to show that the coherence properties of a light source can be precisely measured and we were able to develop algorithmic approaches that can include the effects of partial coherence, delivering a striking improvement to image quality and reliability.

Our successful demonstration of an improvement to coherent diffractive imaging using illumination that is partially coherent inevitably led to the question of the extent to which both lateral and longitudinal coherence requirements can be simultaneously relaxed. To address this question we used experimental X-ray data obtained from a microfabricated test pattern at the Advanced Photon Source to explore the interplay between lateral partial coherence and longitudinal partial coherence and their relative influence on CDI. We found that for iterative *ab initio* phase-recovery algorithms based on those typically used in CDI and in cases where the coherence properties are known, we are able to relax the widely accepted minimum coherence requirements both laterally and longitudinally by an unexpectedly large amount. The improvement is enough to reduce measurement time by orders of magnitude using conventional light sources with emerging detector technology and paves the way for applying CDI to the study of dynamic physical processes at relevant time scales.

VISUALISING CELLS IN THREE DIMENSIONS AT THE NANOSCALE

CXS has led the development of an extension to coherent diffractive imaging (CDI) known as Fresnel CDI (FCDI), which allows an image to be extracted from coherent diffraction data with exceptional reliability. Our subsequent extensions to FCDI with methods of ptychography, phase diversity and tomography allow the method to be applied as a robust form of high-resolution, quantitative three-dimensional microscopy. Applications involving CDI of biological samples are particularly challenging due to the effects of radiation damage that will generally limit resolution. Much of our work has therefore been focussed on optimising the sensitivity and dose efficiency of the technique.

During the period, the program demonstrated three-dimensional FCDI imaging of a whole eukaryotic cell at a spatial resolution below 70 nm. The imaging showed sufficient contrast in the real part of the reconstructed complex three-dimensional transmission function of the cell to distinguish major cellular components, including a parasite that invaded the cell and the parasite's digestive vacuole (Figure 3). For this work, conducted at the 2-ID-B beamline at the Advanced Photon Source, USA, we combined many overlapping projection images at a series of angles and combined them using techniques of ptychography and tomography. This allowed accurate phasing of the diffraction data while keeping the total X-ray dose delivered to the sample to be kept to a minimum. From our data, we



Figure 4. Part of the CXS team at LCLS who are monitoring the acquisition of nanodiffraction data

estimate the minimum dose requirements for FCDI tomography of cells to be lower than other established high-resolution X-ray imaging techniques. Based on the dose, contrast and resolution achievable using FCDI, we anticipate that it will play an important role in tomographic cellular characterisation.

IMAGING ENDSTATION DEVELOPMENT

The Fresnel Imaging ENDstation (FRIEND) is a custom-designed experimental facility that was commissioned at the Advanced Photon Source (APS) in Chicago under a partnership arrangement. In 2012 the endstation was brought home to Melbourne, combining it with a recently constructed dedicated branch beamline. The combined facility will see 'first light' early in 2013, starting a commissioning phase that will result in a highly versatile imaging facility that can uniquely address the growing need to explore the detailed structural properties of materials and biological specimens below 100 nm length scales.

The beamline photon source is an elliptically polarised undulator that can produce high coherent light of variable polarisation over the photon energy range 200 to 2000 eV. This range encompasses the water window, important for natural image contrast in biological samples, and the absorption edges of biologically important elements and technologically important transition metals. With full circular polarisation it is possible to operate the monochromator in zero order to deliver a first harmonic beam with roughly a 4% band pass for fast 'broadband' CDI experiments, i.e. with longitudinal partial coherence.

The endstation has proved to be a versatile instrument that can accommodate three common implementations of two and three dimensional diffractive imaging; plane wave illumination; scanning focused-(ptychographic) and defocused-probe (Fresnel diffractive imaging) The strength of FRIEND lies in its stability and in-vacuum operation which allow for long exposure times, high signal-to-noise and large dynamic range two-dimensional intensity measurements to be acquired. By thorough characterisation of the instrument we have identified opportunities for enhancing its performance that will be implemented in the coming year with support from the Australian Synchrotron and the Lawrence Berkely National Laboratory. These developments, which include state-of-the-art detection systems and high-performance interferometric metrology, will ensure the instrument provides a vehicle for world-class research for years to come. We are concurrently working with the Melbourne Centre for Nanofabrication to develop high resolution X-ray optics and with the Biological Sciences Program to develop supporting facilities for biological sample preparation.

CASE STUDY

ULTRAFAST DIFFRACTION REVEALS TRANSIENT STRUCTURAL PHASE IN NANOCRYSTALS

A team of CXS researchers – comprising members from CXS Experimental Methods, Theory and Modelling and Structure Determinations programs – were the first

Australians to lead an experiment at the hard X-ray FEL (X-FEL), Linac Coherent Light Source (LCLS), at the SLAC National Accelerator Laboratory, operated by Stanford University in California, USA.

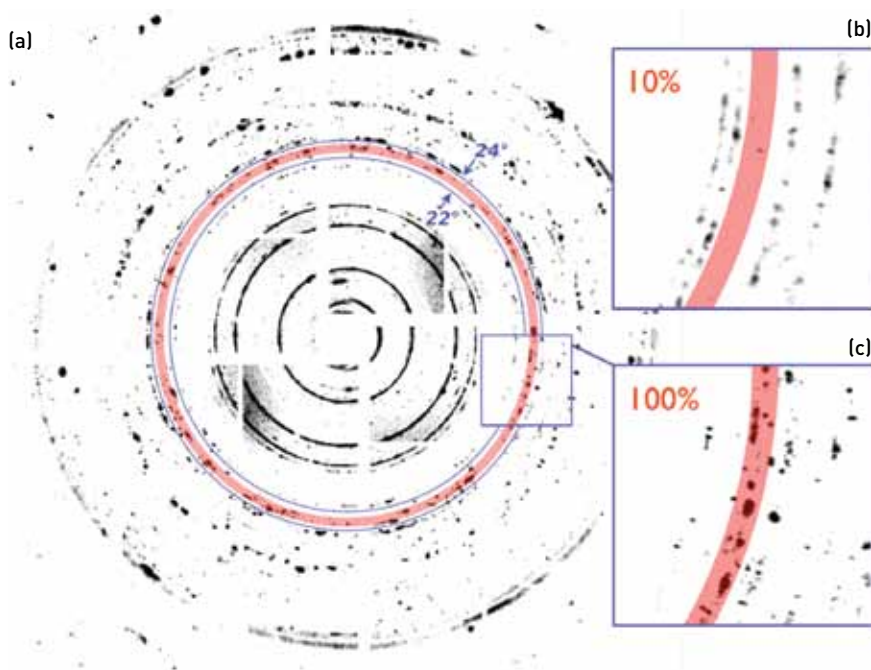
The X-FEL produces pulses of X-rays more than a billion times brighter than the most powerful existing synchrotron sources. The structure of nanocrystals can be probed by the diffraction of these extremely intense and extremely fast femtosecond X-FEL pulses, which occurs before the atomic positions can be affected by sudden photoionisation. However, the power density in an XFEL pulse may be so high that it can modify the electronic properties of a sample on a femtosecond timescale, which is of critical importance to the interpretation of nanocrystallography experiments.

Conducted during April 2012, the experiment explored the interaction of intense coherent X-ray pulses and matter by studying the diffraction of ultrafast (32 fs) nanofocused XFEL pulses of varying intensity by a powder sample of crystalline C60. Forward-scattered diffraction data show a significant dependence on the incident intensity for some diffraction angles (Figure 4). Structural analysis showed that the X-FEL data at 10% of the maximum intensity are similar to synchrotron powder diffraction data and correspond to the expected structure of C60. At 100% X-FEL power the diffraction data is changed in a way that provides direct evidence that the electronic structure of the C60 molecules are modified by the X-FEL pulse without change to the translational symmetry of the C60 crystal. The data suggests a new, albeit transient, structural phase of the C60 crystal has been created through interaction with the nano-focused XFEL beam.

Right: CXS researchers and collaborators from the Advanced Photon Source and SLAC National Accelerator Laboratory during the last day of experiments at the Advanced Photon Source using the X-ray imaging endstation developed by CXS. The endstation has now been relocated to its new home at the Australian Synchrotron.



These startling observations have implications for the accurate determination of membrane protein structure by X-FEL diffraction. We are now analysing data from other nanocrystals to examine the extent of femtosecond electronic rearrangement in molecules of lower symmetry compared to C60. Already our work makes it clear that to understand the conditions produced by highly focused X-FEL beams requires that we move beyond classical electrostatic X-ray diffraction theory, taking into account the electrodynamic changes induced by the measurement process itself.



Above. a) Summed diffraction data from 2500 single X-FEL shots recorded at 100% power. (b) Zoomed region showing Bragg peaks at 10% power at positions consistent with room temperature FCC structure. (c) The same region as in (b) collected at 100% power. The significant variation in peaks at approximately 0.3 inverse angstroms (highlighted in red) represents a phase change of the molecular lattice that occurs on a femtosecond time scale.



SHORT WAVELENGTH LASER SOURCE PROGRAM

The Short Wavelength Laser Source Program (SWLP) 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 imaging studies using X-ray free-electron laser (XFEL) sources currently under development at large international facilities.

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) may 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 electronic acceleration processes and the variation of the molecular or atomic ground state throughout the interaction with the driving laser field play important roles in quantum systems and need to be studied in more detail.

Unlike atoms, molecules are not spatially isotropic systems. For randomly aligned molecules, the HHG spectrum has been shown to have characteristics similar to that produced by atoms; but for aligned molecules, which can be realised by using another laser field, the HHG is influenced by the angle between the molecular frame and the polarisation vector of the femtosecond laser field. An investigation to clarify the roles of intra-molecular quantum processes in field-free aligned molecules is highly desirable, 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 ionisation fraction of the gas; and the difference in the refractive index at the fundamental and harmonic wavelengths. We have been investigating ways of optimising 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.



ACHIEVEMENTS

GENERATION OF NARROW BANDWIDTH EXTREME ULTRAVIOLET RADIATION

The propagation of fundamental and harmonic fields in a gas medium leads to a phase modulation which causes a modulation of the harmonic spectrum. Previous studies have shown that the splitting and blue shift of the harmonic spectrum is due to the intensity-dependent or time-dependent phase shift of the dipole acceleration that is responsible for the harmonic generation. However, different quantum paths also contribute to the harmonic spectrum and it is difficult to study this mechanism in experimental measurements especially when a long laser pulse is used. CXS studies have shown that the macroscopic phase matching plays a significant role in the harmonic generation and the interplay between the single-atom response; and that the macroscopic response is complicated in a long gas cell configuration. With spatial selection, the contribution of the different electron trajectories to the HHG spectrum can be separated (Figure 5a and 5b). In addition, based on these studies, we can determine the conditions for the production of narrow bandwidth, strong harmonics with high coherence (Figure 5c).

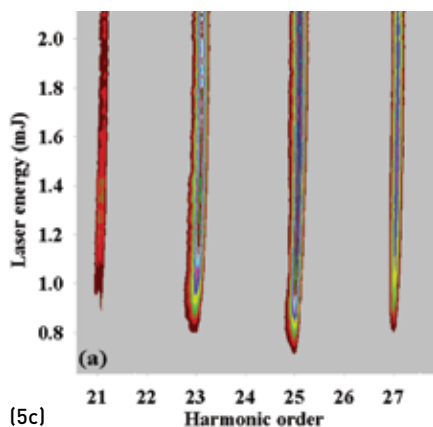
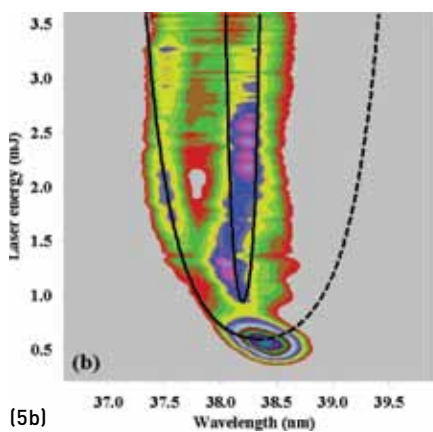
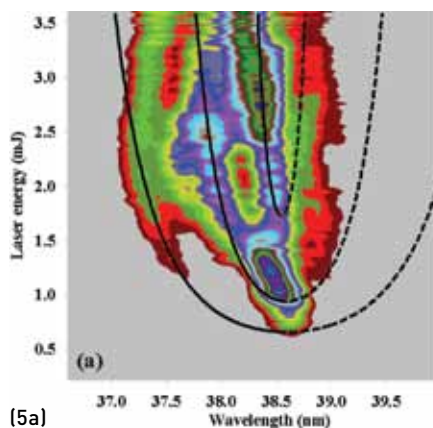


Figure 5. Measured H21 spectrum of the off-axis selection (5a) and the on-axis selection (5b) as a function of the laser pulse energy when the ionisation rate is high. The black lines represent the considering of harmonic phase modulation of two different quantum paths. The phase-matched harmonic spectrum as a function of the laser pulse energy (5c) when the ionisation rate is low.

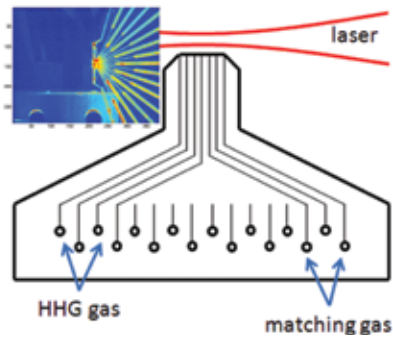


Figure 6. Multiple gas jet array for quasi-phase matched harmonic generation

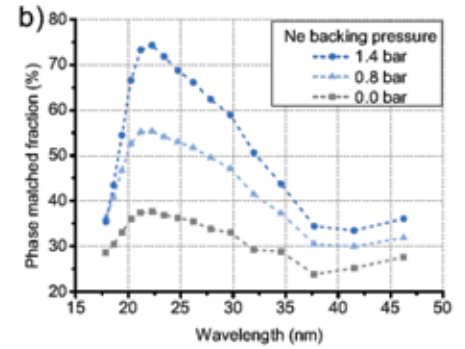
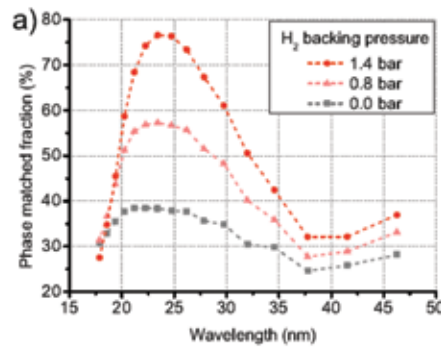


Figure 7. Observed phase matching fraction due to quasi-phase matching when H_2 (a) and Ne (b) were used as the phase-matching gas between two Ar gas jets. Each figure contains the phase matching curve found for backing pressures of 0 bar (squares), 0.8 bar (triangles) and 1.4 bar (circles).

QUASI PHASE MATCHING MECHANISM IN DUAL GAS, MULTI-JET ARRAY

In order to improve the efficiency and properties of the high harmonic source, a new quasi-phase matching technique involving a dual gas, multiple jet array has been designed and used. This technique involves positioning a 'phase matching' (PM) gas jet between the harmonic producing gas jets. The dispersion due to free electrons or neutral atoms in the PM gas can then be tuned by varying the gas jet pressure. A multiple gas-jet channel device, in which the pressure of each jet can be controlled separately, has been designed in collaboration with the Centre for Microphotonics, Swinburne University of Technology, and implemented as shown in (Figure 6). We have conducted experiments to determine whether the ionisation of the matching gas or its low recombination cross-section is the mechanism for efficient phase matching with molecular hydrogen and neon gases because the ionisation potential and also the photo-ionisation cross section of the two gases are different. The results in (Figure 7) indicate that the mechanism by which this quasi-phase matching scheme works is due neither to the phase matching gas being fully ionised nor to its lower recombination cross-section.

HIGH HARMONIC GENERATION WITH TWO LASER FIELDS

Use of multiple colour laser fields to generate high harmonics offers the potential to control the high-order harmonic process. This leads to the generation of attosecond pulse trains with individual pulses separated by a laser period; new approaches to isolating a single attosecond pulse; and the generation of tunable extreme ultraviolet radiation. A pulse at 1400 nm is used for generating high-order harmonics and a second delayed pulse at 800

nm is used for controlling the HHG process. We are able to generate a super-continuum HHG spectrum at 80 eV (14 nm) with ~ 35 eV bandwidth (~120 attosecond) with these two laser fields as shown in (Figure 8).

Use of two laser fields at 1400 and 800 nm to control the high-order harmonic generation.

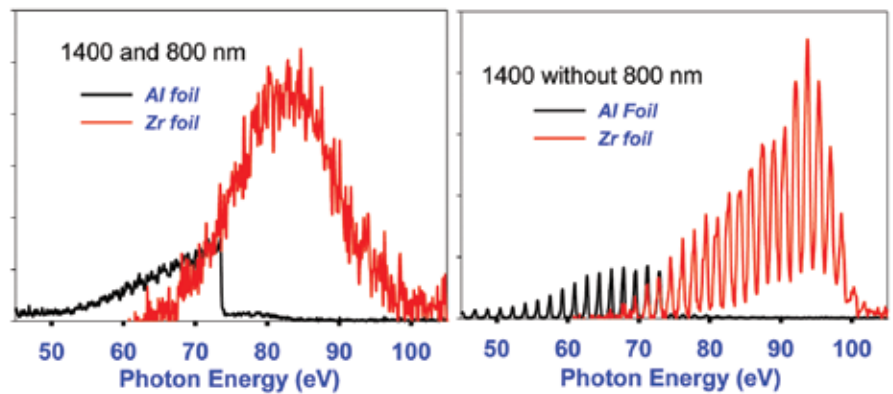
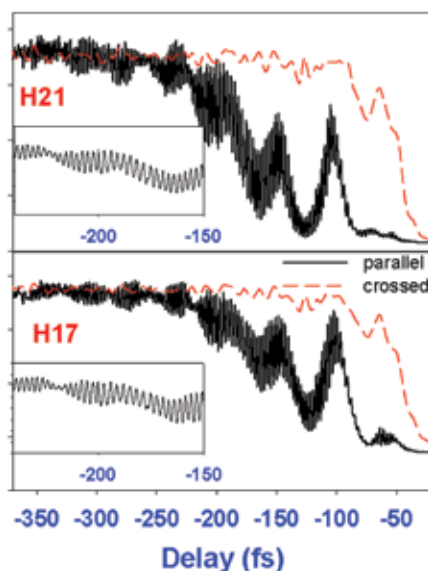


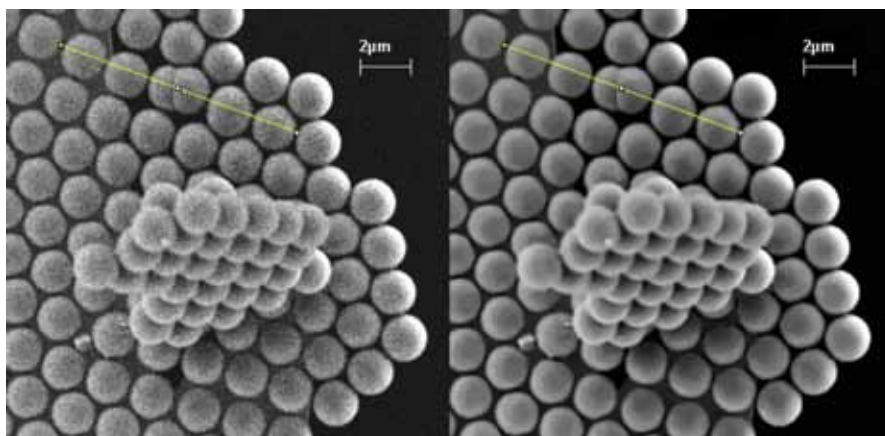
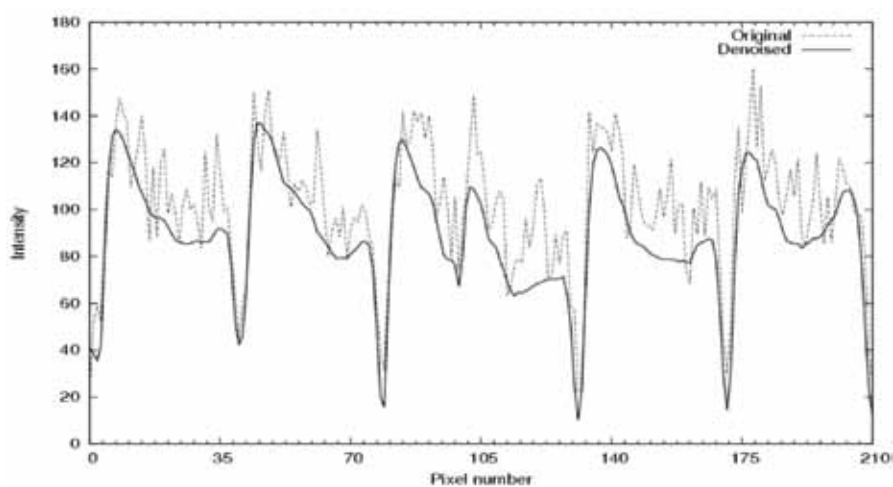
Figure 8. Use of two laser fields at 1400 and 800 nm to control the high-order harmonic generation.

Figure 9. Modulation of the harmonic intensity from oxygen molecular gas versus delay time between two laser fields. This reflects the interference of two free wave-packets. The polarisation of the two fields is crossed and parallel.



DYNAMICS OF A FREE ELECTRON WAVE-PACKET IN HIGH ORDER HARMONIC GENERATION

In conventional pump-probe spectroscopy a strong laser pulse is used to excite an atom (or molecule) and the variation of the optical properties that follows the recovery or excitation of the atoms (or molecules) can be probed by a second delayed pulse. We aim to use pump-probe technology to study HHG. When a strong laser pulse interacts with the atoms, electrons tunnel through the distorted potential to become free electrons or they become trapped in highly excited states. High order harmonic fields are generated through the recombination of the free electron with the parent ion. The propagation and the phase of the fields depend on the optical properties of the medium and will be reflected in the observed harmonic intensity through the so-called phase mismatch factor. A second off-axis delayed pulse is used to perturb the propagation process or to change the harmonic phase which leads to a variation of the total harmonic intensity. Because the laser field varies across the transverse direction, which is perpendicular to the propagation direction, the harmonic phase is also changed across the beam profile. The delay between these two pulses can be controlled or selected with a resolution in the femtosecond and attosecond scale permitting the dynamics of the phase change to be studied with high time resolution. Using a second, long, off-axis laser beam for control of the HHG process we have shown that the dynamics of the excited wave packet can be studied through



SEM image of self-assembled microspheres (left) to be used as a test sample for comparison of a range of super-resolution optical microscopy methods. The plot (top) demonstrates the enhanced contrast achieved by denoising image data (right), a method to be applied as part of our SIM reconstruction software.

the modulation of the HHG intensity. In this case two free wave-packets, which are created by the first laser field and by the second laser field, can interfere with each other as shown in [Figure 9] for oxygen gas.

The experimental approach proposed here will provide a detailed insight of the excited electrons in atomic and molecular systems.



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 2-D crystals and 3-D 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, crystallisation and handling of these samples.

The ongoing study of *purple membrane*, a naturally occurring 2-D crystal of the membrane protein *bacteriorhodopsin*, serves as a useful test case because there is high-resolution structural information available from 3-D X-ray crystallography and 2-D cryo-electron microscopy that can be used for comparison. A collaboration within CXS has helped link into expertise in developing and applying computer programs for deconvolving data for diffraction from 2-D crystal powders and led to alternative ways to explore the use of 2-D 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 2-D crystal powders – a little-explored 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 3-D single-crystal methods.

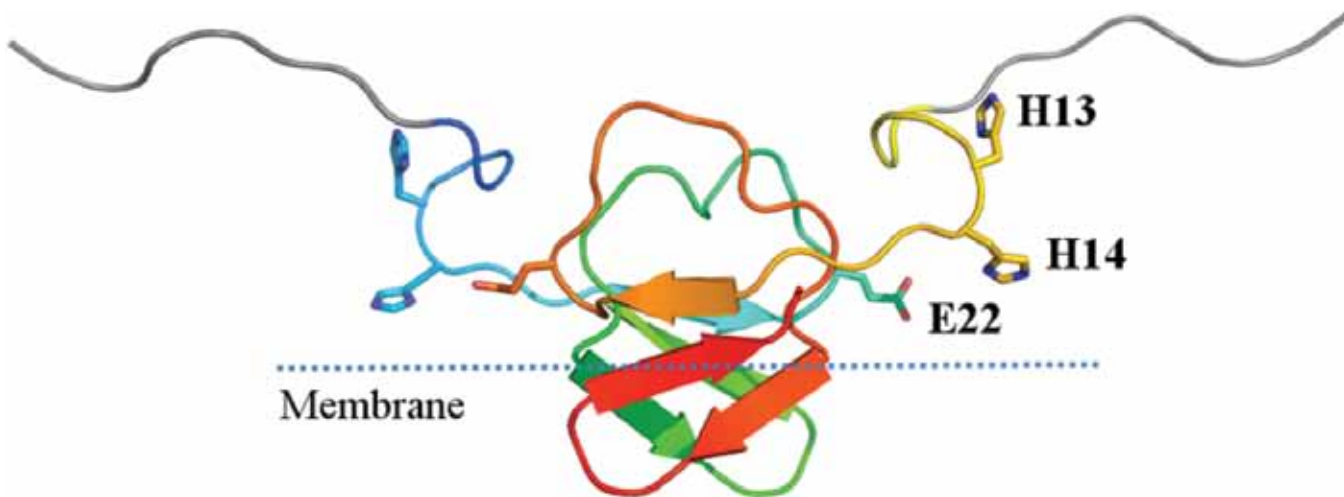
On the CSIRO Molecular and Health Technologies (CMHT) side, work has progressed on the preparation of a number of different types of powder samples of integral membrane proteins consisting of preferentially and randomly oriented 2-D crystal layers.

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 (2-D)

protein crystals in powder samples. The research can broadly be divided into three areas. The first is concerned with fitting 2-D 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 2-D crystal powder diffraction context amounts to reconstruction of a 2-D projection map of the electron density in the crystal. This can be viewed as a technique spanning coherent diffractive imaging and 3-D crystallography and is aimed at high-resolution 3-D structure determination. The advantage of the technique being developed here is that it does not require 3-D crystals, nor does it require 2-D crystals of the size needed for structure determination by electron diffraction.

ACHIEVEMENTS

- Dr Victor Streltsov collaborated with Dr Ruben Dilanian on powder data processing and “nano” crystallography at the XFEL facilities. The resulting paper, Continuous X-ray diffractive field in protein nanocrystallography by Ruben A. Dilanian, Victor A. Streltsov, Harry M. Quiney, and Keith A. Nugent has been published in *Acta Cryst A*. The pair additionally collaborated on low resolution phasing of X-ray powder diffraction data using ellipsoidal construction for molecular envelopes as part of Sophie Williams’ M.Sc. thesis.
- Alberto Cereser (PhD student co-supervised by Dr Victor Streltsov,



Associate Professor Andrew Peele and Dr Grant van Riessen) has collected CDI and XFM data at APS and AS for yeast cell producing fusion GFP-amyloid-beta ($A\beta$) protein.

- Dr Connie Darmanin had the role of preparing protein crystals for the XFELs experiment that is not ideal for proteins. The sample chamber is under vacuum and is at room temperature. The pump down cycle was estimated to take 40 mins and data collection of 3000 crystals (placed in one holder) was estimated to take ~2.5hrs. Lysozyme crystals were prepared for the experiment and were of various sizes to measure radiation damage of the crystals. The crystal conditions were optimised so that the protein crystals were stable at room temp for up to 4 hours. A method was developed to set up the crystals in specifically designed holders to obtain diffraction. This method was tested on a number of Australian Synchrotron trips (Streltsov, Darmanin) where data was collected and crystal quality analysed to ensure crystals survived the XFELs experiment.
- Dr Victor Streltsov had the role of preparing beta-hematin powder samples and testing them as well as C60 samples at the Australian Synchrotron for experiments at the LCLS XFEL, Stanford.
- Low-resolution data for a beta-hematin, C₆₀ and partially for lysozyme have been collected at LCLS XFEL. Data obtained is currently being analysed by the Melbourne uni group (Putkunz, Martin and Dilanian) and paper is in preparation.
- ATP synthase crystal samples from Daniela Stock were also tested and data

collected at XFELs. Data still needs to be examined to see if protein diffraction is present and if so, whether it be included in the next round of XFELs proposals.

- Dr Victor Streltsov received a Fellowship from the Japanese Society for Promotion of Science (JSPS) fellowship through the SPS Invitation Fellowships Program for Research in Japan, to conduct research, attend seminars, give lectures, etc at Nagoya Institute of Technology for a period of 30 days in 2012.
- Lynn Liang, a PhD student co-supervised by Professor Leann Tilley and Dr Connie Darmanin has completed her thesis and as passed with minor corrections.
- Dr Connie Darmanin has organised a Tall Poppies crystallisation workshop at CSIRO, for Year 11 students from Santa Maria College. This workshop has been successfully run for three year now, and is growing in popularity. This year, two workshops are being conducted to cater for the increased number of participants.

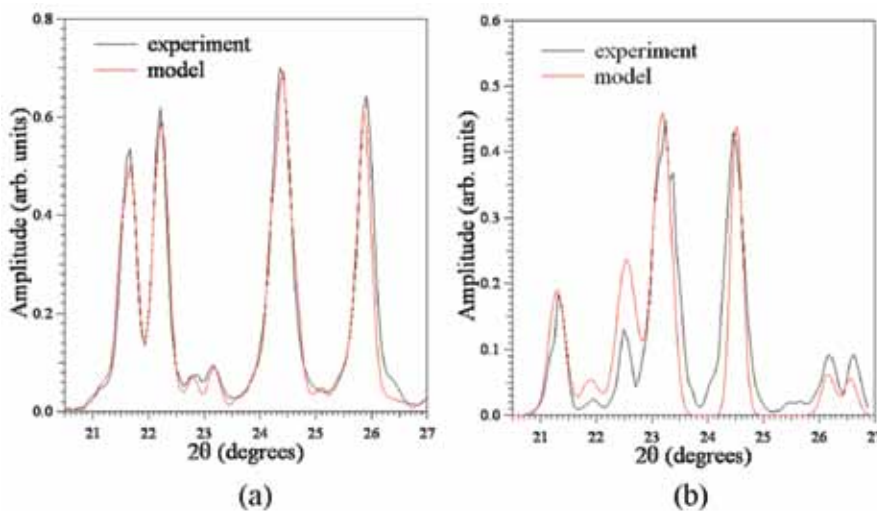
STRUCTURE DETERMINATION PROGRAM CASE STUDY

CRYSTALLOGRAPHIC MODELS FOR AMYLOID-BETA IN ALZHEIMER'S DISEASE

In the rapidly moving neurodegenerative disease field there is a growing realisation of the existence of small oligomeric and metal (Fe, Cu, and Zn) binding forms of amyloid- β ($A\beta$) peptide mediate toxicity in Alzheimer's disease. $A\beta$ is a widely accepted therapeutic target. Crystallographic structural information about $A\beta$ peptide

oligomers and metal binding sites is limited due to the heterogeneous nature of aggregation states formed by the peptide. The problem of spontaneous $A\beta$ aggregation was solved by making use of: 1) a single chain shark antibody, IgNAR [1], to box in the $A\beta$ oligomers as they formed [2]; and 2) immunity protein, Im7, as a scaffold for the stabilization of $A\beta$ metal binding domain, in combination with complex formation using the $A\beta$ specific W02 Fab [3]. Combining the two crystallographic structures [2,3] results in a model whereby the metal-binding site (H13 and H14) of $A\beta$ dimeric oligomer are ideally oriented to mediate oxidative stress *via* Fe or Cu binding and modulate membrane behavior. This discovery finally shows that the structure of oligomers is not like a piece of a fibril, thus potentially providing a model system for non-fibrillar oligomer formation in Alzheimer's disease.

1. **Streltsov VA**, Varghese JN, Carmichael JA, Irving RA, Hudson PJ & Nuttall SD (2004) "Structural evidence for evolution of shark Ig new antigen receptor variable domain antibodies from a cell surface receptor". *Proc. Natl. Acad. Sci. USA*, 101:12444-12449.
2. **Streltsov VA**, Varghese JN, Masters CL, Nuttall SD (2011) Crystal Structure of the Amyloid- β p3 Fragment Provides a Model for Oligomer Formation in Alzheimer's Disease, *J. Neurosci.* 31:1419-1426.
3. Nisbet R, Nuttall SD, Robert R, Caine JM, Dolezal O, Hattarki M, Pearce LA, Davydova N, Masters CL, Varghese JN, **Streltsov VA** (2013) "Structural studies of the tethered N-terminus of the Alzheimer's disease $A\beta$ peptide". Submitted to *Proteins: Structures, Function and Bioinformatics*.



Left. Simulated (red) and measured (black) diffraction pattern of C₆₀ crystal ($2 \leq qD \leq 3$ region of the diffraction pattern). (a) Data collected at 10% power. (b) Data collected at 100% power.

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 involve:

1. The solution of inverse problems.
2. The characterisation of partial spatial and temporal coherence in short wavelength light sources.
3. The relativistic formulation of molecular electronic structure and quantum electrodynamics.
4. The dynamic description of non-linear interactions between molecules and strong coherent fields.
5. Coherent energy transfer processes in biomolecules.
6. The design of efficient computational algorithms.

The Theory and Modelling Program collaborates closely with all of 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 in atomic systems using visible and infra-red light sources and of the interaction of molecules with strong-field high-frequency X-ray free-electron laser (XFEL) sources.
- Non-interferometric phase recovery techniques in photon echo spectroscopy.
- Non-linear interactions involving optical or infrared sources and atoms.

ACHIEVEMENTS

NEW SCIENCE WITH X-RAY FREE-ELECTRON LASERS

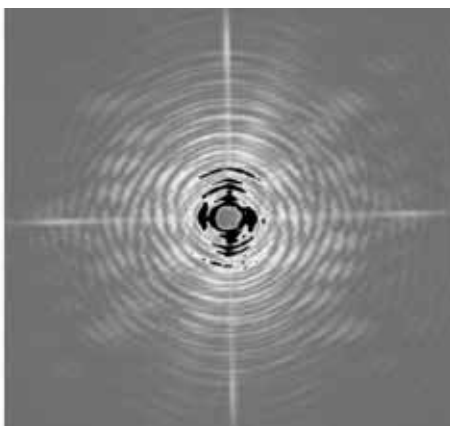
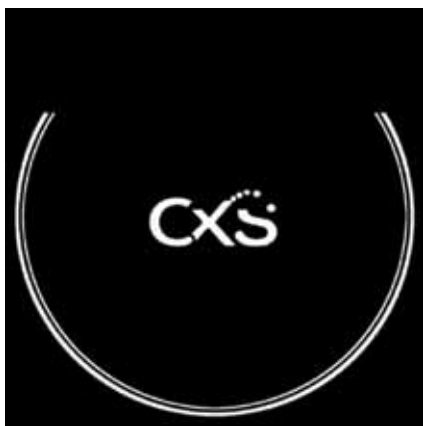
The main focus of 2012 has been the experiment on crystalline C₆₀ at the Linac Coherent Light Source. Dr Andrew Martin and Dr Ruben Dilanian were part of a TMP collaboration with the CXS experimental group to process and analyse the diffraction data. This has been no small task, considering the raw nature of data taken with the custom one-of-a-kind detectors used at XFEL facilities. Having developed methods to extract accurate data from

the measurements, we were struck by the remarkable observation that a long-lived coherent electronic change that can be produced by the X-ray beam has not been predicted by any theory. The Theory and Modelling Group has attacked the problem of trying to understand this effect.

The power density in an XFEL pulse is so high that it can modify the electronic properties of a sample on a femtosecond timescale. Exploration of the interaction of intense coherent X-ray pulses and matter is of both intrinsic scientific interest and of critical importance to the interpretation of experiments that probe the structures of materials using high-brightness femtosecond XFEL pulses. The influence of the nanofocused femtosecond X-ray laser pulse on the structural properties of C₆₀ crystals has been first observed and analysed by TMP.

In our analysis we assumed that the holes created on the C₆₀ molecules by ionisation modify the atomic scattering factors of carbon atoms and in turn, modify the scattering amplitudes of the C₆₀ molecules. The holes induce a dipole moment in each C₆₀ molecule and affect the resulting symmetry of the C₆₀ molecule. The loss of the spherical symmetry of the molecule leads to additional phase contribution to the scattering amplitude. It should also be noted that only the collective alignment of induced dipoles over a large domain of the crystal is a possible explanation for our experimental observations.

A collaboration with Professor. Chapman's group at the Deutsches Elektronen-Synchrotron (DESY) continued strongly. Several projects involving Andrew Martin



Left. The design for the sample that was deposited onto a X-ray transparent window. Right. The measured holographic diffraction pattern at the FERMI light source, which will be analysed in collaboration with the TCMP group.

matured into publications during 2012, including: high resolution XFEL protein crystallography, the first application of XFELs to study the morphology of airborne particulate matter damage studies in nanocrystallography and time-resolved nanocrystallography. Andrew Martin also led the development of dark-field coherent diffractive imaging to study particulate matter and the development of diffractive imaging methods with improved noise robustness.

Ongoing collaborations between researchers at FERMI – the single-pass FEL user facility in Trieste, Italy – and the Theoretical Condensed Matter Group at the University of Melbourne, to develop new holographic imaging methods, produced new experimental results and faster, more-robust algorithms. An example of holographic diffraction for the new methods is shown in the figure below.

Working toward single particle imaging with XFELs, we worked on combining damage theory with the problem of determining molecular orientations. This is a critical problem that must be solved for the future realisation of single molecule imaging with XFELs. We are currently discussing the development of Bayesian methods with collaborators in Electrical Engineering (Manton and Said) at the University of Melbourne.

XFEL imaging work and the C_{60} results were presented at the Coherence 2012 workshop in Fukuoka, Japan; the AsCA 2012 conference in Adelaide; and at the Workshop on Diffraction and Phase Retrieval at Monash University.

T'Mir Julius has continued on the role of software support by developing the NADIA

package for Coherent Diffractive Imaging. This package now includes the ability to incorporate partial spatial and temporal coherence as well as the other signature technologies of CXS, such as Fresnel Coherent Diffractive Imaging and our unified formulation of iterative projective algorithms. The software is distributed freely from the CXS website.

CONTINUOUS X-RAY DIFFRACTION IN PROTEIN NANOCRYSTALLOGRAPHY

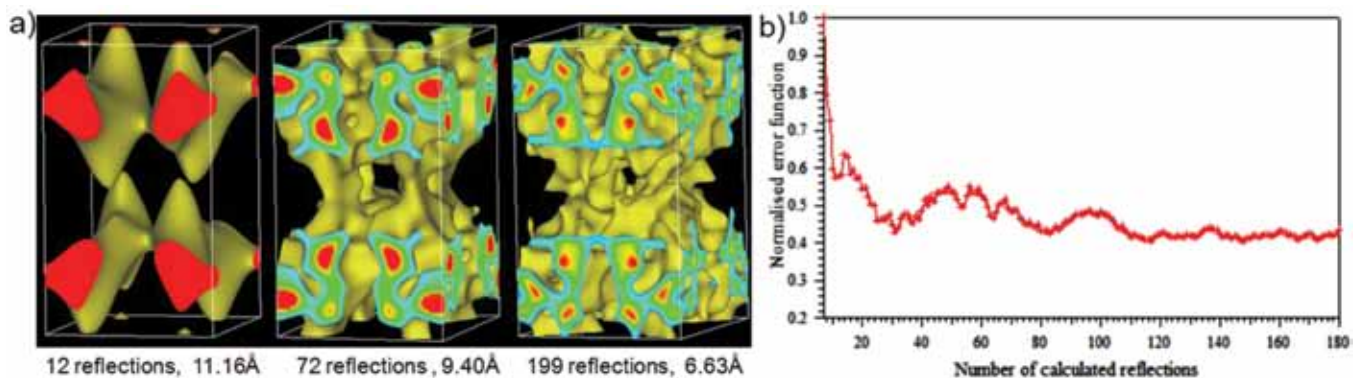
Growing crystals of membrane proteins to a size suitable for high-resolution X-ray structure analysis has always been a major challenge for modern structural biology. The fact that some proteins only form crystals of the nanoscale size indicates, however, that their crystal structures are far from ideal. The structural imperfections such as mutual displacement or misalignment of proteins, particularly at the surface of the nanocrystals, as well as the shape and dimensions of the nanocrystals, play an important role in formation of the diffraction pattern. An approach to data analysis has been proposed and demonstrated that it can properly take these imperfections into account. It is intriguing to note that the analysis proposed here, based on continuous diffraction patterns, offers a unique solution for the structure without the need for additional assumptions or additional data.

STRUCTURE DETERMINATION OF PROTEINS FROM X-RAY POWDER DIFFRACTION

The common structure determination approach of single crystal X-ray diffraction is greatly limited by the difficulties in forming crystals suitable for the study of membrane proteins. Often, membrane proteins tend to form two-dimensional crystals during crystallisation processes, which limits the possibility of obtaining their structures using the standard methods of protein crystallography, or three-dimensional nanoscale crystals, which weakly diffract.

A possible alternative for the study of membrane proteins is presented by X-ray powder diffraction, which can more readily utilise the crystals that are usually formed. X-ray powder diffraction is not widely used for biological structural studies due to the difficulties involved in extracting structure factor amplitudes from overlapping Bragg reflections in powder diffraction patterns. This problem is treated through a combined approach of using the Le Bail method and a new *ab initio* phasing method. This has been applied to test cases of the colicin immunity protein IM and bacteriorhodopsin through simulation studies and to the protein lysozyme from powder diffraction data collected at the Australian Synchrotron (AS).

This approach allows for structure factor amplitudes to be extracted without a structural model. This phasing approach is in contrast to the most common method for biological samples, molecular replacement, in that it does not require atomic structural models. Rather, simple geometric objects and knowledge of the crystal parameters and symmetries are utilised to estimate the phases of low order reflections.



Above. a) Progressive electron density reconstructions of immunity protein IM7 from maximum-entropy reconstructions; b) Normalised error distribution of the maximum-entropy reconstruction of immunity protein IM7

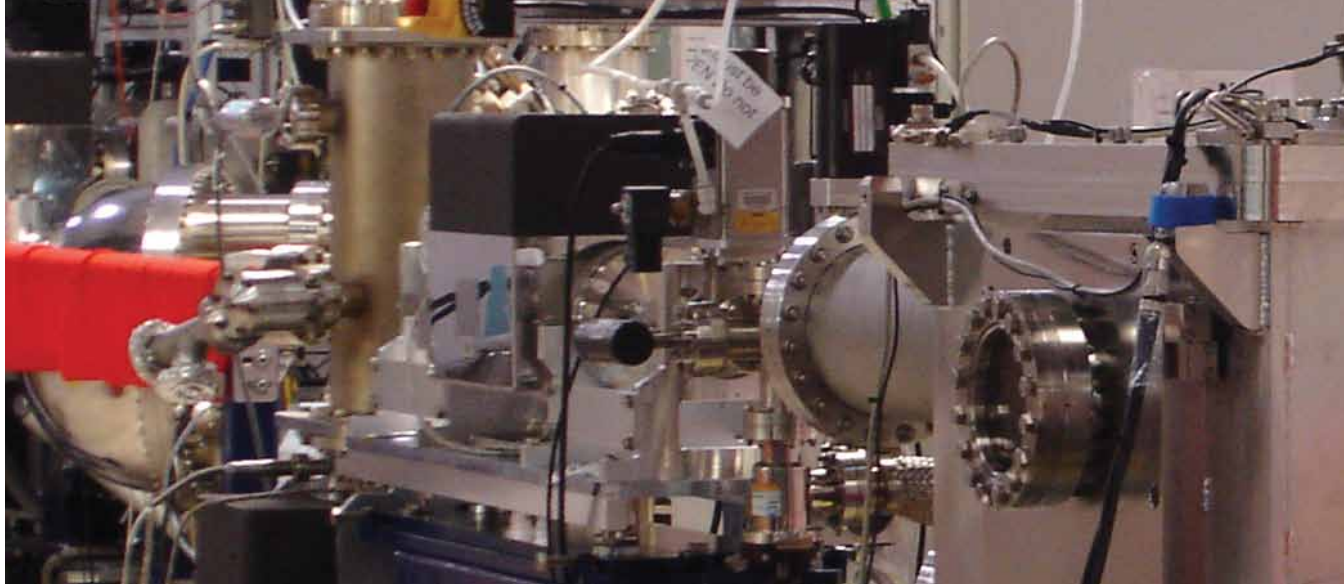
CASE STUDY: THEORETICAL SUPPORT OF NON-LINEAR INTERACTION PHYSICS

Over the past year, Daniel Wells has been working on his PhD as part of the Theory and Modelling group to model the behaviour of atoms exposed to intense femtosecond laser pulses. This research has focussed on developing and implementing methods to numerically integrate the Time-Dependent Schrödinger Equation (TDSE). Solving the Schrödinger equation for laser-atom interactions allows, in principle, for an exact calculation of Above Threshold Ionisation (ATI) or High Harmonic Generation (HHG) spectra. He has developed a new method of solving the TDSE in which the propagation of the wavefunctions is reduced to the solution of a large set of linear equations. The preconditioned conjugate gradient method has been adapted to obtain these solutions to high numerical accuracy, but in a formulation that is readily extended to ultra-strong fields requiring relativistic quantum electrodynamics.

This work is closely tied to the experimental program of the Attosecond Science group at Griffith University. The ATI experiments performed at Griffith use atomic hydrogen as the gas medium. This is particularly amenable to TDSE simulations because the atomic potential experienced by the active electron is known exactly. For this reason this particular system is the best place to look to achieve agreement between the theoretical simulations and experimental data.

A current objective of the Theory and Modelling group is to compile a software

package that will allow for the simulation of these processes across a wide range of parameters. During 2012, Daniel spent a productive week at Griffith University with the Attosecond Science group where the requirements and limitations of such a software package were established. This is expected to be completed in 2013, during which time Daniel will continue his close collaboration with Griffith as part of his PhD.



ULTRACOLD PLASMA SOURCE PROGRAM

The Ultracold 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 most significant aspect of the UCP source and 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. The team is 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. The team has jointly published work based on the Centre's imaging approaches for applications in characterising the cold atom cloud and is now collaborating with the TMP group to employ their expertise on partially coherent X-ray sources for modelling 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 modelling 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 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

In 2011, the CXS Ultracold Plasma Source Program demonstrated the extraordinary potential of its new high-coherence cold electron source which promises unprecedented brightness for diffractive imaging of biological targets. In 2012, we extended the capabilities of the source by demonstrating the production of high coherence picosecond electron bunches.

Our experiments used very fast (femtosecond) laser pulses to ionise cold atoms, and thereby produce short electron bunches with low temperature and high spatial coherence. The results were counter-intuitive because there is a fundamental limit to how short a pulse can be in time, and how narrow in energy uncertainty. The short laser pulses have

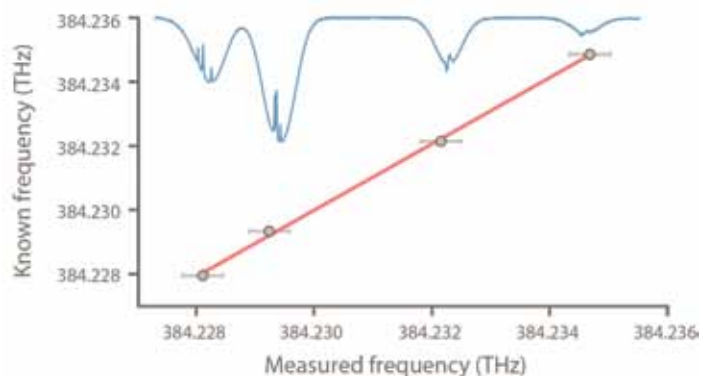
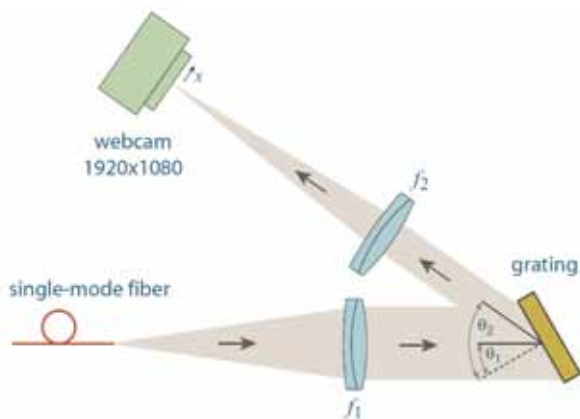


Figure 11. Top left: schematic of the diffraction-based spectrometer, which achieves picometer wavelength resolution with picoWatt sensitivity. A singlemode optical fibre provides a submicron source which is imaged onto a high resolution CMOS imaging sensor via achromatic doublet lenses and a small diffraction grating. Top right: Sample measurement which demonstrates resolution and accuracy by measuring the wavelength of a laser tuned to four hyperfine transitions of isotopically mixed rubidium. From *Review of Scientific Instruments* **83** 113104 (2012).

correspondingly broad energy width which would ordinarily translate into high electron temperatures and low spatial coherence. Using a two-photon sequence to ionise the atoms, and our unique ability to shape the electron bunches spatially, were able to produce and measure ultrafast and bright electron bunches suitable for ultrafast electron diffraction imaging.

A critical assumption in our work is the premise that coherent diffractive imaging (CDI) – so successfully developed and applied by CXS for X-ray imaging – can also be used for electron imaging. Work led by our postdoctoral research fellow Corey Putkunz, in collaboration with the Monash Centre for Electron Microscopy (MCEM), has demonstrated electron-CDI for the first time. The results, published in *Physical Review Letters*, achieved single-atom imaging with enhanced resolution compared to conventional transmission electron microscopy with the same setup.

Demonstration of eCDI was extremely challenging because conventional electron microscopes have poor spatial coherence. The revolutionary cold atom electron source developed by the UCP group has already demonstrated transverse coherence lengths 50 times greater than the \$10mil FEI Titan microscope used in our eCDI demonstration. A detailed study of the spatial coherence has been published in *Optics Express*.

The cold atom electron source can equally well produce cold ion bunches, which are much colder (microKelvin rather than 10K) and travel much more slowly. The long interaction time between source and detector allows ion-ion Coulomb interactions to dramatically affect the shape of the ion

bunches. (Figure 10) is a false-colour image of a detected ion bunch, which began at the source as nine tiny well-separated ion bunches. The Coulomb interactions pushed the mini-bunches into the complex 'wagon wheel' pattern, which can be explained using a complex model incorporating details of the laser-atom and ion-ion interactions.

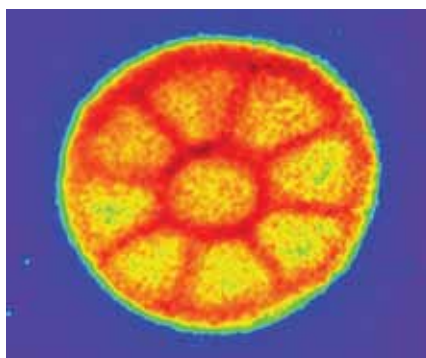


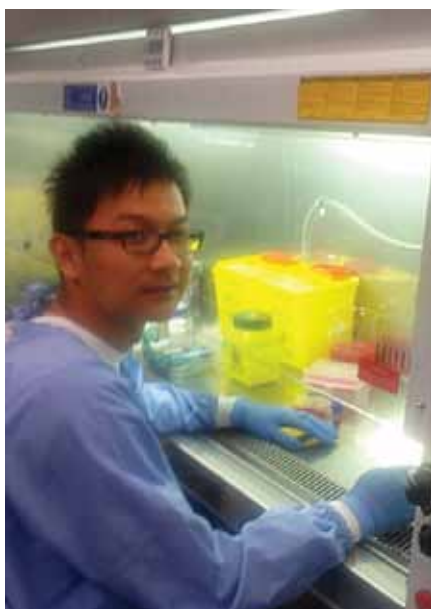
Figure 10.

ULTRACOLD PLASMA SOURCE PROGRAM CASE STUDY

Development of the new electron source has been underpinned by progress in technical areas – in particular, lasers. The group designed a new high-stability external cavity diode laser based on a 'cats-eye' reflector, and a high-resolution wavelength measurement instrument using simple diffraction combined with a modern imaging sensor and single-mode fibre optics, both published separately in *Review of Scientific Instruments*. The latter was reviewed by Nobel laureate Jan Hall, who wrote in his review to the Editor, "It will be interesting to follow the ISI citations for this article – I predict this will turn out to be one of your all-time favorites". (See Figure 11 above)

STUDENT LIFE @ CXS

EXPANDING HORIZONS



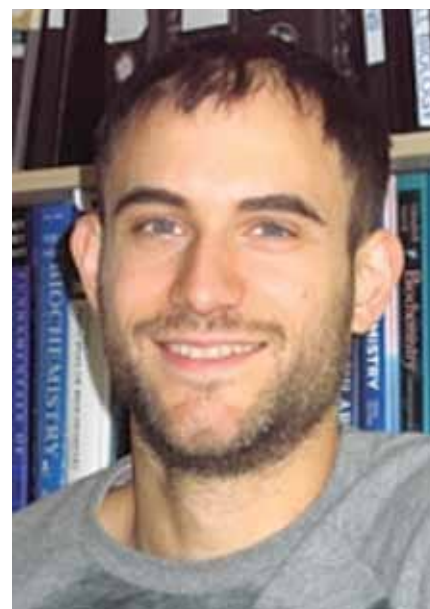
Stanley Cheng Xie

STANLEY CHENG XIE, BIOLOGICAL SCIENCES PROGRAM

UNIVERSITY OF MELBOURNE

I am a first year PhD student in the Biological Sciences program of the CXS under the supervision of Leann Tilley and Nick Klonis. My research focuses on a class of antimalarial drugs, the artemisinins. The aim of my project is to understand the emerging resistance of malaria parasites to artemisinin. It will contribute to the development of new antimalarial drugs in the future.

I have greatly benefited from the environment created by CXS. A series of meetings and seminars have been arranged by CXS, which enables me to interact with researchers and expand my knowledge. As a member of CXS, I have had opportunities to work with colleagues who have expertise in different areas. I have worked with cohorts with maths and physics backgrounds who were able to generate a sophisticated model of parasite responses to artemisinin treatment. This is helping me to understand the data and to make predictions for what might happen during clinical treatment.



Boris Reljic

BORIS RELJIC, BIOLOGICAL SCIENCES PROGRAM

LA TROBE UNIVERSITY

I started my PhD with Professor. Michael Ryan, a senior member of the CXS, at La Trobe University in 2010 and subsequently joined the CXS as a member. During the course of my PhD I am working on elucidating the interaction mechanism of two important mitochondrial outer membrane proteins, both of which play a critical role in mitochondrial induced apoptosis. The mechanisms are not yet fully understood and the CXS provides an excellent environment to address these questions. As a member of the organisation I not only have the opportunity to learn and work with experts in the field of microscopy as well as X-ray sciences, but I also have the opportunity to attend workshops, seminars and meetings to broaden my scientific knowledge. Recently, the CXS provided the opportunity to join an international conference where world leading experts presented their work. The diverse background of biologists and physicists within CXS creates great opportunities for collaborations in which all participants learn from each other. Being part of CXS at an early stage of my scientific career has encouraged me to think in a wider context about my own project and how work in our lab may benefit from an integrated approach.



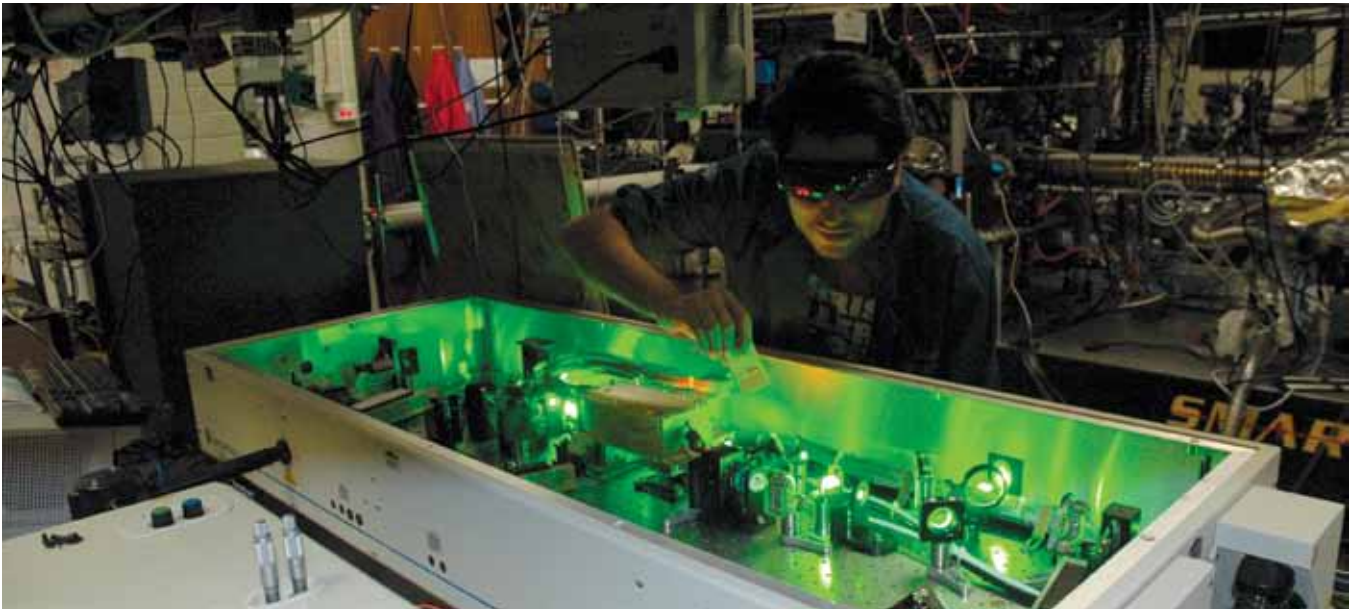
Hoang Vu Le

HOANG VU LE, SHORT WAVELENGTH LASER SOURCE PROGRAM

SWINBURNE UNIVERSITY OF TECHNOLOGY

I joined the Short Wavelength Laser Source program of CXS in early 2011. My project's aim is to enhance the High Harmonic Generation (HHG) source towards the water window region, using this soft X-ray source to perform the CDI experiments. With a bachelor's degree in Electronics and Computer Systems Engineering, I have found it very challenging – but also interesting – to learn new laser physics phenomena. I am also utilising my engineering background to improve the HHG performance, for example, optimising the laser beam pointing stabilisation system. I am interested to use my knowledge and experience in electronics and computer science to improve the stability, reliability and efficiency in our experiments.

Via CXS I have had many great opportunities to learn and share the research experience with scientists and students from different groups through various conferences and workshops. With strong supports from my supervisors, colleagues and other CXS members, I feel this project is very stimulating and I continue to find more inspiration for my research.



Dan Thompson in the Ultracold Lab

DANIEL THOMPSON, ULTRACOLD PLASMA SOURCE PROGRAM

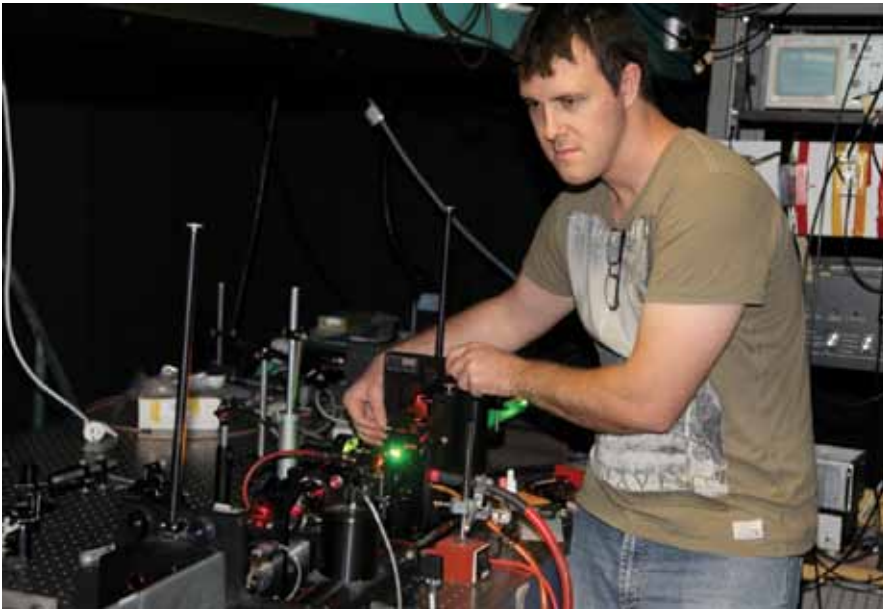
UNIVERSITY OF MELBOURNE

Since the end of 2010 I have been a part of the Ultracold Plasma Source Program (UPSP), under the supervision of Robert Scholten at the University of Melbourne. The source produces a pulsed beam of cold, highly coherent electrons (or ions). The focus of my research is to utilise the 3D arbitrary bunch shaping capability of our source to realise uniformly filled ellipsoidal charge density bunches. It is possible to reverse the effects of space charge expansion within these bunches during free propagation with conventional electron optics, which will allow us to deliver the maximum amount of current to a sample without losing coherence.

Life as a graduate student in the CXS is a tremendously rewarding experience. Being part of an ARC Centre of Excellence enables us to perform research at the cutting-edge. While characterisation of beam dynamics is transient (e.g. the current work on managing Coulomb repulsion), this year we have made significant changes to the original system which will see us perform electron diffraction experiments with our electron source in early 2013. It's truly exciting being in a research environment where the work we're doing will potentially have an impact on the community at large.

In terms of opportunities away from the laboratory this year, being part of the CXS enabled me to attend the inaugural CXS Writers' Workshop; I co-mentored a group of Year 11 students from McClelland College

as part of the Growing Tall Poppies (GTP) program and I was the co-representative for the UPSP at the CXS IP Show and Tell Forum. These activities truly allow students within the CXS to hone their communication skills for a broad range of people as we are trying to establish ourselves as young research scientists. The highlight of my year was definitely attending the Coldbeams conference in France, where I not only learnt a lot but also met with many world leading researchers in the cold monochromatic charged particle beam community.



JAMES CALVERT, ATTOSECOND SCIENCE PROGRAM

GRIFFITH UNIVERSITY

2012 was an interesting year for me as a member of CXS. The year started slowly, but towards the middle of the year I was sent to CLEO 2012 in San Jose, where I promoted some of the work done by the Griffith node of CXS to an international audience, as well as having the chance to find out what else was going on in the world of high resolution imaging. More recently I attended the Griffith node meeting, and became a member of the organising committee for IONS-KOALA 2012, a CXS sponsored student conference for Australasian physicists. The IONS-KOALA preparation has made me appreciative of the people who organise larger conferences, as keeping on top of a small one is considerable work. On the research front this year, I completed a metastable neon source and took preliminary data with the Griffith COLTRIMS device and the AASF laser, with promising results.

HANNAH COUGHLAN, EXPERIMENTAL METHODS PROGRAM

LA TROBE UNIVERSITY

I became a member of the Experimental Methods Program of CXS in 2012 to undertake research as part of a Masters degree. I drew upon my undergraduate background in biochemistry and physics to investigate a new approach to imaging malaria infected red blood cells with coherent soft X-rays. The project involved experimentation, data analysis and simulation work.

Throughout my project, which was based at La Trobe University, I was able to collaborate with researchers from the Bio21 Institute at the University of Melbourne and the ELETTRA synchrotron in Italy. I traveled to ELETTRA to participate in an experiment, which was the highlight of my year.

My aim is to continue working with CXS next year as a PhD student. Being a member of CXS has provided learning experiences and networking opportunities both in the Australian and international scientific communities which have allowed me to expand my scientific horizons.



Left: James Calvert

Above: Hannah Coughlan

N.A.D.I.A PROJECT

DURING THE NATURAL COURSE OF A COMPUTATIONAL-BASED ANALYSIS, A RESEARCHER WILL FIND THEMSELVES WRITING IMPLEMENTATIONS OF THE SAME ALGORITHMS MANY TIMES, WITH EACH ONE SPECIALISED TO THE TASK AT HAND.

It is often difficult to find the time to make this code generic enough to apply to other similar situations and also document the code in such a way that colleagues can change the code for their own purposes. The result is that researchers new to the field, or entering a new area of the field, spend the beginning of their time effectively 'reinventing the wheel'.

NADIA (Nadia's Algorithm for Diffractive Imaging Applications) is a software package that was designed and commenced by previous CXS member, Nadia Davidson. The package aims to collect the inhomogeneous pieces of code that have been circulating throughout CXS for some time, and combine these in to a single, open source package that is accessible to all imaging experiments.

At the time of Nadia's departure, NADIA included iterative algorithms capable of reconstructing coherent planar data as well as coherent Fresnel data using the approach developed by CXS in previous years. This year the code has been expanded to include the algorithms developed at CXS that can reconstruct images taken using partially coherent light sources for both spatially incoherent and temporally incoherent beams. These algorithms more accurately represent the beams available at third-generation synchrotron light sources. By accounting for the use of a partially coherent light

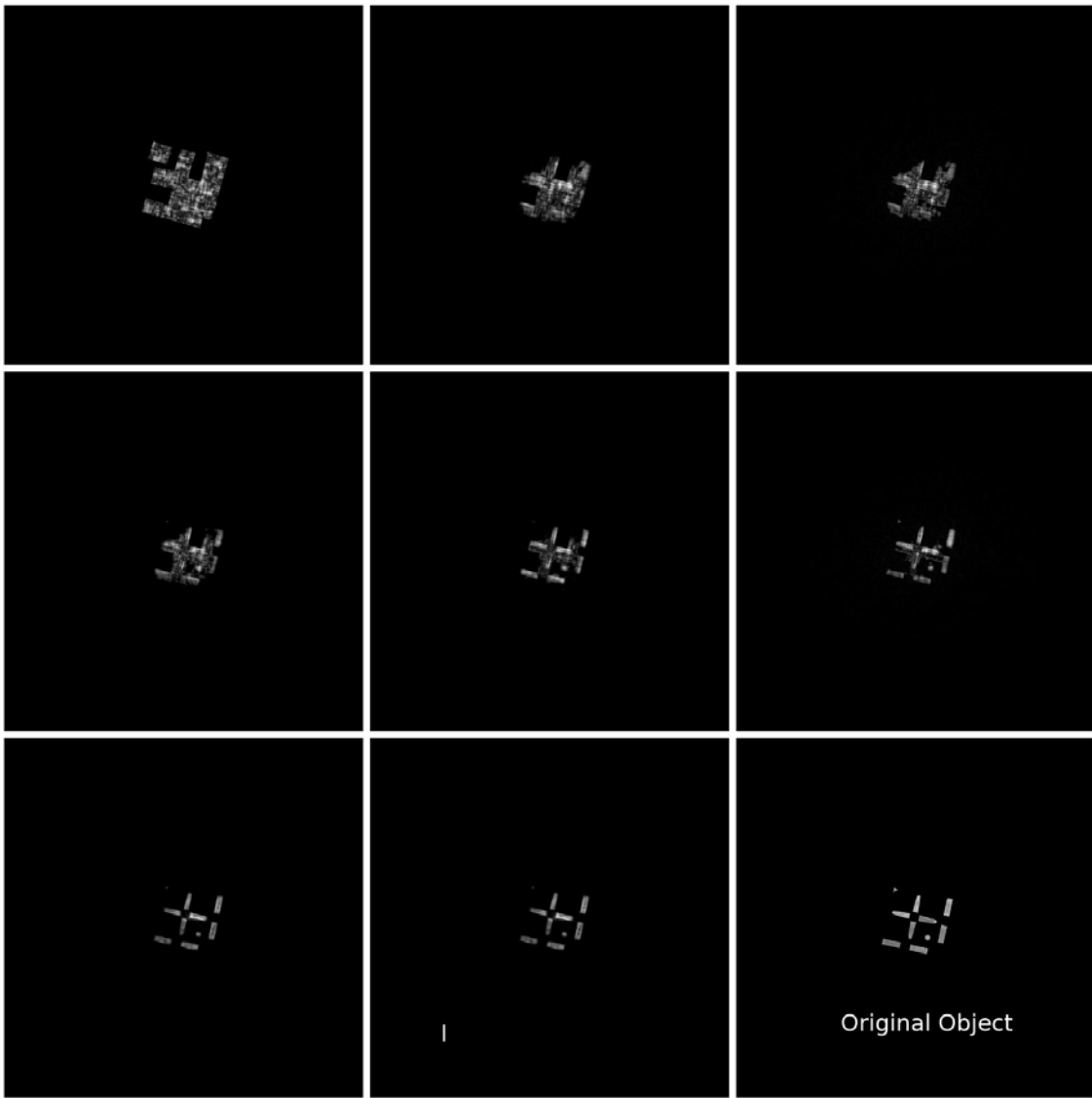
source, it is no longer necessary to filter the beam using a monochromator or a zone plate thereby allowing a much greater illumination of the sample.

The NADIA package aims to become a standard at facilities that perform diffractive imaging, and to do this it must be flexible enough to fit in with frameworks already in use. With this in mind, NADIA comes with a number of usage options. The package has been written in C++, with C++ libraries that can be imported in to a user's C or C++ code. Alternatively, the library can be accessed through a series of command line tools or through IDL using the included IDL routines.

Two workshops designed to explain the theory behind NADIA, and demonstrate the abilities and usage of the software were held in September. The 14 attendees came from a range of software and theoretical backgrounds, and gained hands-on experience in simulating and reconstructing planar data. The workshop also allowed users to write their own piece of code to reconstruct partially spatially coherent data gathered by CXS members.

Extensive documentation as well as installation instructions for Mac OS, Linux and Windows users using Cygwin are available on the CXS website. Examples, sample data and the source code are also available for download.

The NADIA package aims to become a standard at facilities that perform diffractive imaging



Partially spatially coherent data reconstructed using a) the PCDI algorithm and b) planar reconstruction.

FAREWELL TO A FRIEND

OBITUARY: PROFESSOR VASSILIOS SARAFIS, BIOLOGIST, MICROSCOPIST AND PHYSICIST, 1940-2012



T.V. PRICE

**Department of Agricultural Sciences,
La Trobe University, Bundoora, VIC 3086,
Australia**

Professor Vassilios Sarafis died in Hong Kong of a heart attack on 13 June 2012.

Vassilios (Basil/Vasil) was born of a Jewish mother and Greek father in Tel-Aviv, Israel (formerly Palestine) on 16 October 1940. His early childhood was spent in Israel but in 1956, aged 16, he was sent to the United Kingdom where he completed his 'A' Levels. He then went to Queen's University in Belfast where he studied for an external B.Sc. degree of the University of London in Botany and Human Biology. During his vacation he worked at the Department of Cryptogamic Botany, British Museum of Natural History (now the Natural History Museum), South Kensington. His enthusiasm for Botany was greatly influenced by the late Professor Denis Carr who discovered Vasil at 2am one night working in the laboratory in Belfast and promised to give him a job if he passed his Honour's Degree. Vasil was elected a Member of the Institute of Biology (M.I.Biol., UK, now Society of Biology) in 1985.

Vasil's academic career commenced in 1963 as a Demonstrator in Biology at Keele University in the UK. From here he moved to a position of Senior Demonstrator in Plant Physiology at the University of Melbourne in 1965. In 1968 he moved to Massey University, New Zealand, as a lecturer in Botany and Zoology before returning to Australia in 1971 to take up a Lectureship in Biology at Dookie Agricultural College, Victoria. In 1974 he joined Hawkesbury

Agricultural College, New South Wales, as a Lecturer of Biology in the School of Agriculture. In 1980, following the decision by the new Head of the School of Agriculture to abolish the Biology Department he transferred over to the School of Food Science and Technology, where he taught Human Biology, biology of food and alternative crops. Following the amalgamation of Hawkesbury Agricultural College with the University of Western Sydney (UWS, Hawkesbury), he was promoted to Senior Lecturer in 1982 and in 1992 to Associate Professor. He was elected a member of the Council of Hawkesbury Agricultural College and in this role Vasil championed for better staff conditions including promotion criteria and a change of attitudes towards basic research. He supported and mentored many staff and postgraduate students at UWS but in 1997 he opted to take early retirement in order to pursue his varied research interests more widely and without the constraints of working within an institution which he considered stifled his research. Since 1997, until his death in June 2012, Vasil held a number of Senior Honorary appointments at Universities both within and outside Australia in the fields of both Biology and Physics. These included: Adjunct Associate Professor, Horticulture, University of Western Sydney (UWS); Honorary Associate Professor and Reader, Centre for Microscopy and Microanalysis (CMM), University of Queensland; Visiting Associate Professor, Department of Anatomical Sciences, University of Adelaide; Visiting Associate Professor, School of Information Technology and Computer Sciences and Visiting Professor at the Cooperative Research Centre for Sensor Signalling



and Information Processing (CRC CSSIP), University of Queensland as well as Adjunct Associate Professor in the School of Life Sciences; Visiting Associate Professor, Human Biology, University of Adelaide; Honorary Professor of Physics, University of Queensland (2008-2011); Visiting Professor of Optical Microscopy, Department of Physics, Tezpur University and Indian Federal Postgraduate Institution in Assam, India. In 2007, Vasil took up a 3-year appointment as Professor, Institute of Physical Biology, University of South Bohemia, Czech Republic.

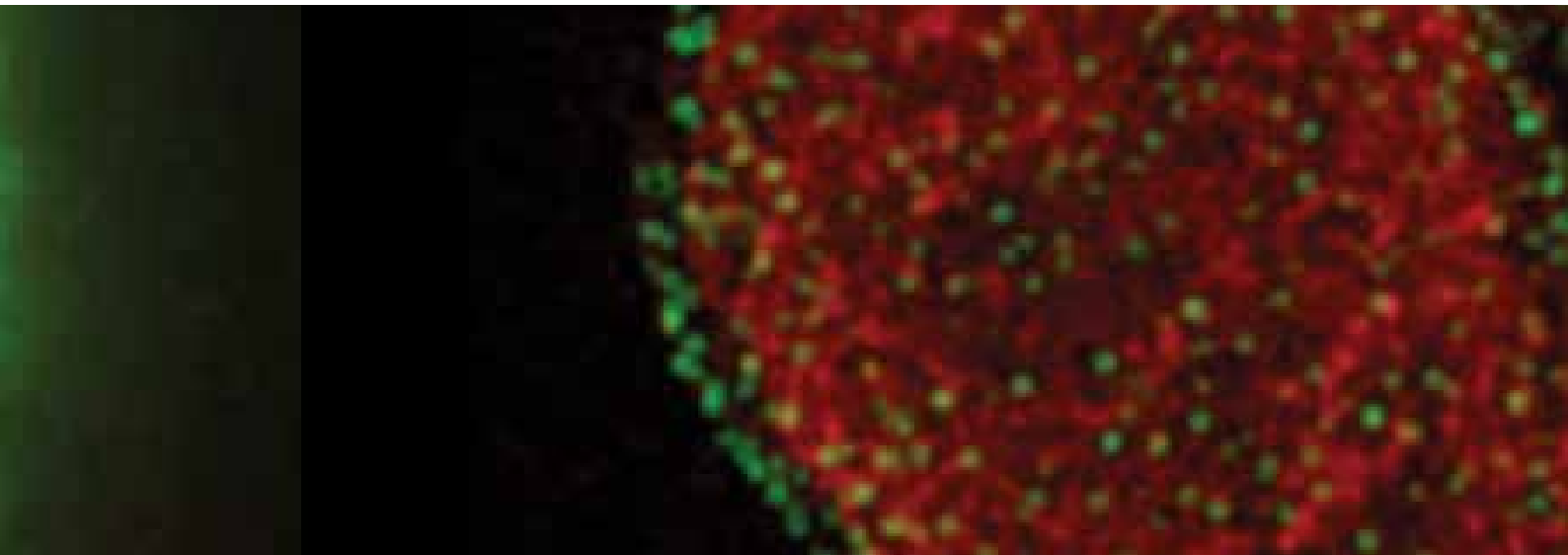
Vasil was an enthusiastic researcher whose biological interests ranged widely from various aspects of Plant and Animal Biology to Human Biology and Microscopy. He successfully obtained competitive research grants from both the Australian Research Council and the Australian Meat Research Corporation. In general his research approach was structural as well as functional and he published papers on methodologies, cell structure, and histochemistry of both plants and animals (Breed and Sarafis, 1979). Vasil had a marvellously inquiring mind that led him into many other disciplines. His early interests included autecology of mosses and evolutionary relationships within plant and animal groups. Vasil was an extremely strong advocate of the need for botanical science as a core discipline that should underpin plant biological research and he knew who was doing good work in this area. He was critical of the way Universities have deviated from the straight and narrow approach, downgrading the need for sound observational science and the overemphasis of molecular biology,

something many will agree with. He was a true polymath who always astounded people with his originality, breadth of knowledge and varied enthusiasms especially for optics and microscopy. His particular interest in super-resolution began in New Zealand in the late 1960's and he undertook further study in this area with the late Professor. H.Lipson in 1975 and this interest was further nurtured by Professor. Colin Sheppard at Sydney University. He was the first person to introduce confocal microscopy to Australians in the then ASEM Newsletter and was always pushing the development of super resolution as a new technique in optical microscopy. Vasil's ideas were always fascinating and credible and just outside the ambit of conventional thinking. He was ahead of his time in this area of super-resolution and this is evidenced by the fact that commercial instruments are just coming on the market today – Vasil had been talking about this technology at least 10 years ago. More recently, his interests concentrated of use of non-invasive imaging techniques in biology and especially the use of confocal microscopy and superresolution. In addition, he had a continuing interest in Bioresources and Food and made contributions in that area. He was saddened that a coursework Graduate Diploma in Food Resources that he and I had jointly compiled in the 1970's, which was approved by the Higher Education Board of NSW, was shelved and never delivered by Hawkesbury College. Because he was restricted in his research at Hawkesbury he tended to collaborate widely with scientists based at other Universities and Institutions both within and outside Australia (especially Germany, UK and Israel) who shared

his research interests and possessed the equipment and facilities he needed especially for his basic research.

One of Vasil's earliest papers was published in the prestigious journal *Nature* (Giles and Sarafis, 1972), but almost 50% of his papers were published after he retired from UWS. His most significant papers include: Survival and reproduction of chloroplasts *in vitro* (Sarafis, 1998); introducing confocal microscopy as a new methodology to re-evaluate the structure of chloroplasts *in vivo* (Spronsen et al., 1989; Sarafis, 1990); the development of super-resolution in microscopy through the use of spatial filters (Hegedus and Sarafis, 1986; Boyer and Sarafis, 2001); the application of nuclear magnetic resonance microscopy as a non-invasive tool for plant structure, histochemistry and physiology (Sarafis et al., 1990); the application of nuclear magnetic resonance (NMR) imaging and confocal microscopy to meat (Tingle et al., 1995) and scald of apples (Golding et al., 1997); applications of X-ray microscopy to the study of plant cells and organelles (Sarafis, 1986) and the identification by cryofluorescence microscopy of chloroplast photosystems (Vacha et al., 2007).

Vasil had a long association with the Centre of Microscopy and Microanalysis (CMM) at Queensland University and organized a workshop on super-resolution at the Australian Conference of Electron Microscopy in Adelaide in 2002. The papers from this meeting were published in a separate issue (Vol 34, 6-7) of the journal *Micron* (Sarafis, 2003). Vasil contributed four papers at this meeting. He also helped organize an International Topical Conference on Super-resolution and



Photonics held at Kolkata in 2005 and presented three papers again published as a special issue (Vol 38, 2) of *Micron* (Harza and Sarafis, 2007). More recently he gave a lucid report on the Third International Super and High Resolution Conference held in Lipica, Slovenia in 2010, again published as a special issue of *Micron* (Sarafis, 2011) of which he again contributed his time, energy and enthusiasm and this unfortunately was to be his last conference in this series. Of course Vasil was larger than life in more ways than one. For one whose interests ranged from plant science to human biology, he was remarkable and he was more than willing to push when he needed to do so in his own interest. Vasil was a good networker and always amazed colleagues by the people in high positions he knew personally and could easily access. These included Vice Chancellors, politicians and important members of the community who could always expect a visit from Vasil when he was in town!

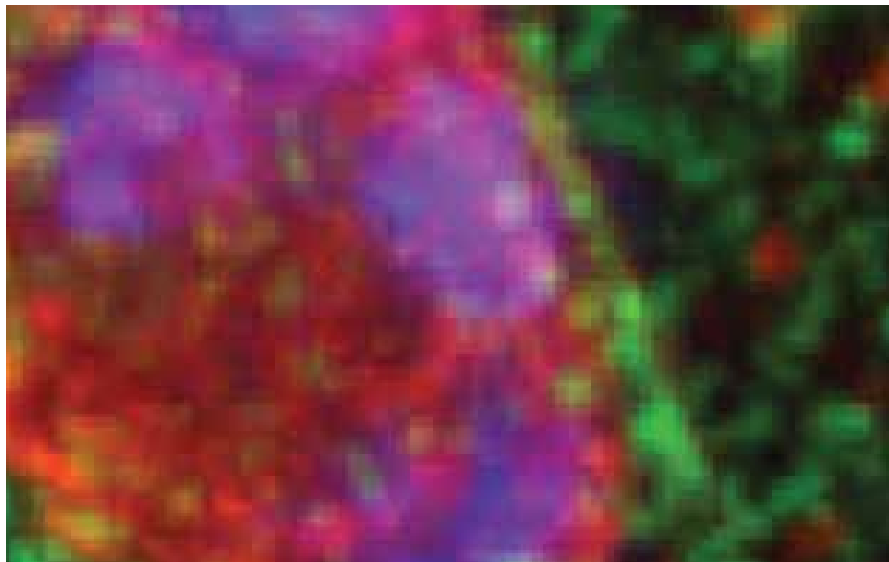
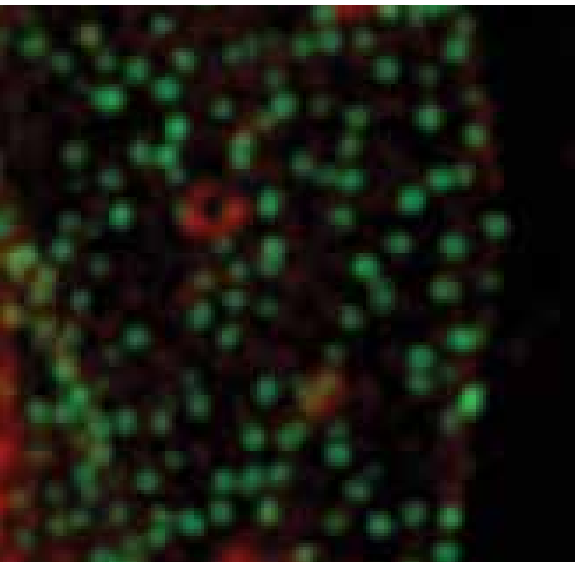
Vasil was fluent in a number of European languages and he travelled widely throughout Europe, Asia, Israel and South America. He was an accomplished pianist and a walking gourmet, who loved to discover new edible plants on his travels. He thoroughly enjoyed arranging discussions over a meal, often at places he chose, with scientific and academic colleagues and friends, wherever he went. One of my earlier experiences was Vasil going to the Sydney fish market, purchasing and bringing the fish by train to Richmond, taking it to the local Chinese restaurant, going straight through the swing doors into the kitchen and asking the chef to cook it for our lunch! Vasil always managed to get

his way! Vassilios, as he liked to be called by some, has been quite an institution, often turning up at a friend's home in Queensland with little notice from time to time, usually laden with mud crabs, mangos etc. for the children. He was thoughtful and generous in purchasing presents of 'goodies and delicacies' to be taken back home, after a meal, for consumption by one's spouses, mothers or children. He had a long memory and continuously reminded all those who had supported him during his undergraduate days and throughout his scientific career, and also those who sent him balloons when he was ill with cancer in Adelaide, of how thankful and grateful he was for their help. Vasil was one of life's characters. He frequented the CSIRO Entomology Laboratory at Canberra in the early 1980's where he interacted with scientists with a liking for both his enthusiasm for science and gastronomy. Vasil spent some time working in India and often reminisced with fellow scientific travellers, who had also worked in India, on the joys and influence they experienced whilst there, frequently mentioning his beloved tree *Ficus bengalensis*.

In the last few years Vasil's physical health declined and this curtailed his overseas travels. In March 2012 I chauffeured him to his annual visit to Cement Creek in the Dandenong Ranges to collect specimens of his favourite moss *Dawsonia* for his researches. Unfortunately he slipped and fell whilst collecting and sustained a fractured leg and we both knew this was to be our last expedition to collect moss specimens together. He was subsequently hospitalized in Adelaide but continued to suffer from other health problems.

He came to Melbourne at the end of May en route to China and insisted on dining with me and my wife at a gourmet French restaurant and sharing some of the courses the day before he departed for China; a fitting last memory!

Vasil never married and he is survived by his sister Nitsa and her family in Israel. His death is a loss to the scientific community, his friends and family.



ACKNOWLEDGEMENTS

I thank Esther and Professor Bill Breed, Professor Emeritus Brian Gunning, Professor Shelley Bergin, Professor Guy Cox, Professor Graham Swain, Dr Barry Filshie, Dr Colin Beaton, Dr Garth Everson, Dr John Drennan and Dr Peter Dart for their assistance in kindly providing me with some background information and useful comments from their association with Vasillios which have been incorporated into this obituary.

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CXS MANAGEMENT & GOVERNANCE

CXS is a collaborative research program between the University of Melbourne, La Trobe University, Monash University, Swinburne University of Technology, Griffith University and CSIRO. It is funded under the Australian Research Council (ARC) Centre of Excellence program.

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

DR HARRY QUINEY
Assistant Director of Research

MS TANIA SMITH
Chief Operating Officer

EXECUTIVE COMMITTEE

During 2012, the administration of CXS was overseen by the Executive Committee, which comprises:

MS ROSSLYN BALL
Executive Officer to Committee

ASSOCIATE PROFESSOR DAVID KIELPINSKI
Attosecond Science Group Leader

PROFESSOR KEITH NUGENT
Research Director

DR HARRY QUINEY
Theory and Modelling Group Leader

ASSOCIATE PROFESSOR MIKE RYAN
Biological Sciences Group Leader

ASSOCIATE PROFESSOR ROBERT SCHOLTEN
Ultracold Plasma Source Group Leader

MS TANIA SMITH
CXs Chief Operating Officer

ASSOCIATE PROFESSOR TREVOR SMITH
Short Wavelength Laser Source Group Member

DR VICTOR STRELTSOV
Structure Determination Methods Group Leader

PROFESSOR LEANN TILLEY
Deputy Research Director

PROFESSOR LAP VAN DAO
Short Wavelength Laser Source Group Leader

DR GRANT VAN RIESSEN
Experimental Methods Group Leader

ADVISORY BOARD

The CXS Advisory Board met in December 2012 at the University of Melbourne CXS office. The meeting focussed on the recommendations of the CXS Scientific Advisory Board, which was tabled for discussion and focused on the proposed bid for the next round of Centres of Excellence beginning in 2014.

CXS would like to thank George Collins and Garth Moorehead for their contribution to this years meeting.

The Advisory Board is comprised as follows:

MR DAVID KRENUS (CHAIR)

Chief Executive Officer Cyclotek

PROFESSOR JAMES MCCLUSKEY

Deputy Vice Chancellor (Research)
The University of Melbourne, or nominee

DR CAL DRUMMOND

Chief of CSIRO Materials Science and Engineering

PROFESSOR GEORGE COLLINS

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

PROFESSOR JOHN HELLIWELL

Professor of Structural Chemistry
University of Manchester

PROFESSOR TIM BROWN

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DR STEPHEN LANE

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

PROFESSOR EDWINA CORNISH

Deputy Vice Chancellor (Research)
Monash University, or nominee

PROFESSOR BONNIE WALLACE

Professor of Crystallography
Birkbeck College

BRUCE WHAN

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

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University of Manchester

DR STEPHEN LANE

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

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CXS Director of Research
University of Melbourne

PROFESSOR LEANN TILLEY

CXS Deputy Director of Research
LaTrobe University

PROFESSOR BONNIE WALLACE

Professor of Crystallography
Birkbeck College

PROFESSIONAL STAFF

The Centre's Professional Staff provide valuable support to research and academic teams. The professional team includes:

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PA to Director & Administrator,
University of Melbourne

KATHY PALMER

Finance and Administrative Officer,
University of Melbourne

NICOLE ANDERSON

Administration Assistant, University of
Melbourne

FABIENNE PERANI

PA to Deputy Director & Administrator,
La Trobe University

TATIANA TCHERNOVA

Administrator, Swinburne University

RESEARCH TEAMS

CXS researchers are second-to-none and their work is held in high esteem around the world. Individual team members have received global recognition and collaboratively, the Centre's groundbreaking work is widely published. Each team is comprised as follows:

ATTOSECOND SCIENCE PROGRAM

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Research Fellow, Griffith University

MALCOLM KELSON

Technical Officer, Griffith University

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Program Leader, Griffith University

DANE LABAN

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Research Fellow, The University of Melbourne

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DR JOSE VARGHESE
Group Leader, CSIRO, Parkville

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DENE MURPHY
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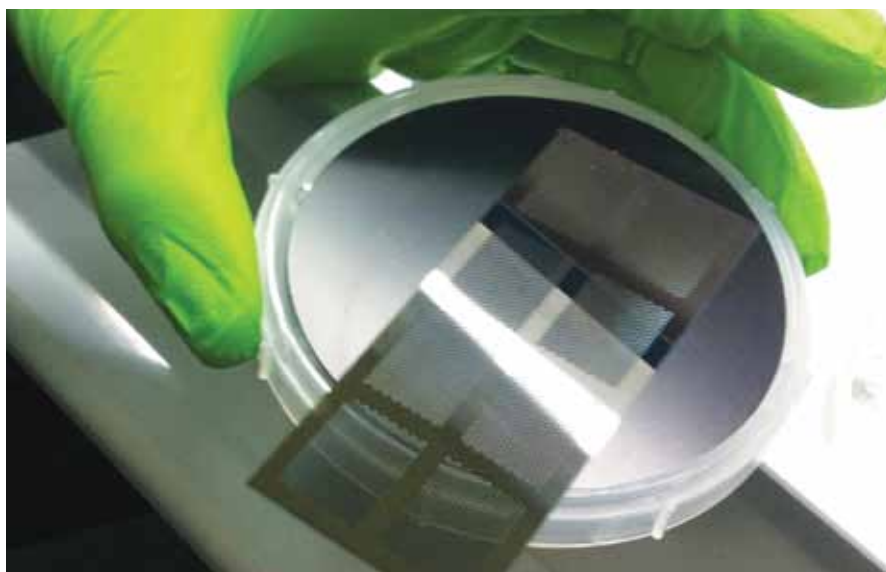
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RORY SPEIRS
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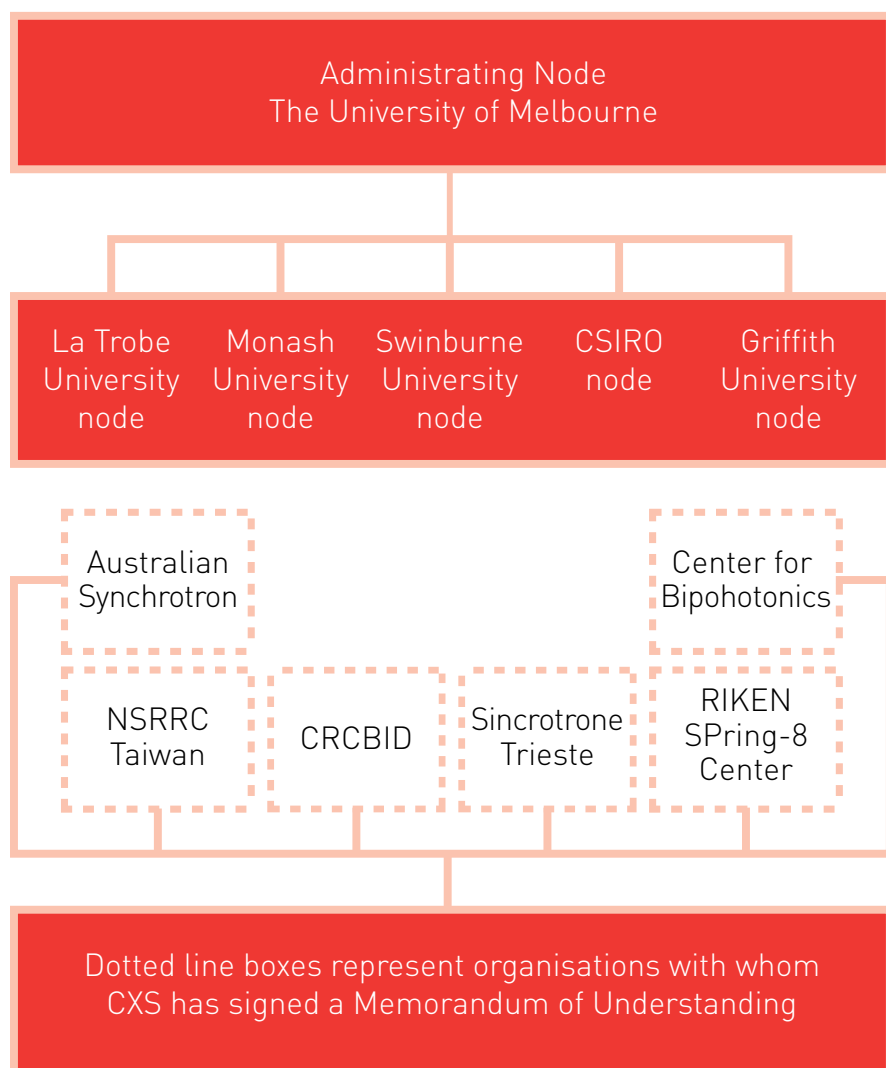
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DANIEL THOMPSON
PhD Student, The University of Melbourne

JOSHUA TORRANCE
MSc Student, The University of Melbourne



ORGANISATIONAL CHART AS OF JUNE 2012



PRESENTATIONS, CONFERENCES & LABORATORY VISITS

DR BRIAN ABBEY

- Attended – Sixth Coherence Workshop, Japan, June 2012
- Invited Speaker – “X-ray nano tomography”, The International Conference on X-ray microscopy 2012, China, August 2012
- Attended – CXS II follow up meeting, Australia, September 2012
- Attended – CXS II Integration Meeting, Australia, October 2012

DR BO CHEN

- Attended – Sixth Coherence Workshop, Japan, June 2012
- Speaker – “X-ray Diffraction Imaging: the limits of partial coherence”, International Conference on X-ray Microscopy 2012, China, August 2012

MEGAN DEARNLEY

- Speaker – “Electron microscopy in a 3D World”, Electron Tomography Workshop, Australia, October 2012.

KHUONG BA DINH

- Attended – Ultrafast Phenomena, Lausanne, IUPAC Conference on Photochemistry, Portugal, August 2012

DR RUBEN DILANIAN

- Attended – CXS Planning Meeting, Australia, May 2012
- Invited Talk – “Electronic phase transition in fullerene crystals induced by the nanofocused femtosecond X-ray laser pulses”, 5th International Workshop on FEL Science, Korea, November 2012

MATTHEW DIXON

- Invited Speaker – Material of Life Symposium, Australia, August 2012

DR MICHAEL JONES

- Attended – “Coherent diffractive imaging of the malaria parasite *P. falciparum*”, Italo-Australian workshop on Synchrotron Radiation X-ray Imaging for Life Sciences and cultural Heritage, Australia, May 2012
- Attended – Bio21 Electron Tomography “Hands-On” Workshop, Bio21 Institute, Australia, October 2012

PROFESSOR DAVE KIELPINSKI

- Poster Presentation – “Benchmarking strong-field physics with atomic hydrogen”, American Physical Society DAMOP, USA, June 2012
- Attended – The Ultrafast Phenomena Conference, Switzerland, July 2012
- Poster Presentation – Mo-214, “Precision attosecond physics with atomic hydrogen”, The International Conference on Atomic Physics, France, July 2012

DANE LABAN

- Attended – The Ultrafast Phenomena Conference, Switzerland, July 2012
- Attended – Frontiers in Optics Workshop, USA, October 2012

MAC LUU

- Speaker – “Multi-wavelength elemental contrast absorption imaging”, Italo-Australian Workshop on Synchrotron Radiation X-ray Imaging for Life Sciences and Cultural Heritage, Australia, May 2012

DR ANDREW MARTIN

- Attended – Conference 2012, Japan, June 2012

PAUL MCMILLIAN

- Invited Speaker – “A cellular nano-imaging facility: 3D Structured Illumination Microscopy.” RAPD Symposium, Bio21, Australia, March 2012

DR PAUL MCMILLAN

- Speaker – Seattle Biomedical Research Institute, USA, August 2012

VED MOOGA

- Poster Presentation – International Keystone Symposium on Mitochondrial Dynamics and Function, Canada, March 2012

PROFESSOR KEITH NUGENT

- Attended – Premier’s Award for Health and Medical Research, Australia, June 2012
- Attended – Australian Academy of Science – New Fellows’ and Medallists Symposium, Australia, June 2012
- Attended – Sixth Coherence Workshop, Japan, June 2012
- Attended – 11th International Conference on Synchrotron Radiation Instrumentation, France, June 2012
- Judge – 2012 Victoria Prize and Fellowship, Australia, July 2012
- Attended – CXS IP Show and Tell Forum, Australia, July 2012
- Attended – Australian Research Council Centre Director’s Forum, Australia, August 2012

- Attended – Australian Nuclear Science and Technology Organisation National Science Week: Fact of Fiction, Australia, August 2012
- Attended – CXS II Follow Up Meeting, Australia, September 2012
- Attended – Celebration of SIEF's Promotion of Science (Science an Industry Endowment Fund, Australia, September 2012
- Attended – *"Innovation Series – Enhancing Innovation through Open Innovation"*, Australia, September 2012
- Invited Speaker – Colloquium to the School of Physics, Monash University, Australia, September 2012
- Invited Guest – Collaboration with Adrian Mancuso, European XFEL GmbH – SPB Instrument, University of Hamburg, Germany, October 2012
- Invited Opponent – Attended as faculty opponent at the defence of a thesis, Uppsala, Switzerland, October 2012
- Attended – CXS II Integration Meeting, Australia, October 2012

ASSOCIATE PROFESSOR ANDREW PEELE

- Attended – Hon Andrew McIntosh, Minister for Crime Prevention Forum, Australia, February 2012
- Attended – Briefing to the Federal Member for Chisholm, Australia, February 2012
- Attended – Australasian Industrial Research Group National Meeting, Australia, February 2012
- Opening Address – Australian Synchrotron IMBL Specialist Workshop, Australia, March 2012
- Speaker – CSIRO MMM Postdoc Symposium, Australia, March 2012
- Invited Speaker – *"Synchrotron to the Laboratory: Better methods for understanding microstructure"*, CSIRO Computational and Simulation Sciences Transformational Capability Platform and eResearch Microstructures Workshop, Australia, March 2012
- Invited Speaker – *"Imagining at the AS"*, Monash Business Breakfast, Australia, May 2012
- Attended – Composites Australia Workshop, Australia, June 2012
- Attended – IR Beamline Workshop, Australia, June 2012
- Opened – The Infra-red Beamline Data Analysis Workshop, Australia, June 2012
- Attended – Conferring of an honorary degree for Professor Rolf-Dieter Heur, University of Melbourne, Australia, July 2012
- Opened – New User Symposium, Australian Synchrotron, Australia, July 2012
- Attended – CSIRO National Characterisation Council Workshop, Australia, July 2012
- Attended – DIISRTE National Research Investment Plan Forum, Australia, July 2012
- Poster Presentation – International Conference on X-ray Microscopy, China, August 2012
- Attended – CXS II follow up meeting, Australia, September 2012
- Attended – CXS II Integration Meeting, Australia, October 2012

ISAAC PETERSON

- Speaker – *"Bragg Ptychography of GaP Nanowires"*, Advanced Photon source, Chicago, USA, April 2012

DR COREY PUTKUNZ

- Invited Speaker – *"Towards Atomic Resolution Ptychographic Electron Diffractive Imaging"*, Coherence 2012, Japan, July 2012
- Poster Presentation – *"Femtosecond XFEL Induced Transient Electronic Phase Change Observed in Fullerene C60"*, 2012 LCLS Users meeting at SLAC, California, USA, October 2012

ASSOCIATE PROFESSOR HARRY QUINEY

- Attended – Biomolecular Imaging using Free-Electron Lasers, Seminar at European XFEL, February 2012
- Attended – Biomolecular Imaging Using Free-Electron Lasers; a bright future for structural biology, Centre for Neural Engineering, Australia, April 2012
- Attended – Max Planck Symposium: The future of structural biology, Hamburg, Germany, May 2012
- Attended – CXS Planning Meeting, Australia, May 2012
- Attended – CXS Writing Workshop, Australia, June 2012
- Invited Speaker – European XFEL Seeding Workshop, Hamburg, Germany, July 2012



PROFESSOR MIKE RYAN

- Session Chair – Lorne Protein Conference on Protein Structure and Function, Australia, February 2012
- Invited Plenary Speaker and Session Chair – International Keystone Symposium on Mitochondrial Dynamics and Function, Canada, March 2012
- Speaker – Institute for Biochemistry and Molecular Biology, Germany, June 2012
- Speaker – Department of Cell and Developmental Biology, University College London, United Kingdom, June 2012
- Invited Seminar Speaker – The Baker Heart and Diabetes Institute, Australia, July 2012
- Co-Chair – Dynamite 2012, the 4th International Symposium of Mitochondria, Japan, August 2012
- Invited Speaker – European Bioenergetics Conference, Germany, September 2012
- Invited Speaker – “*Tubulointerstitial Disease in Diabetic Nephropathy*”, ISN Forefronts Symposium, Australia, October 2012

ASSOCIATE PROFESSOR ROBERT SANG

- Speaker – Conference on Lasers and Electro-optics, “*A High Order Harmonic Radiation Zeptosecond Phase Interferometer*”, USA, May 2012

ASSOCIATE PROFESSOR MARTIN SCANLON

- Attended – FBLD2012, San Francisco, USA, September 2012

ASSOCIATE PROFESSOR ROB SCHOLTEN

- Invited Speaker – “*Diffraction imaging with arbitrarily shaped high-coherence electron bunches from cold atoms*”, Banff Meeting on Structural Dynamics, Canada, February 2012
- Speaker – Quantum Measurement in Living Cells, and High-Coherence Electron Bunches from Cold Atom, CNRS, France, March 2012
- Invited Speaker – “*Arbitrarily shaped ultrafast high coherence electron bunches from cold atoms for coherent diffractive imaging at the nanoscale*”, 24th Spring Symposium of the Plasma Physics Division of the Royal Dutch Physical Society, The Netherlands, March 2012
- Invited Speaker – “*Arbitrarily Shaped High-Coherence Electron and on Bunches from Laser-Cooled Atoms*”, The 56th International Conference on Electron, Ion and Photon Beam Technology and Nanofabrication (EIPBN), Hawaii, USA, June 2012

TANIA SMITH

- Master of Ceremonies – CXS IP Show and Tell Forum, Melbourne, July 2012
- Invited Chair and Set the Agenda – Australian Research Council Centre of Excellence Director’s Forum, Chief Operating Officer and Manager’s Workshop, Australia, August 2012
- Attended – The Australasian Research Management Society Conference, Australia, September 2012

ASSOCIATE PROFESSOR TREVOR SMITH

- Invited Speaker – “*Time-Resolved Microspectroscopy of Conjugated Polymer Films*”, 2nd Molecular Materials Meeting (M3), Singapore, January 2012
- Attended – Focus on Microscopy, “*Structured Illumination Microscopy of Living Cells*”, Singapore, April 2012
- Invited Speaker – at Workshop on Optical Microscopy in Life Sciences, Britton Chance Center for Biomedical Photonics, Huazhong University of Science and Technology, China, August 2012
- Attended – Ultrafast Phenomena, France, August 2012
- Attended – IUPAC Conference on Photochemistry, Portugal, August 2012
- Invited Guest – and Annual Meeting on Photochemistry 2012, Tokyo Institute of Technology, Japan, September 2012
- Invited Guest – “*Recent Development of Nanomaterials: Structures, Dynamics and Applications*”, Taiwan, October 2012

PROFESSOR LEANN TILLEY

- Attended – Molecular Approaches to Malaria Conference, Australia, February 2012
- Speaker – London School of Hygiene & Tropical Medicine, United Kingdom, March 2012
- Speaker – Liverpool School of Tropical Medicine, United Kingdom, March 2012
- Speaker – Department of Microbiology, Monash University, Australia, June 2012
- Speaker – Adelaide Protein Group, Australia, June 2012



- Speaker – Super-Resolution Microscopy Facility Opening, Australia, August 2012
- Session Chair – Women in Medical Research Colloquium, Australia, August 2012
- Session Chair – Material of Life Symposium, Australia, August 2012
- Speaker – School of Botany, The University of Melbourne, Australia, September 2012
- Attended – The Australian Synchrotron Career Development Forum, Australia, September 2012
- Attended – Mahidol Oxford Tropical Medicine Research Unit, Thailand, October 2012
- Attended – *X-rays for biological microscopy*, 5th International Workshop on FEL Science, Korea, November 2012
- Attended – CXS II follow up meeting, Australia, September 2012
- Attended – CXS II Integration Meeting, Australia, October 2012

PROFESSOR LAP VAN DAO

- Attended – High Intensity Lasers and High Field Phenomena, *“Generation of Coherent Radiation in the Water Window”*, Germany, March 2012
- Invited Speaker – *“Coherent X-ray diffraction with high order harmonic radiation”*, Time resolved X-ray Imaging, Euro LaserLab Foresight Workshop, Greece, May 2012
- Presented – *“Generation and application of coherent radiation in the water window”*, 13th International Conference on X-ray Lasers, France, June 2012
- Invited Speaker – *“The Workshop on Super Intense Laser-Atom Physics (SILAP 2012)”*, China, September 2012

DR GRANT VAN RIESSEN

- Invited Talk – *“Progress and challenges in coherent diffractive imaging with soft*

AWARDS & HONOURS

It has been another successful year with a number of CXS members receiving awards and honours. We extend our congratulations to each of them for their efforts in achieving such significant recognition.

CXS is the first Australian team to be awarded access to the Linac Coherent Light Source X-ray free-electron Laser at SLAC National Accelerator Laboratory in the United States of America. This world-class research facility, launched in 2009, has attracted thousands of scientist from all over the world each year. The demand to use the facility is extremely high. The CXS proposal was rated in the top ten percent of the 114 international proposals. The selection panel said the CXS proposal of investigation structure determination of biomolecules with X-ray XFEL is considered to be very promising.

Professor Keith Nugent was appointed the Deputy Vice-Chancellor and Vice-President Research at La Trobe University. Professor Nugent will lead the reinvigoration of La Trobe's research capacity to realise the

university's new 'World Ready' Strategic Plan. This aims to return La Trobe University to the ranks of the top 300 global universities by 2017.

Dr Victor Streltsov was awarded the Japanese Society Fellowship for the Promotion of Science 2012. Victor was selected based on nominations made by the Social Science Research Council Japanese Advisory Board. The award has provided Victor the opportunity to conduct research in Japan under the leadership of a host researcher to advance their own research, while closely collaborating with young Japanese researchers, and contributing to the Japanese research community.

Dr Eroia Barone-Nugent was a finalist in the Science Teaching Eureka Prize awarded by the Australian Museum. Dr Barone-Nugent was recognised for his work with



Melbourne Protein Group Poster Session



SCHOLARSHIPS AND STUDENTSHIPS

the Growing Tall Poppies Program, giving students authentic science experiences with real scientists at CXS. Learning science is contextualised and shows how the field solves complex world problems. The inspiring Growing Tall Poppies Program has increased the number of girls studying physics by 93% at Santa Maria College Northcote.

Professor David Kielpinski and his student Ben Norton won second place in the Canon 'Extreme Imaging' Competition 2012. This competition focuses on imaging of science projects where students make equipment that can produce images beyond the boundaries of creative photography and video. Ben is supervised by Professor David Kielpinski who helped him develop techniques to take some of the highest resolution images of atoms ever made, including the first ever image of the shadow of a single atom. Imaging single atoms is important for understanding physics, the new field of quantum computing and may also have applications for ultra-high resolution imaging of biological cells.

The Melbourne Protein Group 2012 awarded the ASBMB-Vic Branch Poster Prize to Veg Mooga. Veg's poster was chosen from a field of 40 posters. The Melbourne Protein Group provides opportunities for young Victorian researchers interested in topics related to all aspects of protein's function, structure and their role in health and disease. It also provides an opportunity for students to present their research data, network with other students, guest speakers and trade delegation, and to gain experience presenting their research at either the annual Melbourne Protein Group student meeting or biannual postdoc meeting.

We would like to congratulate the following students for their successful applications in 2012:

- Daniel Thompson, CXS Top Up Scholarship and CXS Travel Scholarship, Ultracold Laser Source Program, The University of Melbourne
- Megan Dearnley, CXS Top Up Scholarship, Biological Sciences, Program, The University of Melbourne
- Silvia Teguh, CXS Travel Scholarship, Biological Sciences Program, The University of Melbourne
- Boris Reljic, CXS Travel Scholarship, Biological Sciences Program, La Trobe University
- Aidan Jessen, CXS Vacation Scholarship, Attosecond Sciences Program, Griffith University

RESEARCH TRAINING & PROFESSIONAL EDUCATION

The Centre met all of its recruitment and professional education targets for 2012, and met all expectations in the areas of *Postgraduate Recruitment and Presentations to Schools and/or Teaching Communities*.

CXS SPONSORED EVENTS

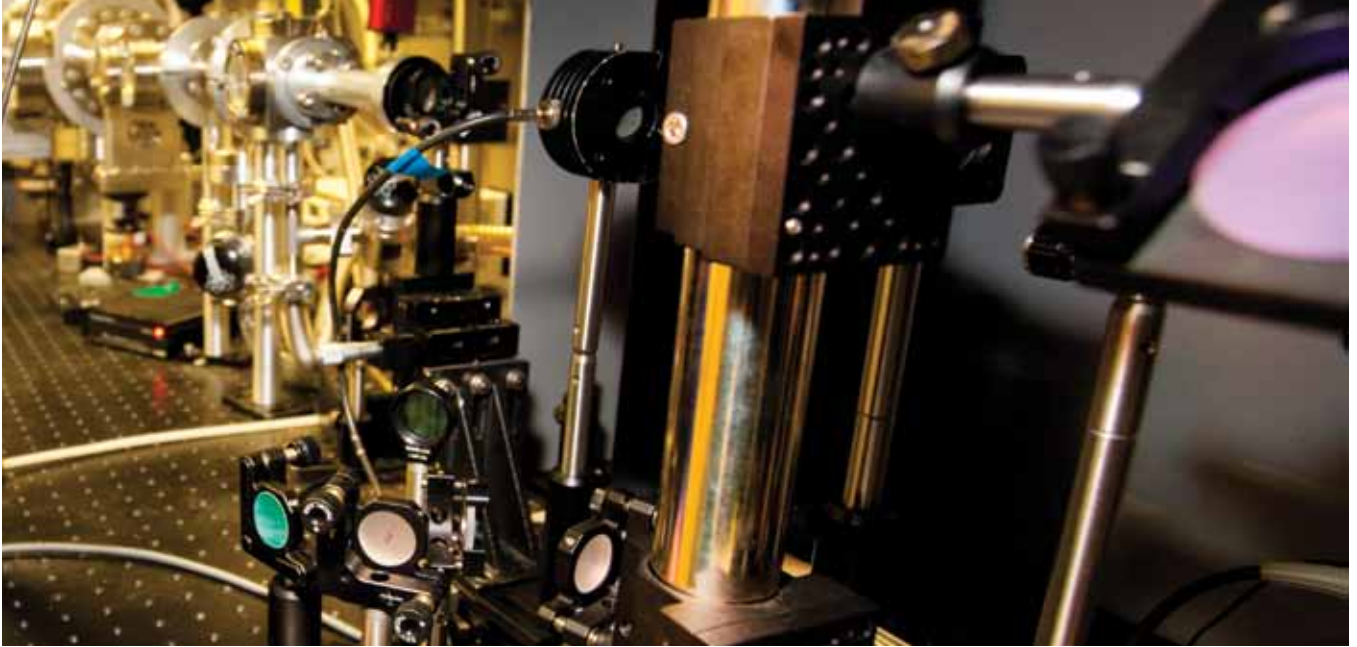
CXS sponsored the following events in 2012:

- Italo-Australian Workshop, ELETTRA, Italy, Session Sponsorship
- Melbourne Protein Group Post Doc Symposium 2012, Oral Award Prize
- Melbourne Protein Group Post Doc Symposium 2012, Poster Award Prize
- 20th AIP Congress 2012, Session Sponsorship
- IONS-KOALA Conference 2012, Gold Sponsorship
- Coldbeams Workshop 2012, France, Sponsorship and attendance of Associate Professor Scholten
- 38th Lorne Conference on Protein Structure and Functions 2012, Session Sponsorship
- Women In Science – Passionate Minds, General Sponsorship
- Materials of Life Symposium 2012, Session Sponsorship
- Bragg Symposium and Dinner 2012, General Sponsorship

WORKSHOPS

CXS conducted the following interdisciplinary workshops in 2012:

- LCLS Experiment Workshop, La Trobe University, 13 April 2012
- CXS 2 Retreat, Daylesford, Victoria, 28-30 May 2012
- CXS IP and Commercialisations Information Session, The University of Melbourne, 6 June 2012
- CXS Writer's Workshop, Stonelea, Acheron, Victoria, 12-13 June 2012
- CXS IP Show and Tell, The University of Melbourne, 11 July 2012
- CXS 2 Retreat – Stage II Planning Workshop, Mantra Southbank, Victoria, 3 September 2012
- N.A.D.I.A Workshop, The University of Melbourne, 21 September and 28 September 2012
- CXS 2 Integration Planning Workshop, The University of Melbourne, 16 October 2012
- CXS Writer's Workshop, La Trobe University, 1 November 2012
- Ultrafast Non-linear Microscopy Workshop, Swinburne University, 7 December 2012



CELLULAR NANO-IMAGING CONSORTIUM

The Cellular Nano-Imaging Consortium (CNIC) is an affiliation of scientists with interests in Super-Resolution Optical Microscopy managed under the auspice of CXS. Its inception is the direct result of a joint initiative undertaken by CXS Director Professor Keith Nugent, Deputy Director Leann Tilley and CXS member Associate Professor Trevor Smith, School of Chemistry, University of Melbourne, to bring together institutions and research leaders with cross-disciplinary expertise and an interest in using and/or developing nano-imaging optical methods.

CNIC provides online access to information about conventional and super-resolution optical imaging techniques and what resources are currently (and potentially) available to interested parties. Through CNIC, workshops and conference sessions will be organised to inform Australian scientists about new high-resolution imaging modalities. CNIC aims to co-ordinate efforts to generate a super-resolution imaging capability in Victoria, providing information and access to the new techniques.

CNIC is working to ensure that all Victorian scientists have access to the Super-Resolution Microscopy format they need to be competitive as international research leaders.

The CNIC website can be visited at www.coecxs.org/cnic



THE MATERIALS OF LIFE SYMPOSIUM

THE CXS-SPONSORED MATERIALS OF LIFE SYMPOSIUM WAS HELD AT THE UNIVERSITY OF MELBOURNE ON 29TH JUNE, 2012.



Professor Elizabeth Blackburn delivering her Plenary Lecture



Professor John Sedat and Leann Tilley at the Materials of Life Symposium

This cross-disciplinary workshop brought together physical and biological scientists around two special guest speakers, Professor Elizabeth Blackburn and Professor John Sedat. The Symposium attracted 309 registrants, from 36 institutions, including many interstate visitors.

Professor Elizabeth Blackburn was awarded the 2009 Nobel Prize in Physiology or Medicine for co-discovering telomerase, an enzyme that replenishes structures called telomeres at the ends of chromosomes. Elizabeth presented recent work that provides a molecular explanation for observation that health risks such as chronic life stress and smoking are linked to shorter telomeres and dampened telomerase activity. Similarly sub-optimal telomere maintenance is associated with an increased risk of a range of disease states such as coronary artery disease, depression, diabetes and immune system failure.

Professor John Sedat was a leader of the consortium that developed the Optical Microscope eXperimental (OMX), a 3D-Structured Illumination Microscope (3D-SIM). The OMX can image cellular components with an 8-fold better volume resolution than conventional microscopes. John spoke about his work developing pulsed light sources and filtering algorithms that permit the collection of useful imaging data using up to one

thousand times fewer photons. He also described the use of adaptive optics to enable aberration-corrected imaging of thicker tissue samples.

Professor Tilley and other CXS colleagues were successful in obtaining funds from an

ARC LIEF grant and partner institutions to purchase and commission an OMX-BLAZE 3D-SIM. The 3D-SIM has been installed as part of Melbourne University's Advanced Microscopy Facility at the Bio21 Institute. Professor Sedat officially opened

the Super-Resolution Facility on 2nd July, 2012.

The Symposium also featured talks from early to mid career researchers including CXS member, Dr Matt Dixon.

The Symposium attracted 309 registrants, from 36 institutions, including many interstate visitors.

SCIENTIFIC LINKAGES

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



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



CRC for Biomedical Imaging Development



The Centre for Biophotonics Science and Technology

COMMERCIAL- ISATION

The Ultracold Plasma Source Program developed the MOGLab's range of external cavity diode laser (ECDL) controllers.

The logo for MOGLabs, featuring the word "moglabs" in a stylized, lowercase, blue font. The letters are connected and have a modern, rounded appearance.

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.

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

OUTREACH

THE AUSTRALIAN INSTITUTE OF PHYSICS YOUTH LECTURE TOUR 2012



This year Associate Professor Robert Sang had the honour of delivering the 2012 Youth Lecture Tour for the Queensland Branch of the Australian Institute of Physics.

The motivation behind the tour is to raise the profile of physics with high school students by exposing them to physics research, and the real-world outcomes produced. Ultimately, it is hoped that these lectures may inspire high-school students to undertake science-based programs in their tertiary studies. The tour also gives students in remote areas access to interesting research that they would not have the opportunity to engage with unlike their metropolitan counterparts.

This year Robert spoke on the research carried out in the Attosecond Science node of CXS. He presented concepts of the exciting research being conducted in the discipline of attosecond, high-field atomic physics. He reviewed laser technology

and how one can create high-intensity and ultra-short light pulses and investigate their interactions with matter. Such interaction processes are highly non-linear and occur on time scales of attoseconds (a billionth of a billionth of a second). This is the timescale in which it takes an electron to orbit the nucleus of an atom. It is possible to interact light from these lasers with atoms and molecules and create new light sources which can be used in turn to dynamically probe matter on the attosecond (10^{-18} s) time scale. One can view such a laser system as a time machine that can effectively 'freeze time' and investigate, as well as control, these very fast atomic and molecular processes. Robert also presented the ground-breaking research being made at the *Australian Attosecond Science Facility* at Griffith University, Nathan Campus in Brisbane and the connection of this research with the goals of CXS.

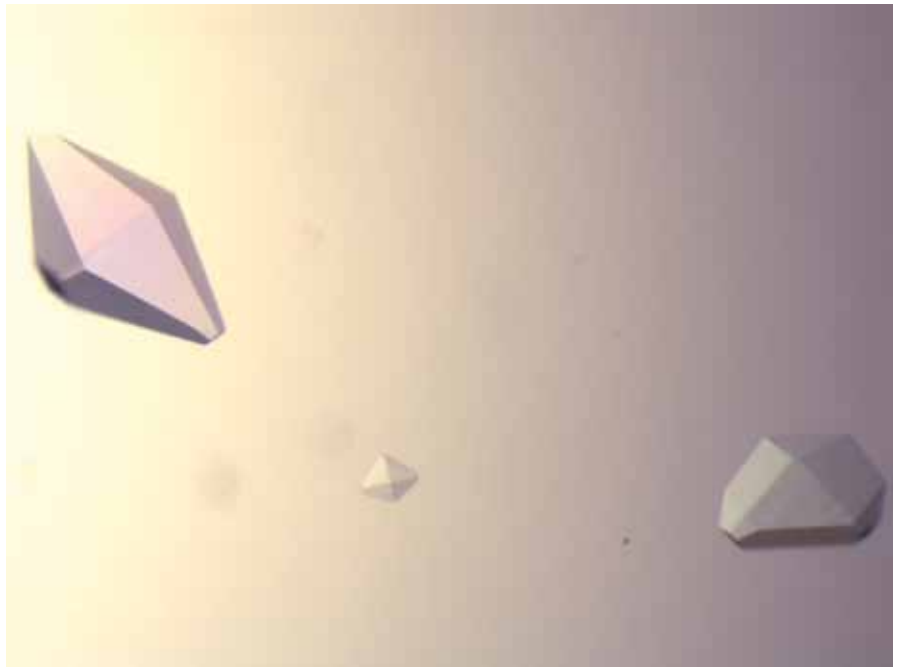
The lectures were delivered around the state of Queensland and in two weeks during August Robert presented nine lectures to over 1000 students. This year the lectures were delivered in Brisbane, Hervey Bay, Toowoomba, Rockhampton, Mackay, Cairns, Townsville, Mt Isa and the Sunshine Coast and required ten flights in ten days travelling approximately 12,000km. It was fascinating and encouraging to see the enthusiasm of the students in the lectures and the great depth of questions that they asked. Robert was also amazed to see relatively large classes of students studying physics in remote towns like Mt Isa and he believes this is a testament to the wonderful skills of their teachers encouraging them to take up senior sciences. We would like to thank Mark Young and Chris Langton from the Queensland Branch of the AIP for organizing the logistics of the tour and the Australian Institute of Physics, Griffith University and CXS for sponsorship of the tour.



GROWING TALL POPPIES CRYSTALLISATION WORKSHOP

A Growing Tall Poppy crystallisation workshop was conducted at CSIRO laboratories in Parkville, Victoria. The students were engaged in growing Lysozyme crystals and introduced to the C3 crystallisation facility, which houses a number of crystallisation robots. The students had the opportunity to manually set up two different crystallisation experiments, which allowed them to see the challenges involved in crystallising proteins and then experience the crystallisation robots in action. At the end of the day the students could take their crystals back to school and proceed with the next step of data collection at the synchrotron.

This was a fun experience for all. The students were pleasant to teach and very enthusiastic to learn as they were intrigued with the science in which they were participating.



A Lysozyme crystal grown by the Growing Tall Poppies students





SANTA MARIA COLLEGE REFLECTS ON THE GROWING TALL POPPIES

DEBORAH BARKER
PRINCIPAL, SANTA MARIA COLLEGE,
NORTHCOTE

At Santa Maria College we promote the ethos of 'dare to do as much as you are able'. We are a Good Samaritan school devoted to education that nurtures the search for truth and a love of learning. We seek to form leaders of the future who are connected with what and why they learn. The Growing Tall Poppies in science program reflects the integral component of our learning and teaching ethos which is to strive for excellence in understanding and rise above the ordinary to become extraordinary. Students in years 10 and 11 go on a journey of not only discovering the interconnected aspects of science through this immersion program but a journey to discover their own capabilities. Our students have increased their literacy of science in the real world, and we have derived an increased retention of students in Physics and an elevated attention to how important studying science is to being a thinking and purposeful member of society. These students create their own networks of professionals that support their transition from school to further study or work and they form a strong sense of the importance of being a life-long learner and connecting what they learn with their reflective inner voice that makes them rise to a higher level of understanding. The philosophy of the Growing Tall Poppies nurtures our students to emerge as the Tall Poppies of the future who will lead themselves and others to greater states of awareness.





BRYAN O'REILLY TEACHER, SANTA MARIA COLLEGE, NORTHCOTE

I have been involved with the Growing Tall poppies authentic learning environment for five years. Year 10 is an important year level to get students thinking about how sciences can provide exciting career paths, which is especially difficult when we get to the physics topics. Even though students do practicals at school and have undoubtedly gone on many excursions they have not been with scientists in the work place and seen how it's done or what the scientists are like.

Young people often have the image of scientists being old, bearded men and so cannot see themselves in their place. This is especially true for girls. We all know what it's really like but imparting that to students is not straightforward in the confines of a classroom; not even with all the best equipment – and our students get to use some of the most amazing equipment! So being able to place students to work with scientists on real projects develops their inquiry skills, curiosity, and encourages them to see with their own eyes that scientists are young and of both genders is inspiring for our students. It opens them up to the possibilities of what career paths are available and that the diverse range of jobs are interesting; contribute to making the world a better place and pay quite well.

The structured experience students get in this program gives them the contextual learning that is impossible to provide at school. It demonstrates the relativities of different science disciplines to each other and connects the importance of scientists' work to real questions that matter. The program immerses students in a real thinking-inquiry environment where their participation is real, fun and memorable. The content becomes secondary to the experience and so becomes authentic learning to explain what they really need to address on the day rather than something artificial to regurgitate in a test.

How wonderful to be part of such a novel way of teaching science. It invigorates my students and it has reinvigorated my teaching by linking the classroom with a wider range of real science possibilities for the girls.





VERNON CURTIS TEACHER, SANTA MARIA COLLEGE, NORTHCOTE



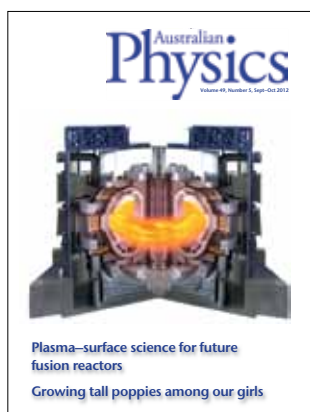
I have been a Science teacher for four decades and well appreciate the difficulty teachers have encouraging students to pursue a career in Science – especially electing Physics to Year 12.

For some reason, students believe that only those with 'brains' study science. Even though the opening up of possibilities is put to them, it is hard to put 'old heads on young shoulders'. Experiencing science via the Growing Tall Poppies program has had a very positive impact on students' opinions about science especially Physics. The program enables them to experience connectedness and relevance which are vital to their decision making.

It is with pride that I have seen temerity give way to confidence by the end of the immersion process of the Growing Tall Poppies program. Observing the care, attention and commitment that students invest in their work and the wonderful mentor-mentee relationship formed with the enthusiastic scientists that assist them has been a revelation.

Thank you for the opportunity of enriching my own learning through the Growing Tall Poppies program.

MEDIA RELEASES



MEDIA COMMENTARIES

CXS members appearing in the media in 2012 have had a worldwide reach, with the following 26 countries reporting our activities:

Argentina
Australia
Bangladesh
Brazil
Canada
Chile
China
Denmark
France
Hungary
Germany
India
Iran
Italy
Japan
Korea
Mexico
Norway
Romania
Russian Federation
Spain
Taiwan
Ukraine
United Kingdom
United States of America
Vietnam

NEWSPAPER AND MAGAZINE ARTICLES

- National Geographic Daily News, *Extreme Scientific Imaging: Best of 2011 Named*, 22 February 2012
- Cosmos Ultimate Science Guide 2012, *In the Detail*, p 20, March 2012
- Cosmos Magazine, *Where in the Cosmos?*, p 10, March 2012
- Sunday Herald Sun, *Our Marvellous Medical Women*, p 20-21, 8 July 2012
- BioChem Babble, *Melbourne Scientists Solve 130-year-old Mystery*, p 3, July 2012
- MUSSE, *New Super Resolution Microscopy Capability at Bio21 Institute*, 12 August 2012
- Swinburne Venture, *Through the Water Window*, p 18-19, August 2012
- Australian Teacher, *Science Retention: Tall Poppies join forces for future*, p 44, August 2012
- Australian Physics, *Growing Tall Poppies*, p 141-147, September-October 2012
- Northcote Leader, *Putting the fizz in physics*, p 19, 7 November 2012
- EurekAlert!, *Webcams offer a low-cost way to tune lasers for serious science*, 4 December 2012

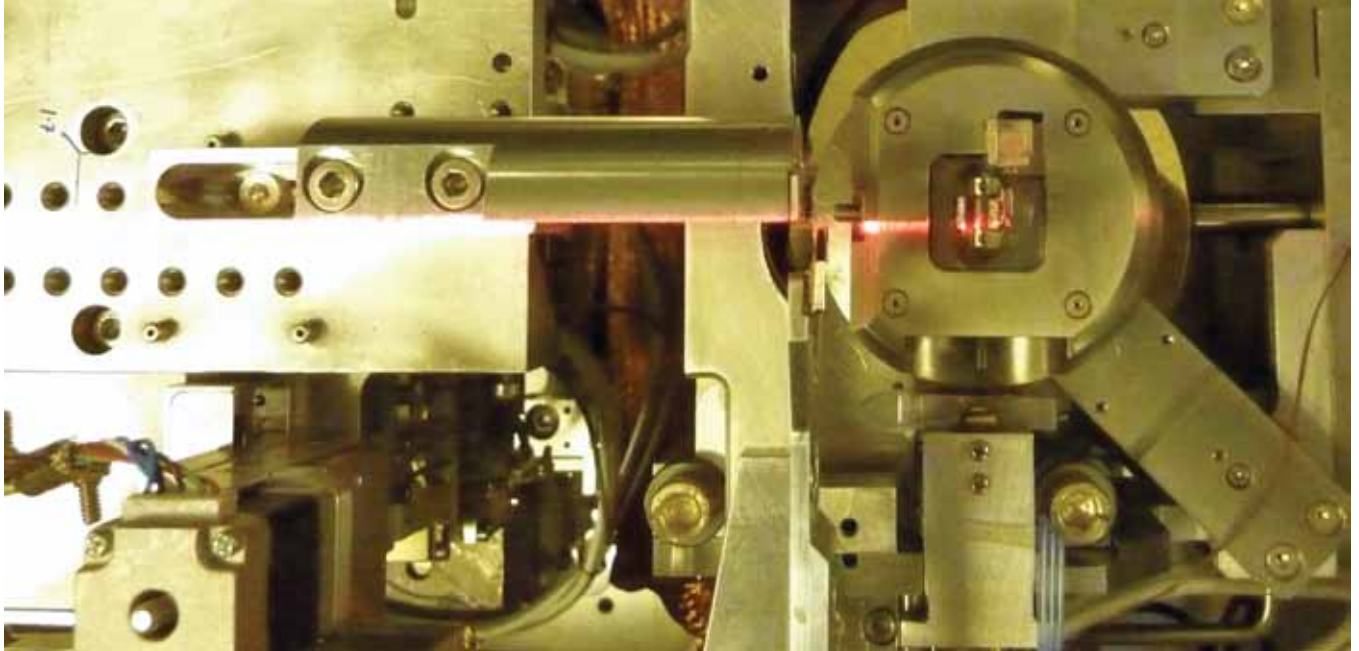
ELECTRONIC MEDIA

1. The Australian, National Affairs, *Lifeline needed as light dims on scientific research*, 13 January 2012 www.theaustralian.com.au/national-affairs/opinion/lifeline-needed-as-light-dims-on-scientific-research/story-e6frgd0x-1226242986847

2. Australian Institute of Physics, *Recognising physics achievements, science in space and diamond computing*, 25 January 2012 www.aip.org.au/news/250
3. Phys.Org, *Study supports role of quantum effects in photosynthesis*, 26 January 2012 phys.org/news/2012-01-role-quantum-effects-photosynthesis.html
4. Port Macquarie News, *Australia Day Honours list*, 26 January 2012 www.portnews.com.au/news/local/news/general/australia-day-honours-list/2433821.aspx
5. Griffith University, *Griffith takes prize in imaging science*, 10 February 2012 www3.griffith.edu.au/03/ertiki/tiki-read_article.php?articleId=35062
6. The Medical News, *Study shows how malaria parasite changes into banana form before sexual reproduction*, 14 February 2012 www.news-medical.net/news/20120214/Study-shows-how-malaria-parasite-changes-into-banana-form-before-sexual-reproduction.aspx
7. Science Alert, *Parasite goes bananas before sex*, 15 February 2012 www.sciencealert.com.au/news/20121402-23115.html
8. First Science, *Malaria parasite goes bananas before sex: New Study*, 15 February 2012 www.firstscience.com/home/news/infectious-and-emerging-diseases/malaria-parasite-goes-bananas-before-sex-new-study_121411.html

9. Science Daily, *Malaria parasite goes bananas before sex*, 15 February 2012
www.sciencedaily.com/releases/2012/02/120214100940.htm
10. Daily India, *Sex makes malaria parasite go bananas*, 15 February 2012
www.dailyindia.com/show/485165.php
11. Hamara Photos, *Sex makes malaria parasite go 'bananas'*, 15 February 2012
hamaraphotos.com/news/general/sex-makes-malaria-parasite-go-bananas.html
12. AndhraNews.net, *Sex makes malaria parasite go 'bananas'*, 15 February 2012
www.andhranews.net/Technology/2012/Sex-makes-malaria-parasite-go-bananas-799.htm
13. MediLexicon, *Malaria Parasite Goes Bananas Before Sex: New Study*, 15 February 2012
www.medilexicon.com/medicalnews.php?newsid=241646
14. Laboratory Equipment, *Malaria Parasite Changes Shape to Breed*, 16 February 2012
www.laboratoryequipment.com/news/2012/02/malaria-parasite-changes-shape-breed?xmlmenuid=51
15. Bright Surf, *Malaria parasite goes bananas before sex: new study*, 16 February 2012
www.brightsurf.com/news/headlines/72964/Malaria_parasite_goes_bananas_before_sex_new_study.html
16. Bio-Medicine, *Extreme imaging wins science praise*, 18 February 2012
www.bio-medicine.org/biology-news-1/Extreme-imaging-wins-science-praise-23752-1/
17. Griffith University, *Single atoms talk to electric circuits at Griffith*, 21 February 2012
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BROADCASTS

- Professor David Kielpinski appeared in an episode of Channel 10 science show SCOPE. The episode was titled Green, (3/3) 9 February 2012

PUBLICATIONS

CXS published 82 papers in peer-reviewed journals in 2012.

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CONFERENCE PROCEEDINGS

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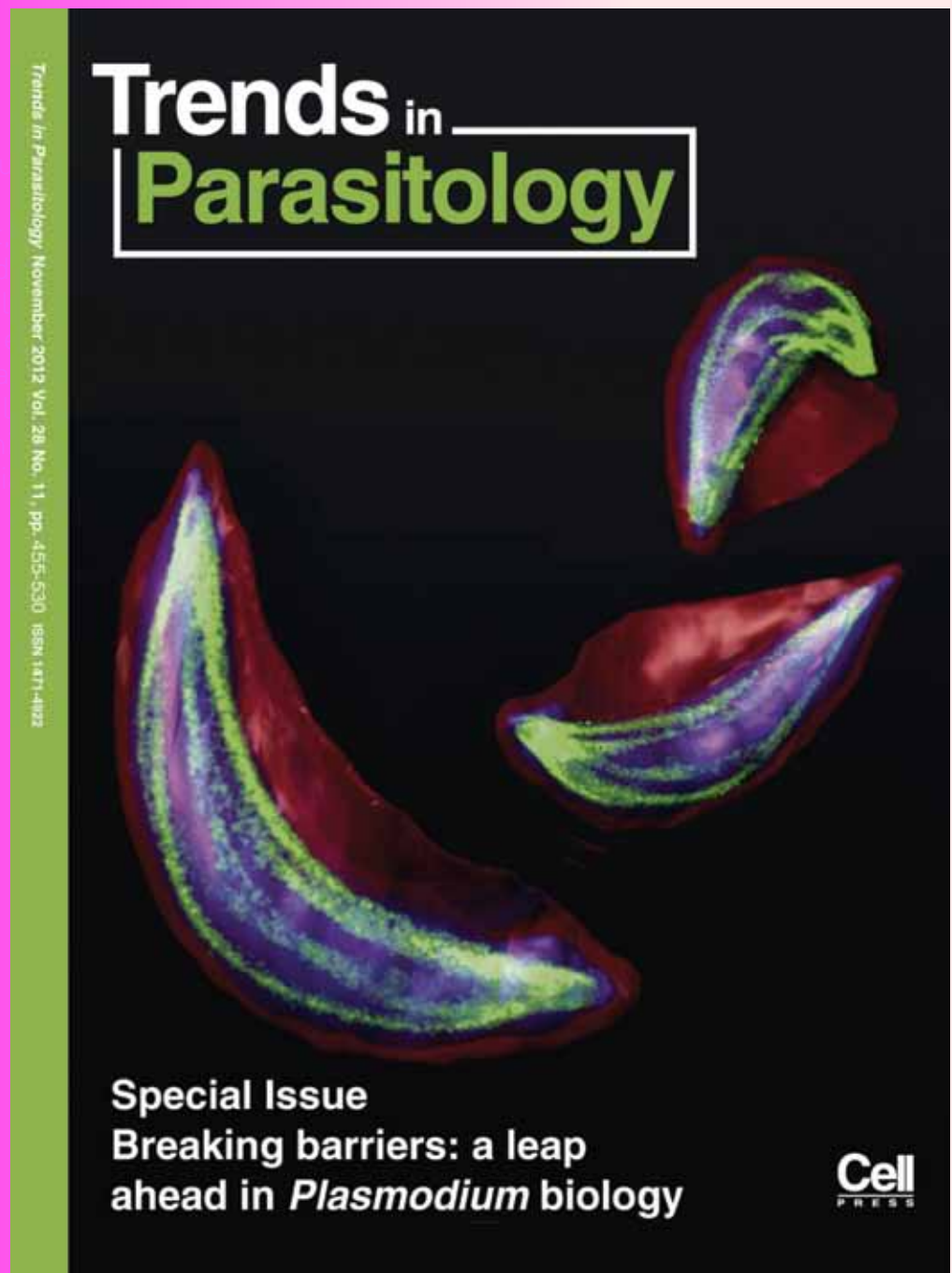
GRANTS



CXS members have attracted \$3,206,993 in additional support in 2012.

ARC	
LIFE – Melbourne and La Trobe rapid integrated X-ray diffraction facility	360,000
LIFE – A cellular nano-imaging facility: Probing cellular complexity	350,000
LIFE – Advanced surface imaging and spectroscopy facility	600,000
DECRA	375,000
NHMRC	
Transforming the diagnosis of mitochondrial disorders using high throughput sequencing, functional prediction and experimental validation	648,675
Mechanisms regulating mitochondrial outer membrane permeabilisation during programmed cell death	296,175
Protein interactions facility	24,323
University of Melbourne	
Major Bids NRIC	15,000
UoM collaborative grant with Lastek	19,500
Major Bids ARC COE	30,000
LTU Faculty of Science, Technology and Engineering Research Grant	
Standard method for mounting non-reproducible biological specimens for correlative imaging	4,800
Probing electronic interactions in dimensionally reduced systems	7,000
Other	
ISAP	11,000
International Synchrotron Access Program Grant	11,300
AINSE Travel Support	220
MRGSS	45,000
US Air Force Office of Scientific Research	389,000
Ian Potter Foundation	20,000

2012 JOURNAL COVERS



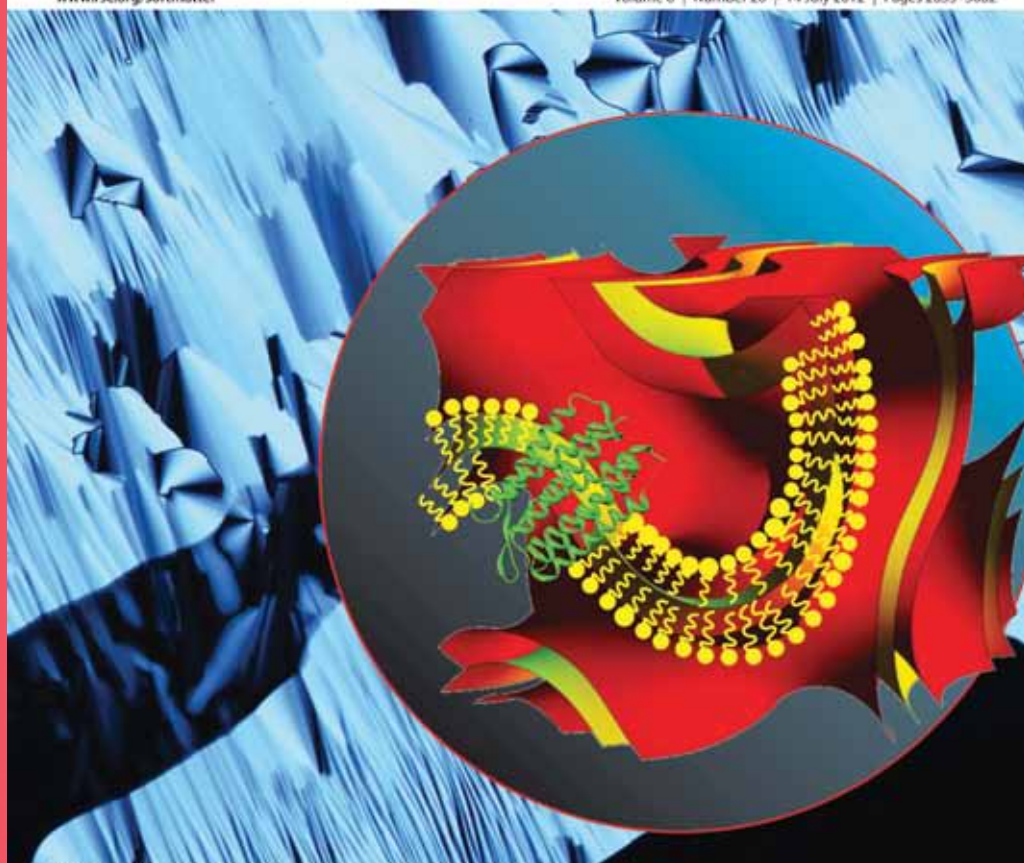
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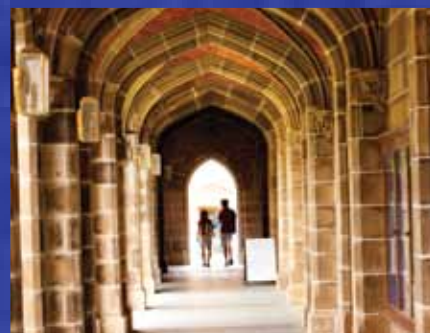
Charlotte E. Conn et al.

Effect of lipid architecture on cubic phase susceptibility to crystallisation screens



1744-683X(2012)8:26;1-8

CXS LOCATIONS



PARKVILLE CAMPUS

Corner Swanston Street and Tin Alley, Parkville

PHYSICS BUILDING CXS Head Office

The Experimental Methods Program (also at La Trobe University)

The Theory and Modelling Program

The Ultracold Plasma Source Program

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SCHOOL OF BIOMOLECULAR AND PHYSICAL SCIENCES

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MOLECULAR AND HEALTH TECHNOLOGIES

The Structure Determination Methods Program



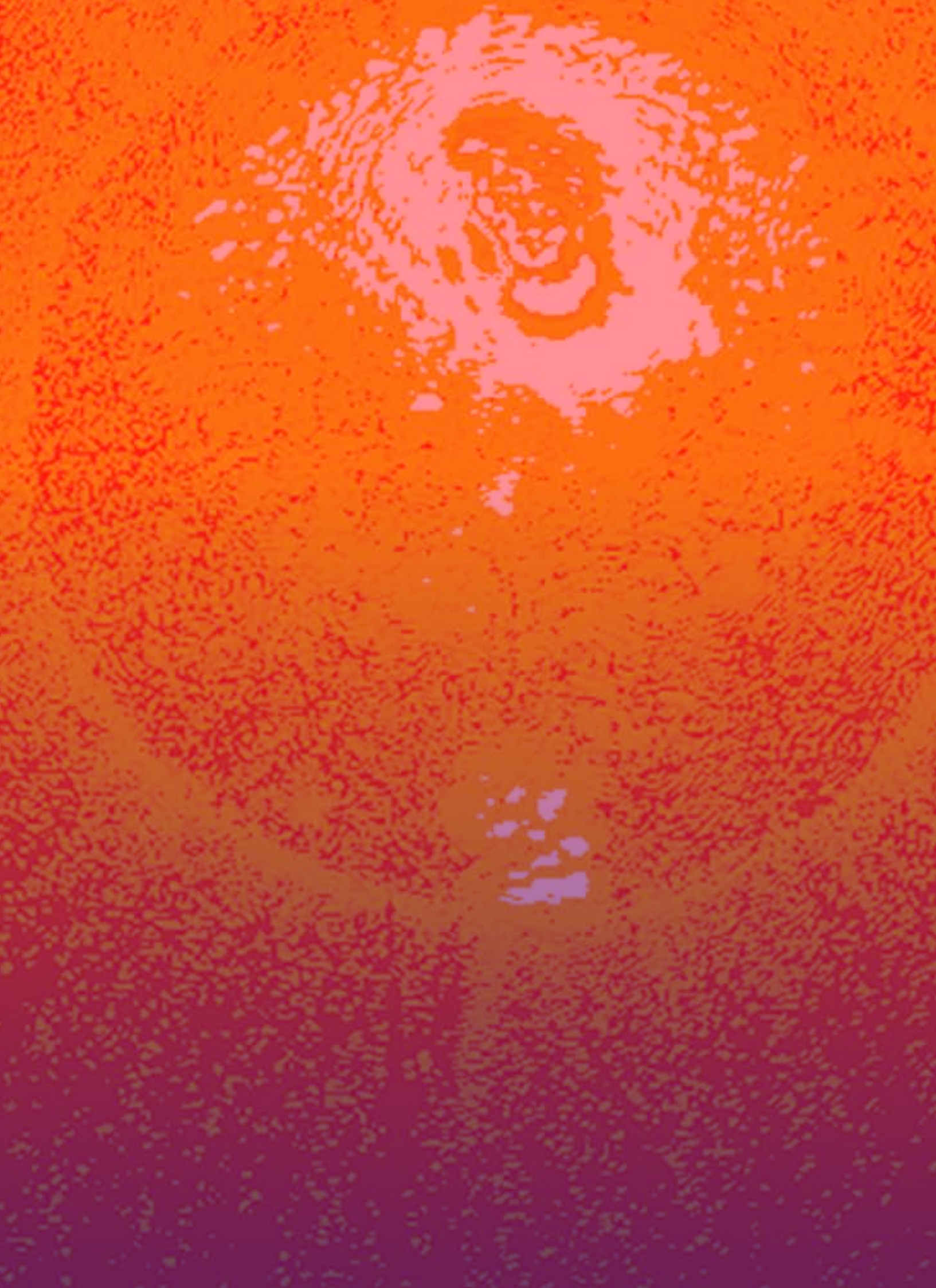
FINANCIAL STATEMENT

CXS FINANCIAL REPORT JANUARY – DECEMBER 2012

	2012 REPORTING PERIOD (\$)		2013 REPORTING PERIOD (ESTIMATED) (\$)	
Carry Forward	\$2,910,559		\$2,658,596	
Other Funds	\$2,200,000	ARC Income	\$2,200,000	ARC Income
	\$96,767	ARC Indexation	\$309,733	ARC Indexation
	\$837,271	Node Contribution	\$1,041,829	Node Contribution
	\$183,050	Refund from Monash EMP Close down		
Total Income	\$6,227,647		\$6,210,158	
Expenditure	\$2,075,515	Salaries	\$2,885,920	Salaries
	\$443,058	Equipment	\$598,574	Equipment
	\$308,899	Travel, Accommodation and Conference	\$215,000	Travel, Accommodation and Conference
	\$302,267	Materials, Provisions and Services	\$553,557	Materials, Provisions and Services
	\$125,601	Scholarships	\$152,000	Scholarships
	\$92,377	Marketing, Outreach and Sponsorship	\$157,400	Marketing, Outreach and Sponsorship
	\$40,902	General	\$52,800	General
	180,432	Payment to LU EMP Detector Project	\$145,000	2014 Operations Admin Commitment
			\$306,000	LTU End Station
			\$162,500	Chemistry Arrears Transfer
			\$981,407	2014 Project Completions
	\$3,569,051		\$6,210,158	

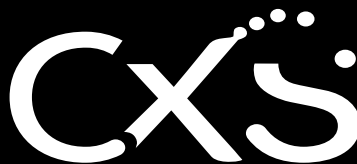
IN-KIND REPORT JANUARY – DECEMBER 2012

University of Melbourne	\$4,147,061
La Trobe University	\$1,892,283
Monash University	\$94,172
Swinburne University of Technology	\$736,363
Griffith University	\$495,875
CSIRO	\$99,161
Total	\$7,464,915





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