Australian Synchrotron Development Plan
Project Submission Form

Section A: Summary and Proponent Details

Project Title

Soft X-ray Microscopy and Spectroscopy Cluster

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Executive Summary (approx. 100 words)

Following a series of community consultations there is strong support in the soft X-ray community for the development of a **Soft X-ray Cluster** that encompasses a new undulator beam line and bending magnet beam line facility.

- The new undulator beamline would be optimised for micro-focus, imaging soft X-ray spectroscopy comprising a "Super-STXM" endstation,
  - combining STXM-AFM capabilities simultaneously on the same sample,
  - introducing new zone plate advances to achieve sub-10 nm resolution.
- The new bending magnet beam line could have up to three branch lines to cover the 10 eV up to perhaps 1500 eV energy range. One line would be able to accommodate the new toroidal analyser and another to cover possibly general XAS and/or full field microscopy.

Longer term objectives include:

- Development of the XPEEM and LEEM communities followed by the acquisition of a SPELEEM endstation.
- Access to "tender" photon energies, e.g. up to 4keV on a bending magnet beamline

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Section B: Detailed Description

B1: Description of Proposed Beamline/Development Project

The proposed project involves the development of a new soft X-ray beam line cluster as part of the bid for the next suite of beam lines at the Australian Synchrotron (AS). This cluster will consist of an undulator beam line source (with provision for a main line and a branch line) co-located with a bending magnet source (with provision for up to 3 independent lines). The vision of the soft X-ray community is the long-term development of Australian soft X-ray synchrotron science by establishing a suite of beamlines that will cater both for the immediate needs of the community as well as its anticipated future requirements. As such, the proposed soft X-ray beam line cluster involves a phased development of beamline capabilities. Phase 1 involves the combined development of an undulator-based scanning X-ray microscopy beamline and a bending magnet based low energy and environmental spectroscopy beamline. Phase 2 would involve upgrading the bending magnet facilities with the provision of additional beamlines for accessing the higher energies and full field microscopy. This proposal is focused on establishing Phase 1 of the soft X-ray beam line cluster as part of the first suite of beamlines funded by the Australian Synchrotron Development Plan.

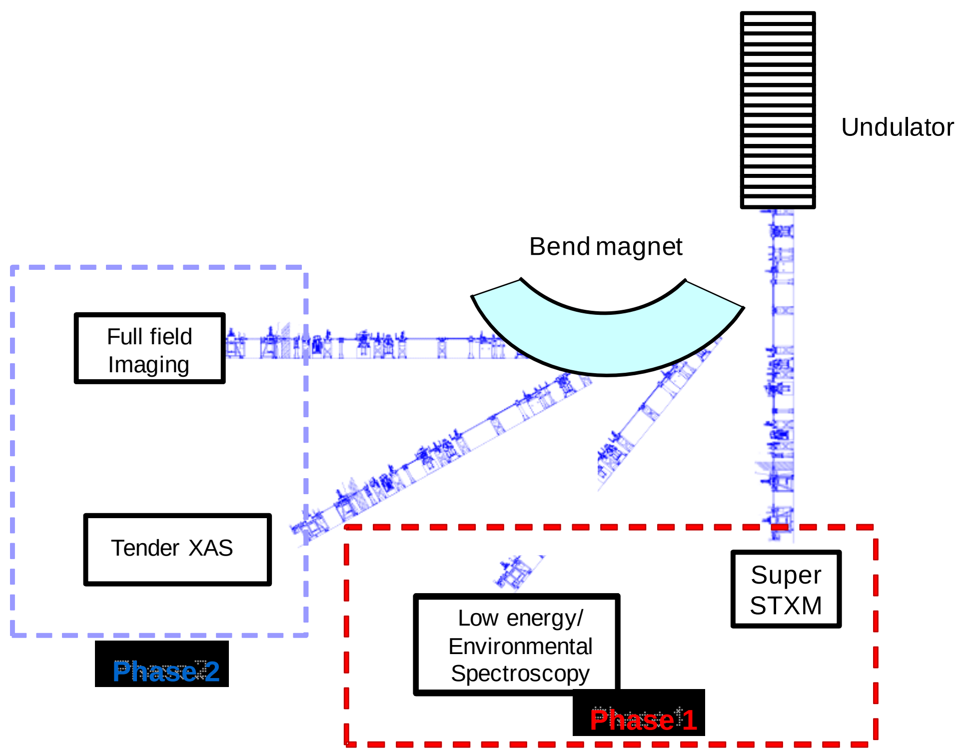

Figure 1: Schematic of proposed Soft X-ray Cluster at the Australian Synchrotron

Phase 1: Undulator Soft X-ray Spectromicroscopy Beam Line

Synchrotron-based soft X-ray microscopy is a unique technique for mapping the chemical composition of surfaces with sub 30 nanometre resolution. Currently there are more than 10 such facilities worldwide with substantial oversubscription for general user access with a number more under construction. In addition, recent zone plate advances involving doubled Fresnel zone plate architectures are able to achieve sub-10 nm resolution.

This project will involve the development of a unique "Super STXM" scanning X-ray microscopy facility that combines X-ray microscopy with scanning probe microscopy on the same sample. This new facility would allow the simultaneous measurement of topological and chemical maps of the surface, thus overcoming one of the major limitations of current X-ray microscopy systems. A similar facility is currently under construction at the Swiss Light Source but on a bending magnet beamline. In addition, the new facility would build in the capability for coherent diffractive imaging (CDI) and new zone plate architecture to achieve sub-10 nm resolution.

The technical requirements of the new beamline is anticipated to involve a Danfysik Apple II EPU together with a collimated plane grating monochromator with grating multilayers to provide for a new extended range scanning X-ray microscopy system. Ideally, the new facility would incorporate both transmission X-ray detection (STXM) together with photoelectron emission detection thus providing surface and bulk chemical sensitivity. Indeed, Detection across a range of modes including: transmission, fluorescence, photoelectron, secondary electron and X-ray emission would be highly desirable and would open up still further avenues for research. Importantly, the new system would involve an integrated in-situ scanning probe microscopy capability, which in the first instance is likely to be atomic force microscopy (AFM) although a variety of other scanning probe microscopies would be possible. The energy range of the facility would be ideally 200 – 3000 eV with a flyscan resolution of resolution of better than 10nm. Ideally, the dedicated endstation would allow the provision of some degree of variable pressure operation (ranging from ultra high vacuum (UHV) conditions to higher pressures and "environmental control" (ie. temperature, redox, etc). The sample handling facility will be designed to handle a wide variety of samples, from simple powders, to thin films to largish chunks of metals, concretes, plastics etc. the system and sample presentation design considerations should include compatibility with the hard X-ray EXAFS and microprobe XRF beam lines, including sample handling and detection systems so that users have sample compatibility across several beamline facilities.

A preliminary costing for the undulator beamline has been prepared by the soft x-ray beamline scientists based on the component costs of the exisiting soft x-ray undulator spectroscopy facility (Table 1).

Item	Cost ($'000)
Beamline	4 500
Undulator	850
Front end and straight	400
End station	2 500
Total	**8 250**

Table 1: Initial cost estimates for undulator-based Super-STXM Beamline

Phase 1: Low Energy/Environmental Bending Magnet Soft X-ray Beamline

In addition to the undulator beamline there is also considerable demand from within the soft X-ray community for a number of advanced synchrotron techniques and facilities that would need to be accommodated on a bending magnet beamline. In particular, there is a significant immediate demand for spectroscopies that cannot be readily accommodated by the existing soft X-ray beamline. Specifically, there are four main areas that are currently not supported:

1. **Low energy spectroscopy**
2. **Environmental XAS**
3. **Tender XAS**
4. **Full-field imaging**

This project will involve the development of a bending magnet soft X-ray facility designed to accommodate both the current and future needs of the soft X-ray community. The long term vision of the cluster is for the development of 3 lines each based around a collimated plane grating monochromator. Line 1 (which is included in Phase 1 of the soft X-ray cluster as part of the first suite of beamlines funded by the Australian Synchrotron Development Plan) would comprise a low energy and environmental line. For low energy work, the beamline would have an energy range of 20 – 1600 eV under windowless operation, whereas for environmental studies a windowed operation would ensure that the facility could cope with a wide range of environmental samples that require analysis under much higher pressures approaching 1 atm. The low energy beamline would exploit the 3rd Generation toroidal analyser system currently under construction at La Trobe University and which is due to be delivered to the Australian Synchrotron in 12 months time. This new instrument has the best angular resolution and speed of analysis of any comparable system internationally. The environmental line would alleviate the current inability of the existing soft X-ray facility to cope with samples requiring (or not suitable to) non-UHV conditions. The smooth output characteristics of the bending magnet would be well-suited to the requirements of both low energy spectroscopy and environmental XAS.

A preliminary costing for the bending magnet beamline has been prepared by the soft x-ray beamline scientists (Table 2) assuming that the end-station facilities will be coming from other sources.

Item	Cost ($'000)
Beamline	4 000
Front end	300
Total	**4 300**

Table 2: Initial cost estimates for Low Energy/Environmental Bending Magnet Beamline

Thus the total cost of Phase 1 of the new soft X-ray cluster incorporating a combined undulator and bending magnet facility is approximately $12 – 13 M and will lead to the immediate development of 2 beamlines. The proposed cluster is designed for cutting-edge microscopy and spectroscopy and caters to the immediate needs of scientists and technologists in the soft X-ray community.

Phase 2: Future Needs of the Soft X-ray Community

Through its consultation process, the soft X-ray community has also attempted to foreshadow the emerging trends and hence the future needs of the community. The key areas that were identified for future development were the establishment of a higher energy (Tender) beamline and a full-field microscope beamline capable of operating in the soft X-ray range. In the case of the Tender line there are a number of users interested in going to higher energies (~1.5 – 4 keV) with a number of applications in the areas of minerals and materials analysis using XAS. In the case of the full field microscope, there is strong support from Biosciences for work in the water window. In addition, based on feedback from current LEEM and PEEM users, a spectroscopic photoemission and low energy electron microscope (SPELEEM) is also foreshadowed. This system will provide, LEEM, XPEEM, LEED, XPD measurements providing surface morphology (3D) and structure, chemical state and magnetic domain imaging and would be located on an undulator branch line. Only three SPELEEM facilities are currently in operation including Diamond, Spring 8 and ELETTRA, which has the highest resolution of 14 nm in LEEM mode. These facilities are heavily oversubscribed and are not easily accessible to Australiasian scientists. The SPELEEM facility will provide spatial resolution in the order of 2nm in LEEM mode enabling magnetic dichroism studies and electronic structure determination of individual nanoparticles. Expected applications include the study of nanocatalysts, quantum dots, chiral templates, magnetic nanostructures, carbon nanotubes, conducting polymer films, earth and environmental science and minerals processing. Furthermore, with the soft X-ray cluster in place, many and varied endstation-specific instrumentation & techniques may be easily accommodated, e.g. X-ray emission spectroscopy (XES), imaging XPS, etc.

B2: Applications and Potential Outcomes to Australian Scientific Community

This project represents the most significant advance in the development of soft X-ray synchrotron science since the establishment of the soft X-ray beamline at the Australian Synchrotron. The proposed new facilities will result in significant scientific outcomes for Australian science and, importantly, would contribute to a new of the key national priority areas. Indeed, the number of projects that would be supported by this new facility are considerable and a few examples are given below:

An Environmentally Sustainable Australia

- The development of organic photovoltaic (OPV) technology offers the prospect of inexpensive, flexible solar cells fabricated over large areas but the performance of these materials is critically dependent upon the nanoscale morphology of the polymer blends. STXM is the only technique that is capable of providing chemical contrast in these systems with nanoscale resolution.
- Hyperaccumulating plants accumulate extremely high concentrations of trace metals in specific cells (e.g., Ni in epidermis cells, Mn in mesophyll cells). STXM will allow the investigation subcellular localization of target elements with a high spatial resolution, which provides insight into the physiological mechanisms of heavy metal tolerance and hyperaccumulation in the plants.
- The only sustainable and enduring source of green energy in sufficient abundance to supply humankind’s needs is sunlight. Producing hydrogen by the photocatalytic splitting of water using the visible portion of the sun’s radiation provides sustainable, carbon-neutral green power. Catalysts for this process are based on semiconductor nanoparticles immobilized within the pores of mesoporous materials. Imaging of the supported materials using the STXM would provide invaluable complementary data to electron microscopic studies in establishing the distribution of the nanoparticles on the mesoporous supports.
- As a means of process intensification, with the aim of reducing the footprint of chemical manufacturing plants by conducting separations on the nano-, rather than the macro level, we have encapsulated catalysts within successive layers of polyelectrolyte membranes to enable two otherwise incompatible catalysts to function in the same solution. The STXM would be used to image the nanocapsules to establish the integrity of the encapsulating membranes and to test the fundamental question of whether catalysts are in fact, encapsulated within, or merely associated with the polyelectrolyte nanocapsules.
- STXM will provide correlated ultrastructure-chemistry information leading to enhanced understanding of the uptake and metabolism of toxic and nutrient metals in the environment. Having this facility in Australia will allow many analyses to be performed on plant and animal tissues that are prohibited from transport overseas.
- The STXM technique allows investigation of functional group chemistry of natural organic molecules from soil. Humic and fulvic acids can be isolated, and carboxylic acid concentration analysed, and are of particular interest in understanding the C cycle in soil(s).
- Arbuscular mycorrhizas are symbiotic associations formed between the majority of terrestrial plant species (approximately 80%) and a specialized group of soil fungi. Formation of these associations can lead to significant improvements in plant nutrition. They therefore have an important role to play in natural and agricultural ecosystems. SXM would enable detailed

analysis of the physiology of these associations, at a previously unparalleled level of resolution. Studies involving Zn in this context are of particular interest.

Safeguarding Australia

- The development of simple, safe, non-intrusive, rapid, portable, direct, cost-effective sensing equipment that is more sensitive and selective for detecting traces of concealed explosives and narcotics would greatly enhance the ‘dual-tasking’ capability of law enforcers in controlling security (i.e. protection against threat of terrorism) and preventing drug trafficking at entrance portals and other domestic situations such as in buses, trains, buildings. Molecular imprinted polymers (MIPs) are stable, robust, re-usable and can be generated, in principle, for any type of target and, thus, have significant advantages over the widely used biosensors. The new facility would provide the ability to characterise these polymer blends on the nanometre length scale.

Frontier Technologies for Building and Transforming Australian Industries

- Mineral processing invariably begins with grinding of ores. Fracture surfaces produced by fine-grained ores, containing a range of mineral types (sulfides, oxides, aluminosilicates, etc.) may be dominated by internal, reacted layers and films at the interfaces between dissimilar phases. Chemical imaging of the nature of these interlayers, particularly of low Z elements, via STXM, will be invaluable for determining processing strategies.
- Ultrafine (<2 microns) mineral particles impact heavily on reagent adsorption, froth and foam stabilisation, gel formation and dewatering processes and are of increasing concern in toxicity in the environment. Both STXM and CDI will enable direct visualisation and chemical contrast in monitoring the effects of chemical conditions on ultrafine particle distribution and interactions in industrially-, and environmentally-relevant systems.
- The properties of TiO_2 are a major focus of research in a number of areas, covering optical, catalytic and energy applications. The dispersal and particle-particle association of TiO_2 and surface-modified TiO_2 particles in various polymer matrixes as a function of fabrication parameters will need to be correlated with the distribution of organic chemical additives. STXM is the only method available that can combine the physical (transmitted X-ray imaging) and chemical (NEXAFS mapping) information required on this dimensional scale. The coupling of STXM measurements with the 3D visualisation of TiO_2 aggregate structures via CDI is an area of great potential.
- Access to high resolution STXM will provide critical information for the improvement of the adsorption/desorption reactions of porous geomaterials, including soils, filters and clay-based barriers. It will also enable important insights into controlling porosity changes in geomaterials; minimising fault fractures in building materials including cements, concretes, asphalts and metals; and controlling corrosion, dissolution and/or salt-impregnation in cements, concretes, asphalts and metals.
- The facility will provide a state-of-the-art test bed for the development of novel techniques in coherent x-ray optics. These projects will continue in parallel with the STXM developments.

Promoting and Maintaining Good Health

- Coherent diffractive imaging methods can be used to obtain additional information about cellular architecture of parasitised erythrocytes at a resolution of 10 nm or better.
- The high spatial resolution of the STXM microscope will enable the study of heme aggregation in normal and sickle red blood cells with the goal of determining the actual spatial location of these aggregated hemes are difficult to determine.
- A critical question in the field of malaria research is how drugs accumulate in the food vacuole of the parasite. Some studies suggest that drugs like chloroqine bind to preferential sides of the haemozoin aggregate (malaria pigment) but there is no definitive proof of this occurring. We would like to trial a range of anti-malarial drugs and determine whether such preferential binding does exist using scanning transmission X-ray microscopy.

B3: Match to Selection Criteria

Selection Criteria	Match to Selection Criteria
Meet the demands of an identified group of researchers for new techniques	The soft X-ray cluster proposal is based on an extensive consultation process with the soft X-ray community, which numbers some 80 – 100 academics, researchers and students. This proposal addresses the key demands of this community in the immediate term and provides for the future development of this community over the next ten years.
Take advantage of the existing third generation light source	The proposed X-ray microscopy and spectroscopy facilities exploit fully the existing light source at the Australian Synchrotron. The proposed advanced surface mapping would not be possible without a 3rd generation source and indeed would be ideally positioned to make maximum benefit of the proposed upgrade of the source to top-up mode. The low energy and environmental lines both require a 3rd generation source to reach their full potential.
Will position Australasian scientists at the leading edge of their field	The proposed new combined surface probe and soft X-ray microscopy capabilities of the Super-STXM line together with advanced zone plate construction would place Australasian scientists at the leading edge of their field. In addition, the establishment of a low energy beamline with a 3rd generation toroidal analyser places Australian science again at the leading edge of soft X-ray developments. Together, this soft X-ray cluster is a unqiue facility with unique capabilities not available elsewhere.
Can be demonstrated to be feasibly constructed within a 3 year timeframe	The development of the Super-STXM line would build on the expertise already in Australia through the STXM working group and the CXS centre. The advanced capabilities (combined SPM and zone plates) are under development at other facilities and could be implemented in Australia in a 3 year timescale. The toroidal analyser

	is already under construction and is scheduled for delivery to the AS in 2010. Thus, the development of the soft X-ray cluster facility is certainly feasible in a 3 year timescale.

B4: Potential Users

In response to the call for preliminary input to Science Case II for the next suite of beam lines, a series of community meetings and discussions have taken place with a view to defining the needs and expectations of the soft X-ray community with regards to Science Case II. A wide range of input was received from experienced Australian users with a diverse range of research interests (encompassing Physics, Chemistry, Mineralogy and Geochemistry) and from a number of institutions in NSW, VIC and SA. In addition, advice on the state-of-the-art capabilities of related overseas SXM facilities from an international perspective has been provided by colleagues at overseas facilities. This proposal for the development of a new soft X-ray beam line cluster is the result of this extensive consultation process and as such directly addresses the immediate and long term needs of the soft X-ray community.

As part of this consultation process the community noted that synchrotron-based soft X-ray microscopy and spectroscopy are unique techniques for mapping and analysing the chemical composition of surfaces with sub 30 nanometre resolution and sub 0.1% sensitivity. In addition, there is a large and growing Australian soft X-ray community across the full range of science and technology disciplines encompassing Physics, Chemistry, Biology and Earth Sciences including Geochemistry and Mineralogy, and Soil Sciences amongst others. The driver for the growth of this community is the ability of soft x-ray microscopy to provide quantitative chemical maps of surfaces with unprecedented resolution.

In order to further develop soft X-ray microscopy (SXM) in Australia, a SXM Working Group has been formed and has already successfully achieved LIEF funding for a prototype joint STXM/CDI end station to attach to the soft X-ray beam line at the Australian Synchrotron. However, it is already apparent that the capacity and capability of the planned joint STXM/CDI system will be limited and that planning is urgently needed for the development of a new dedicated soft X-ray microscopy beam line. In addition, the present soft X-ray beam line is already heavily oversubscribed and a number of proposals are having to be rejected on the basis of a lack of capacity (Figure 2). The provision of additional spectroscopy capability would thus alleviate this additional demand as well as providing new soft X-ray facilities thus providing a strong case for additional spectroscopy based soft X-ray beam-lines.

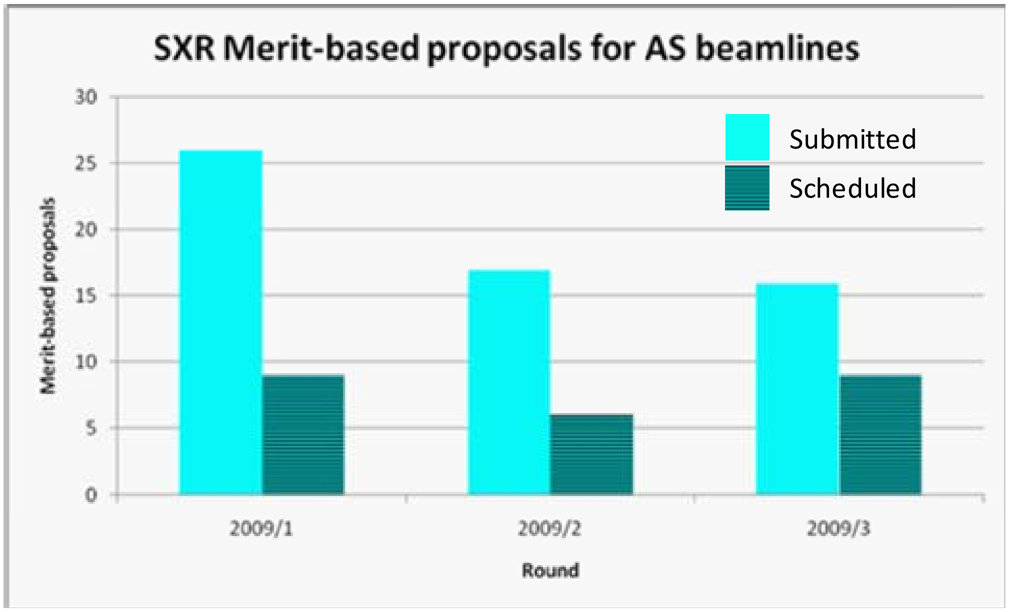

Figure 2: User Statistics for the Current Soft X-ray Spectroscopy Beamline

Although applicable to a wide range of materials, the capabilities of soft X-ray spectroscopy and microscopy are particularly relevant to organic and biomaterial surfaces where it is now possible to differentiate materials on the basis of subtle differences in molecular structure rather than crude elemental composition. For example, these capabilities now enable differentiation between organic components (e.g. live cellular vs humic materials) as well as inorganic components (e.g. various carbonate minerals) simultaneously within a single sample. The proposed dedicated soft X-ray cluster will also be able to take soft X-ray data under a variety of pressure conditions. This capability would enable the expansion of soft X-ray techniques to the biological sciences as well as to the study of predominantly organic species (like coal), and methods have been developed that enable the study of fully hydrated samples. The unique energy and spatial scanning system of soft X-ray microscopy minimizes radiation damage to tissues and provides the ability to scan a large portion of the periodic table (from Be K to Kr L) within a short time-frame.

Summary

The Australian soft X-ray science encompasses a large and growing community with a broad range of disciplines and a wide geographic spread. As part of the consultation process in preparation for Science Case II, this community has developed a clear vision of community needs in the near and long term. This soft X-Ray cluster proposal represents the culmination of this vision and involves the development of a combined undulator and bending magnet facility designed for cutting-edge microscopy and spectroscopy. This facility will cater to immediate needs of Australian scientists and technologists and is designed around a phased development. Phase 1 seeks an investment of $12 – 13M from the Australian Synchrotron Development Programme for an undulator and bending magnet beamline with cutting edge soft X-ray microscopy and spectroscopy capabilities. The long term vision is for the development of an expanded co-located X-ray cluster facility with a built-in capacity for future upgrades and developments including a long term plan to build full-field and SPELEEM facilities at the AS.