# Report

SPring-8 Academic Review Committee
(SPARC)

January 23, 2009

## *1. Introduction*

SPring-8 started operation in 1997, and celebrates its 11th anniversary in the fall of 2008 with a broad portfolio of ongoing activities. To reach this mature stage required constant efforts on the part of SPring-8. Periodic critical assessments and warm and thoughtful encouragements and advice from colleagues nationally and internationally have helped to shape the developments.

International reviews in the past include,
1. International Advisory Councils in 1991, 1992, 1993, 1995 and 1996.
2. SPring-8 Advisory Council in 2000.
3. JASRI International Advisory Council in 2006.

SPARC (SPring-8 Academic Review Committee) this time was held on November 16-19, 2008. The terms of SPARC given by the Director General of JASRI are as follows,

1) To measure or evaluate the peak height of the academic outputs
2) To explain their scientific values in a manner that can convince public community
3) To advise on the future plans for SPring-8

In contrast to previous review committees, the mission of SPARC has been straightforward, i.e. to focus only on scientific achievements in the past and on the presented future plans.

Based on the presentation and documents made available, SPARC had intensive and extensive discussions on the scientific activities which SPring-8 has so far achieved. Through these discussions, it has become clear that SPring-8 has a high degree of capability to meet scientific needs once they become clear and well defined. This is impressive and highly commendable.

In this report, the Summary of the Review is presented as an Executive Summary on scientific achievements and recommendations in Section 2, followed by a detailed assessment of each subfield in Section 3. The relationship to society, especially the educational program, is briefly assessed in Section 4.

## *2. Executive summary*

The results of the assessment of the scientific achievements made by SPARC are presented first, followed by the general recommendations.

### [A] *Outstanding achievements*

**** In-vacuum Undulator Sources***

By placing the magnet structure inside the vacuum chamber, the undulator gap can be reduced, and hence much shorter magnetic periods can be built without compromising the strength of the magnetic field. This extends the energy-range of undulators at SPring-8 and all other light sources. The brilliant success of this approach has been leading the way for other facilities and for new sources with medium size accelerators which nowadays even operate at smaller emittance than the first 3 facilities, APS, ESRF and SPring-8. It is also worth pointing out that this concept promises presently a cost saving option for future XFEL sources. Clearly, this development has had a profound worldwide impact.

****Advanced Beamline Technology***

From the start the SPring-8 beamline team has tried to develop new beamline concepts using the source properties in the most optimised way. This has led not only to new designs of monochromators and polarisers, but also to new measurement strategies such as a 1km beamline, modulation spectroscopies and several more.

**** Structural Studies on Membrane Proteins.***

It is known that up to 30% of human proteins are located in the cell membrane. These membrane proteins play crucial roles in many biological functions and are of key importance for medicine. We recognized that research on $Ca^{2+}$ -ATPase, bovine Rhodopsin, bacterial multidrug efflux transporter are truly outstanding and to the highest international standard. High flux X-ray beams at BL41XU and BL44XU were essential for these experiments.

**** Structural Studies on Macromolecular Assemblies.***

The study of macromolecular assemblies is a particular challenge for structural biology. The flagellum is a huge molecular complex made of 20 to 30 thousand subunits containing about 30 different proteins. High resolution X-ray structures of flagellar component proteins were solved using the brilliant X-ray beams at BL41XU and BL44XU. By combining these single crystal X-ray results with the low resolution structures obtained using cryo-EM and X-ray fibre diffraction, the structures of three distinct parts of the flagellum were determined.

****Real-time SAXS Analysis of Periodosome***

The process of assembly/disassembly of the periodosome (a multimeric complex of Kai proteins) was followed in real time by SAXS experiments at BL45XU, which could indeed verify that this was controlled by the phosphorylation of one of the Kai proteins and provided an overall picture of the periodosome in its different states. This real time elucidation of the circadian clock mechanism by Small Angle X-ray scattering is a unique example of the application of real time SAXS experiments. Other examples include the successful investigation of protein folding.

***Motion of Potassium Channel revealed by Single Molecule Tracking.***

By using a novel technique based on monitoring the movements of a gold nanoparticle attached to the KscA potassium channel and irradiating it with white X-radiation, the motion of the protein could be monitored in real time by following the motions of the diffraction spots from the gold crystal. These experiments showed how the potassium channel upon gating was twisted around the pore and that gating could be prevented by adding an open-channel blocker. Single molecule tracking opens unique opportunities to study molecules in action and this was made possible on BL44B2.

***Rational Design of Nanoporous Materials with Chemical Functionality***

An impressive range of new metal-organic frameworks (MOFs) and Porous Coordination Polymers (PCPs) compounds exhibiting specific chemical functionalities have been synthesized. These compounds have significant commercial potential as potential gas storage, as well as catalytic, media for clean and renewable energy solutions. This program benefits and interplays synergistically with the world-leading small molecule crystallography program at BL02B2.

***Probing Bulk States of Correlated Electron Systems by High-Resolution Resonance Photoemission***

At a helical undulator beamline, equipped with a varied line space grating monochromator, high-resolution and high-photon flux soft X-ray beamline was realized at BL25SU. This has been successfully utilized in soft-X-ray resonance photoemission experiments of strongly correlated systems. Thanks to a much longer escape depth, bulk electronic states were observed, which previously had been revealed only weakly with a low photon energy photoemission spectroscopy (PES). These results demonstrate the effectiveness of high energy, high resolution PES for the study of strongly correlated 4f electronic states.

*** *Phase Change Mechanism of Rewritable Optical Media***

X-ray diffraction pinpoint measurements at BL40XU demonstrate the interest in time resolved X- ray diffraction for academic and industrial use. Optical recording on DVD media is due to the amorphous to crystalline phase transition of the $Ge_2Sb_2Te_5$ (GST) and $Ag_{3.5}In_{3.8}Sb_{75.0}Te_{17.7}$ (AIST) materials. A direct measurement of the crystallization processes has been studied on a 0.32 micron surface of the DVD itself at nanosecond time resolution. Comparison between GST and AIST suggests that crystal growth control may be a key for designing faster phase change materials. The quality of the micro beam is paramount for investigating the ultra fast physics of photo- and thermo-excited phase transitions or chemical reactivity, by time resolved studies

**** Post-perovskite Phase of $MgSiO_3$ at 120GPa: Nature of the Mantle-Core Boundary***

Under the high-pressure and high-temperature conditions (125GPa, 2500K) corresponding to a 2700km depth at the mantle-core boundary, where the D" seismic wave velocity discontinuity is observed, the crystal structure of the post-perovskite phase of $MgSiO_3$ was successfully analysed, based on the in-situ X-ray diffraction measurements at the state-of-the-art high-pressure station BL10XU. This newly-solved crystal structure has a striking high-density layered-structure. This feature can solve successfully long standing mysteries, such as the discontinuous seismic change and the seismic anisotropy in the D" layer.

**** Advancing the Understanding of Automobile Exhaust Gas Catalysts***

Researchers from Toyota are advancing their understanding of Ceria Zirconia – a 3-Way automotive exhaust catalyst. Extended X-ray absorption fine structure (EXAFS) measurements were made on the Ce K-edge (40.45 kev) and Zr K edge (18 keV) at BL01B1 and BL16B2 to understand the local structure around these atoms and a clear relationship between the oxygen storage/release capacity of the material and its local structure was determined. Through the end of 2006, over 30 million Toyota vehicles have been fitted with this type of exhaust catalyst. This, and other work, clearly has made an impact on Toyota as they are now in the process of constructing an insertion device beamline (BL33XU) at the SPring-8 facility.

In other work on catalysis, scientists from Daihatsu are using BL14B1 to further their understanding of so-called intelligent catalysts with the goal of developing a more durable exhaust gas catalyst. They found that precious metal ions such as palladium, entered and exited the ceramic crystals repeatedly as if they had "intelligence", and that the ions did not grow larger in size which can reduce the efficiency of their catalytic activity. This information has allowed Daihatsu to achieve a substantial reduction of palladium in their automotive catalysts.

These two examples clearly demonstrate the fact that the basic research with strong motivation can lead to real break-through in applications. Such efforts should be encouraged more.

** Interfacial Magnetism between FM/AFM Bilayers in Magnetic Sensor Heads*

It is the goal of many hard disk drive manufacturers to reach a recording density of 1 Tb/in$^2$. With this increase in density, instabilities in the exchange coupling between the ferromagnetic (FM)/antiferromagnetic (AFM) bilayers have been seen where the magnetization in the ferromagnetic layer has changed unexpectedly. Higher robustness is required in the fidelity of the data on hard drives and so experiments were performed at BL25SU to better understand the mechanism of exchange coupling and the control of magnetic structures at FM/AFM interfaces. Previously the existence of pinned interfacial AFM spins had been reported, but the mechanism that stabilises this process was unclear. This work verified the existence of pinned interfacial spins in the anti-ferromagnetic layer.

[B] *General Recommendations on Future Plans*

**Revolutionary Instrumentation Development*

Relying on the development (together with Osaka University) of the Elastic Emission Machining of mirrors to reach atomically smooth surfaces, a microfocus of 48nm x 36 nm has already been demonstrated on the 1 km beamline, with remarkably low stray scatter. Furthermore, focusing to 8 nm has been demonstrated in one dimension. This is clearly a remarkable record. Particularly exciting plans were announced to extend this technology to the 1 nm level by the use of multilayers. In fact, a Kirkpatrick-Baez microprobe with any spot size in the sub-10 nm range will be revolutionary!

** Compact XFEL*

The use of a thermionic gun followed by several bunch compression stages, a C-band warm linac and micro-undulators as emitters, was considered by many specialists, again similar to the in-vacuum undulator approach in the early 90's, a high risk approach. A prototype was built, which has demonstrated brilliantly the viability of the approach, and is now used as a successful user facility with a 20 – 25 eV FEL. Knowing that the prototype is working, the opportunity to realise a short and cost efficient version of an XFEL has become even higher. There are plans to use the FEL as a pump, to be combined with beams from SPring-8, as a stroboscopic probe of time evolution. This will be a unique capability. Furthermore, electron bunches from the linac will also be available to be injected into SPring-8 to create capabilities for very short X-ray pulses. This would give additional unique scientific opportunities.

** Improvement of life-science BL*

More and more complex biological systems will be targeted in the future that will require the use of different synchrotron radiation based techniques, *e.g.* diffraction, small angle scattering and imaging. The combination of techniques in the study of biological systems is already taking place and it is important that SPring-8 continues to facilitate applications of complementary methods. Structural biology evolves towards the study of more and more complex systems that are characterized by small and poorly diffracting crystals. It is therefore necessary to examine many crystals of the same sample to find the one most suitable for the measurements.
The proposed improvements of the MX beamline complex, that aims at creating a beamline portfolio, with each beamline fulfilling a specific role, seems best suited to meet the demands of structural biology in the future and to keep the macromolecular crystallography at SPring-8 at an internationally competitive level.

** Theoretical Modeling*

Due to their quality, the experimental results sometimes deserve a more thorough theoretical approach, as for example the pioneering work on myoglobin. Similarly, combined with MEM, systematic use of multipolar analysis of electron density would allow better description of inter-atomic interactions and bonding.

** High Resolution Inelastic X-ray Scattering*

At BL35XU non-resonant meV resolved Inelastic X-ray Scattering should be developed in the future in order to investigate atomic scale correlations in electronic excitations. This requires the construction of a new beamline which will enable important higher resolution measurements of electronic excitations.

**Synthesis of Nano-Polycrystalline Diamond: Potential Applications for HPT Experiment*

A nano-polycrystalline diamond, named "HIME-DIA", was successfully synthesised with a special capability of hardness exceeding diamond and low thermal conductivity, potentially accessible to the center of the earth (364GPa, 5,500K). It will benefit also fields such as material and environmental sciences.

## *3. Detailed Assessment of Scientific Achievements in Each Subfield of Science*

[Instrumentation]

## *General Statements*

SPring-8 used in-vacuum undulators as the standard insertion device in order to cover a wide energy range, particularly in the higher energy region and to reduce heat-loads on optical components. Most of the instrumentation and methodologies now characteristic of the facility stemmed from this decision. Even at the beginning of SPring-8 operation, the undulator technology itself was in its infancy. While undulator development at SPring-8 continued, the extremely intense, highly-directional, quasi-monochromatic and well-polarized X-rays generated by the undulators, demanded a new approach to instrumentation. To take full advantage of the undulator radiation requires a low emittance of the electron beam circulating in the storage ring. Deliberately careful alignment of the accelerator components has made it possible to minimise the vertical and horizontal emittance coupling, resulting in a vertical source size < 10 μm. This small source size combined with the long distance between source points and sample positions enables delivery of hard X-rays with a very high degree of coherence. From these partially coherent X-rays, fully coherent hard X-ray beams can be extracted by placing an appropriate pinhole in the centre of the beam.

## *Highlights*

Tightly collimated X-ray beams are very well matched to X-ray optics based on perfect crystal components, in which dynamical diffraction occurs within an angular range of only a few μrad around the Bragg condition. This even allows building optical devices such as the diamond phase retarder which converts X-ray polarisation from linear to circular. The phase retarder can produce both right- and left-hand circular polarized X-rays in a specified energy range. It can even switch the helicity by changing the X-ray angle of incidence by < 1 mrad. SPring-8 has pioneered techniques for operating an X-ray undulator beamline for magnetic circular dichroism (MCD), by using X-ray phase retarder optics delivering fast helicity-switched of circularly polarized X-rays. Bi-stable flipping of the phase retarder can produce alternating right- and left-hand circularly polarised X-rays with a flipping rate > 30 Hz by using a piezo-electric stage, and of ~1 kHz by using a Galvano motor stage. Such fast flipping rates enable the use of phase-locked measurement technology, resulting in a low noise measurement of the extremely weak MCD spectrum.

High-resolution X-ray monochromators are another example of benefits resulting from perfect crystal X-ray optics with highly directional undulator beams. The performance of both, backscattering monochromators and combined channel-cut monochromators, is much enhanced with highly-directed undulator X-rays. A backscattering monochromator can be utilised very advantageously when only the difference of X-ray energies inbound and outbound is important. A good example is instrumentation at BL35XU used in high resolution inelastic scattering. Energy loss in the meV range is recorded as a function of momentum transfer, thus enabling detection of low energy excitations such as phonons. Combined channel-cut monochromators are preferred whenever the absolute value of the output energy is important, such as in nuclear resonant scattering experiments. The highest resolution achieved so far is approximately 0.1 meV at 14.4 keV. This monochromator was also extensively utilised for a Hambury-Brown-Twiss type intensity interferometer in the X-ray region, and to devise a Fabri-Perot interferometer in the X-ray region. With highly-directional undulator X-rays, even a simple channel-cut monochromator using a higher order reflection can provide energy resolution better than 100 meV. Such monochromators are extensively utilised for hard X-ray photoelectron spectroscopy (HAXPES), which SPring-8 is one of the pioneers in developing. Now HAXPES is attracting growing interest as a promising new tool in materials science. Highly directional undulator radiation has also enabled the realisation of high resolution monochromators in the soft-X-ray region exceeding $E/\Delta E > 10{,}000$.

SPring-8 is unique in having a 1 km beamline (BL29XU). This beamline can provide large area coherent hard X-rays. The coherent property of the beam has been extensively utilized in developing ultra-smooth X-ray mirrors in collaboration with a group from Osaka University using the Elastic Emission Machining (EEM) technique. The collaboration team developed simulation code based on the wave-optical theory, instead of the geometrical theory, and a micro-stitching interferometer, which combines the microscopic interferometric data of the mirror surface figure with the large scale Fizeau interferometer data to measure with high precision the global mirror surface figure. Once the surface figure of the mirrors is accurately measured, the team is able to correct the figure toward the ideal one. These developments led to the construction of a series of Kirkpatrick-Baez (KB) type focusing mirrors. The smallest focal spot size currently achieved is ~ 10 nm. Development toward a ~1 nm focal size is underway. The polishing method is also used to fabricate a speckle-free mirror for XFEL. A 400 mm long elliptical mirror has been prototyped that has a deviation from the designed figure of less than 2 nm. Focusing devices based on reflective optics match well to spectroscopy because their focal position remains unchanged as a function of X-ray energy. One of the most straightforward applications of nano-focused X-rays is high resolution scanning probe microscopy. Some devices for scanning fluorescence X-ray microscopy have been developed and applied to a wide variety of samples, in which the local distribution of specific chemical elements is important. There is a growing interest in applying this technique to biological and medical samples, such as cancer cells.

The enhanced lateral coherence of X-ray beams at SPring-8 has contributed significantly to further develop coherent diffractive imaging (CDI). The collaboration with Miao's group began in 2000, and resulted in a series of milestone experiments applying coherent diffractive imaging to nanoscience and biology. The first 3D reconstruction by CDI was demonstrated for an artificial sample, the first application for a non-artificial sample was completed using a porous silica particle, and the first biological application was made using E-coli bacteria at SPring-8. The image recovery algorithm was improved to solve the missing central cone problem and a new algorithm to get super-resolution was developed. The 3D image reconstruction was applied to a GaN nanodot sample with 17 nm voxel resolution. Especially impressive has been the most recent 3-dimensional visualization of a human chromosome using coherent X-ray diffraction with beamline BL29XU.

In-vacuum undulators, developed as the standard insertion device for SPring-8, have found many applications in various research areas. A 27 m long, in-vacuum undulator was designed and constructed to serve as a light source at BL19LXU. Although photon flux did not increase as the square of the undulator length due to the energy dispersion of the electron beam, the undulator has provided the world's highest photon flux above 10 keV. Having the magnet structure inside the vacuum makes it possible to build shorter period, or mini-pole undulators, because the gap between two magnet arrays can be made very small. The use of mini-pole undulators opens new capabilities for constructing lower electron energy, third-generation synchrotron radiation sources emitting hard X-rays. The first demonstration of a mini-pole undulator was made by collaboration between SPring-8 and the NSLS at Brookhaven National Laboratory (BNL). This proved the capability of low energy storage rings to generate undulator X-rays. With the demonstrated success of this configuration, many lower energy, third-generation, synchrotron light source facilities considered installing in-vacuum undulators. Most of these facilities use the higher order harmonics of the undulator to extract hard X-rays. For this purpose stronger magnetic fields are better, and the SPring-8 team developed a cryogenic undulator which utilizes the magnetic field enhancement of the permanent magnet at a low temperature.

Another important direction is to apply minipole undulator technology to linac-based, free electron lasers. The technical feasibility of in-vacuum undulators opened the possibility to design a compact SASE source. In-vacuum undulators reduced the electron energy required to produce FELs compared with conventional out-of-vacuum undulators, thus reducing the length of the linac. SPring-8 started an R&D program focusing on the compact SASE XFEL in 2001, with an approach that was quite different from the approaches used by LCLS or Euro-XFEL.

Instead of the laser-RF electron gun, a thermionic gun with a single-crystal CeB6 was employed. An electron injector system with velocity bunching was proposed and developed to generate the high density and low emittance electron bunches required for an XFEL. High frequency accelerating tubes operating at 5712 MHz (C-band) further reduce the length of the linac compared with those using the more conventional 2856 MHz (S-band). A 15 mm period in-vacuum undulator was prototyped.

These newly developed components were combined to make a prototype free electron laser (FEL) operating at 250 MeV and generating intense ultraviolet SASE laser radiation at a wavelength of 60 nm. Building upon these results, an XFEL project has been proposed to construct an 8 GeV linac-based XFEL generating SASE X-rays at wavelengths less than 0.1 nm. The total length of this facility will be approximately 700 m, i.e., less than 1/3 of the length of the U.S. and European facilities. The proposal was approved as one of five 'Key Technologies of National Importance' of Japan to start in 2006 and to complete in 2010 fiscal year.

### *Recommendations*

With the completion of the XFEL, Harima will be the unique site where both a third-generation synchrotron light source and an XFEL will be co-located. Several experiments utilising XFEL pump and SPring-8 probe measurement are discussed. The linac for XFEL, which can provide low-emittance and short-pulsed electron bunches, will be used as an injector of the SPring-8 storage ring. Although the current SPring-8 lattice cannot take full advantage of the higher quality electron bunches from the XFEL linac, some planned alterations of the lattice will enhance the SPring-8 performance greatly in terms of emittance and pulse length. The synergistic use of SPring-8 and XFEL will undoubtedly require more innovative instrumentation and development of new methodology. We believe both SPring-8 and XFEL will be excellent and complimentary scientific tools, which will enable entirely new classes of experiments and will further advance the frontiers of science and its applications.

## [Life Science]

### *General Statements*

SPring-8 has been successful in developing a strong program in Life Science. This is demonstrated by fact that 40 % of the most cited papers are in this area. In terms of productivity the macromolecular crystallography beamlines are also leading in the Asian region, 65 % of the depositions in the Protein Data Bank are based on data measured at SPring-8.

The Protein 3000 initiative from 2002-2006 has been important to stimulate the growth in structural biology in Japan, that it now seems possible to continue through the Targeted Proteins Research Programme.

The strength of the Life Science program is illustrated by the relatively large number of very difficult protein targets comprising membrane proteins and macromolecular assemblies for which the structure determination was made possible with the use of SPring-8's beamlines. SPARC recognizes the very high overall quality of protein crystallographic activities at SPring-8.

## *Highlights*

Two of the truly outstanding works are the studies on $Ca^{2+}$- ATPase and on the bacterial flagellum. $Ca^{2+}$-ATPase of sarcoplasmic reticulum is an integral membrane protein, which pumps $Ca^{2+}$ into the sarcoplasmic reticulum from muscle cells using ATP, thereby regulating muscle constriction and relaxation. This pump is a representative member of a group of enzymes called P-type ATPases, which are ion pumps of crucial importance. The structures of this calcium pump revealed its molecular transport mechanism. It is known that up to 30% of human proteins are located in the cell membrane. The hydrophobic nature of membrane proteins, however, makes crystallisation extremely difficult and many of these crystals diffract X-rays only very weakly. Because of these problems, less than 10 mammalian membrane protein structures have been solved so far. To solve the structures of $Ca^{2+}$-ATPase, full advantage was taken of high flux X-ray beams at BL41XU and BL44XU. In collaboration with beamline scientists, very careful data collections were carried out addressing radiation damage occurring during measurement and they solved this important mammalian membrane protein in 6 different conformations. These results and related works have produced more than 40 papers in the international journals including 4 papers in Nature since 2000. This is a truly remarkable example of cutting-edge structural biology studies using synchrotron radiation.

Bacteria swim by rotating a helical filamentous organelle called the flagellum. The flagellum is a huge molecular complex made of 20 to 30 thousand subunits containing about 30 different proteins. The study of macromolecular assemblies like the flagellum is a particular challenge for structural biology. The high-resolution X-ray structures of flagellar component proteins were solved using the brilliant X-ray beams at BL41XU and BL44XU. By combining these X-ray structures and low resolution structures obtained using cryo-EM and X-ray fibre diffraction, models of the structures of three distinct parts of the flagellum have been obtained. These structures in combination with computer simulations have revealed the polymorphic transition mechanism of the flagellar filament, the universal joint mechanism of the hook and the molecular joint mechanism of the hook-filament junction. These are big steps towards a complete understanding of the structure and molecular mechanism of this complex nano-machine, which have led to more than 20 papers in the international journals including two Nature papers. This is another brilliant example of contemporary structural biology studies combining various methodologies and highlights the importance of state-of-the-art synchrotron beamlines like BL41XU and BL44XU.

We also recognized that the studies on bovine Rhodopsin and on the bacterial multidrug efflux transporter AcrB are outstanding and to the highest international standard.

The Rhodopsin structure is a very important contribution to pharmacology and medicine. The structure published in Science in 2000 represents the first structure of the G-Protein coupled receptors (GPCRs), which, at least, 30% of currently available drugs are targeting. The structure determination of this mammalian membrane receptor is a big step towards rational drug design based on GPCR structures. The fact that the paper has been cited over 2000 times highlights the impact of this paper. The structure determination was achieved by a successful application of the Trichromator at BL45XU beamline on MAD phasing of the structure from extremely delicate Rhodopsin crystals. The same group recently solved another important membrane protein structure. The structure of leukotriene C4 synthase, which was published in Nature in 2007, is one of the first X-ray structures of membrane proteins and also an important drug target. BL44B2 was used for this structure determination.

The emergence of bacterial multidrug resistance is an increasing problem in the treatment of infectious diseases. The major cause of the multidrug resistance of bacteria is a multidrug efflux transporter, which exports drugs out of the cells. AcrB is a membrane protein and the major multidrug efflux transporter in bacteria. The structure of drug-free AcrB was published in Nature in 2000. This is the first structure of not only a multidrug efflux transporter but also a secondary active transporter driven by proton motive force across the membrane. In 2006, the AcrB-drug complex structure was also published in Nature. It consists of three asymmetric protomers, each of which has a different conformation corresponding to one of three functional states. This elegant work reveals the drug export mechanism of AcrB by a three-step rotating mechanism in a trimer, in which drugs undergo ordered binding change. The X-ray data collections for these challenging structure determinations were performed at BL41XU and BL44XU as were the data for $Ca^{2+}$-ATPase and the flagellar components. This again highlights the importance the high-flux beamlines at SPring-8 optimised for difficult-to-solve biological structures.

In addition to the highly productive beamlines for protein crystallography at SPing-8 that can catch a static picture of a protein in different states, some outstanding results have recently been obtained at SPring-8 that give real time pictures of the protein in action.

One example is a very elegant experiment recently reported in Cell on the single molecule monitoring of the gating of potassium ion channels. Ion channels transport ions across the cell membrane. They are signal transduction molecules that are able to switch the ion permeation on or off (gating). Though the crystal structures are known of potassium channels in open and closed conformations, knowledge was not available about how the gating actually takes place. By using a novel technique based on monitoring the movements of a gold nanoparticle attached to the KscA potassium channel and irradiating it with white X-ray radiation, the motion of the protein could be monitored in real time by following the motions of the diffraction spots from the gold crystal. These experiments showed how the potassium channel upon gating was twisted around the pore and that gating could be prevented by adding an open-channel blocker. This single molecule tracking opens unique opportunities to study molecules in action and it was made possible at BL44B2.

Another real time investigation of protein movements and protein assembly was published recently in Molecular Cell. The circadian clocks allows organisms to adapt to the daily variations. Three different clock proteins KaiAm, KaiB and KaiC have been identified as being responsible for the control of the oscillations of the circadian mechanism of the cyanobacterium *Synechocossus elongatus* that is controlled by phosphorylation of one of the proteins (KaiC). It had been postulated that the oscillatory mechanism was controlled by assembly/disassembly of the Kai proteins into multimeric complexes (periodosome). The assembly/disassembly of the periodosome was followed in real time by SAXS experiments at BL45XU, which could indeed verify that this process was controlled by the phosphorylation of KaiC and provided an overall picture of the periodosome in its different states. This real time elucidation of the circadian clock mechanism by Small Angle X-ray scattering is a unique example of the application of real time SAXS experiments. Other examples are the successful investigations of protein folding.

Thanks to recent software developments Small Angle X-ray Scattering are being used increasingly by the structural biology community. SPring-8 contributes to this renaissance of SAXS and the potential of this method to give valuable information on protein-protein interactions. One prominent example is the investigations of the fatty acid β-oxidation multienzyme complex carried out at BL40B2. The SAXS experiments revealed that $NAD^+$ binding led to significant domain rearrangement and to a structure that was significantly different from the crystal structure.

With its long beamlines, SPring-8 offers excellent opportunities to effect the imaging of biological samples by computed tomography at different resolution levels. Among the highlights using this technique, are the *in vivo* experiments on rabbits to study the structure of lungs during breathing. These investigations that are carried out by an Australian user group show the excellence state of biological imaging at SPring-8.

*Recommendations*

The proposed improvements of the MX beamline complex, that aims at creating a beamline portfolio with each beamline fulfilling a specific role seems best suited to meet the demands of structural biology in the future and to keep the macromolecular crystallography at SPring-8 at an internationally competitive level.

[Chemical Science]

*General Statements*

SPring-8 chemical science programs presented at the review included structural chemistry, polymer science, nanoporous materials, catalysis and soft X-ray photochemistry. Due to the considerable overlap between chemical science programs with materials science programs, in particular in structural science and polymer science, the highlights and recommendations mentioned in the materials science section will not be repeated here.

Structural chemistry and small molecule crystallography carried out at SPring-8 are clearly world leading. The productivity of this program is extremely impressive, with ~40 publications a year from BL02B2. The program benefits enormously from the high energy, high brilliance and the remarkable stability of the source; as well as from the development in methodology and instrumentation, by the SPring-8 staff.

The structural chemistry program complements and interplays synergistically with world class synthesis capability in Japan, and together a large number of important new and novel structures have been solved at SPring-8. This synergy is best illustrated by the development of Porous Coordination Polymers (PCPs) and Metal-Organic Frameworks (MOFs).

It would be a benefit to SPring-8 portfolio to further widen their chemical user base within Japan and through new international collaborations, possibly through visiting fellowships to overseas scientists.

There is a great deal of opportunity for commercial exploitation in many of the examples that were presented in this section in a similar manner to materials science. The best example is thst of catalysis research. This program clearly should be highlighted more to educate the public about the importance of synchrotron research (see industrial application section.) The success of the catalysis research program is a very good example of how academic and industrial research can work together. It should also be noted that the spectroscopic study on fuel cells and *in situ* observation of catalytic reactions is clearly scientifically world class.

In addition to high resolution structures, most of the chemical science programs have also been able to relate structure to function in some cases, by studying structure evolution under different sample environments and using a variety of external stimuli. e.g. temperature, light, electric field, pressure. The timescale of the current data collections exceeds the time frame for any molecular structural changes or for 'normal' chemical reactions. However, this aspect of chemistry at SPring-8 will become increasingly important as new instrumentation and XFEL come on line, for example, the new high resolution instrument with important time resolved capability.

The question of time resolution was remarked upon by most subject groups in relation to their future plans, which follows from the quality of the SPring-8 beams, the novel instrumentation and innovation from the staff scientists. Additionally several leaders mentioned their plans to exploit the XFEL, which is truly impressive even at this prototype stage. The staff are well poised to exploit XFEL into the future; there is no shortage of bright ideas.

This is particularly true for the soft X-ray photochemistry program. This program focuses on fundamental spectroscopic measurements that underpin our understanding of X-ray interactions with matter. It takes advantage of the little known fact that SPring-8 is the superb source for soft X-rays. The activity at SPring-8 in this area is world leading. This program has engaged in research using the UV-FEL source and will likely be important for the SPring-8 X-ray FEL program as well.

### *Highlights*

#### **Interaction of hydrogen with metal nanoparticles*

The development of economically viable hydrogen storage materials is one of the key challenges in addressing the global energy problem. In-situ high resolution powder diffraction was used to characterize the core-shell structure of Pd/Pt nanoparticles under hydrogen atmosphere at BL02B2. The results revealed that most of the adsorbed hydrogen atoms are trapped to the interfacial region between the Pd-core and Pt-shell and suggested a route to design better hydrogen storage materials.

***Visualization of adsorbed gas molecules in framework structures***

At BL02B2, the combination of very high quality powder diffraction data with sophisticated data analysis methods and in-situ experimental system has allowed the determination of the structure of adsorbed gas molecules in $[Cu_2(pzdc)_2(pyz)]_n$. The high resolution structure provided insight into the chemical bonding and mechanism of gas adsorption. The same methodology has been applied further to a wide range of molecules in nano-porous framework materials and has resulted in many important scientific findings and potential industrial applications.

***Development of Porous Coordination Polymers (PCPs) and Metal-Organic Frameworks (MOFs)***

Porous Coordination Polymers (PCPs) and Metal-Organic Frameworks (MOFs) are new framework compounds exhibiting a wide range of structural characteristics from the very rigid to the very flexible, corrugated and interleaved. PCPs and MOFs respond differently to adsorbed gas molecules and are potential gas storage media for clean and renewable energy solutions.
In-situ high resolution powder diffraction has been instrumental in determining the structure of PCPs and MOFs as well as understanding the adsorption/desorption mechanism.

***In-situ time-resolved study of surface reactions***

Mechanism of surface reaction at the Pt/C cathode in a fuel cell under the operating conditions of the fuel cell was revealed by a new in-situ time-resolved X-ray absorption spectroscopy technique developed at BL01, SPring-8. The quality of the data was extremely good, thus provided high resolution structural data for the initial stages of the reaction for the first time. This opens up the way to 'seeing' chemical reactions in a wide range of industrial applications.

***Complete measurement of inner-shell excitation in $N_2$***

High resolution X-ray photoelectron, Auger electron as well as multiple electron –ion coincidence spectroscopy were carried out for gas phase $N_2$, at BL 27SU, to follow the inner-shell excitation process completely. These measurements provided fundamental spectroscopic results that put stringent test on our understanding of

X-ray interactions with matter. It confirmed a long standing prediction of difference in bond length for the two core-hole states, and provided strong evidence that the core-hole is not localized. This study has generated a great deal of interest in the community.

*Recommendations*:

*The proposed high-resolution single crystal program is very important and should be implemented as soon as possible. It will further enhance the strength of this world class program.

*Time-resolved studies with time-resolution down to pico-second are important for all areas in chemical sciences. These programs should take advantage of the significant expertise exists at SPring-8. They will also help to generate future scientific use of the FEL.

*The programs should be encouraged to use and exploit fully the capabilities at SPring-8. For example, most of the chemical science programs could benefit from using both spectroscopy and diffraction.

* World class studies using high resolution powder diffraction across the chemical sciences and exploiting the time structure of the beam should be continued.

[Materials Science]

*General Statements*

A longstanding cooperation well-organized among solid state physicists, chemists and material scientists in Japan has resulted in continuous production of novel materials and high-quality crystals of a wide variety of compounds such as superconductors, multiferroics and molecular complexes. SPring-8 has accepted such exciting themes very timely and produced excellent outputs by utilizing its full capability.

Highly accurate atomic and electronic structure results are produced on SPring-8' beamlines which are of utmost importance for understanding physical properties of newly designed materials. This is mostly due to an excellent combination of the high quality of the scientific and technical staff with an excellent synchrotron machine, symbolized e.g by the top-up mode operation, and due to outstanding instrumentation on the beamlines. Due to their quality, the experimental results may deserve a more thorough theoretical approach, as for example the pioneering works on metallofullerenes and myoglobin. The electron density modelling is only based on MEM methods and multipole modelling which is widely, used should be introduced and compared to MEM results.

On the other hand, systematic experimental and theoretical works have been conducted for inelastic scattering studies particularly on strongly correlated electron systems.

The Material Science Subfield has two components

STRUCTURE

X-ray diffraction and absorption experiments in SPring-8 are highly accurate, up to date, original and develop forefront techniques as for example demonstrated by the benchmark powder diffraction data collected on silicon and diamond. The precise structural description of complex materials such as thermoelectrics, metallofullerenes, host guest crystals serves now as world structural reference. The quality of these data permits realistic modelling of disorder and/or of electronic structure; such a structural accuracy is a necessity to understand and design materials' physical properties.

SPECTROSCOPY

Electronic and Magnetic Properties

Resonant and Non-Resonant X-ray Inelastic Scattering have been largely developed and optimized in SPring-8 in order to study the lattice/charge dynamical properties and the electronic structure of materials in the meV to eV range. Fermiology studies of materials are also very well recognized combining photoemission spectroscopy, ARPES and Compton Scattering. SPring-8 has a beamline devoted to magnetic Compton scattering applied to strongly correlated systems as for example to probe the orbital nature of the valence band of perovkites manganites. X-ray absorption and diffraction experiments under high magnetic fields were successfully performed on f-electron systems to induce valence and structural phase transitions.

*Highlights*

STRUCTURE

** Phase change mechanism of rewritable optical media*

As selected as one of Outstanding achievements, X -ray diffraction pinpoint measurements demonstrate the interest of time resolved X-ray diffraction for academic and industrial use. The quality of the micro beam is the key for photo and thermo excited phase transition studies and this beam should also be applied to ultra fast physics (BL40XU).

** 100nm single crystal data*

X-ray diffraction data collected on a 100nm single crystal of $BaTiO_3$ is a world record and the corresponding crystal structure quality is also a world record. This shows the possibility to move from powder diffraction to more accurate single crystal experiments using crystalline grains. It is predicted that there will be increased novel applications for the use of micro beams with single crystalline grains (BL40XU).

** MEM crystal structure of metallofullerenes*

MEM is an excellent method of structure analysis to locate the metal atoms in the fullerene framework .The systematic use of MEM in crystal structure determinations was introduced in SPring-8 and was of importance to visualize guest atoms in host –guest materials in $Sc_2@C_{66}$. This method is now applied to more complicated compounds for rational drug design (BL02B2).

* *The liquid-liquid transition in phosphorus*

The striking discovery of the phase transition in monatomic liquid (phosphorus) between the low-density and high-density states with a change of the coordination number as a function of pressure. SR X-rays at SPring-8 played a major role in the observation of a high-contrast image and in analysis of liquid diffraction patterns (BL14B1).

** X-ray magnetic scattering experiments*

This was used to probe the coupling between spin and orbital momentum in $Sr_2IrO_4$: A large unexpected angular momentum of the 5 d electrons was observed which may induce a large electromagnetic response (BL29XU, BL46XU). The first-order phase transition in $YbInCu_4$ was successfully observed through the lattice distortion resulting from the valence transition of the Yb ion at magnetic field B=26T (T=32K) with a pulse magnet reachable to 41T synchronized with X-ray diffraction (BL22XU).

** Resonant X-ray Scattering (RXS) study on ferroelectricity in charge-frustrated* *system $LuFe_2O_4$*

The ordering of $Fe^{2+}$ and $Fe^{3+}$ on triangular lattices was distinctly observed by RXS and thus evidenced the presence of an electric polarisation consisting of distributed electrons arising from the repulsive property of electrons (electron correlations) acting on a frustrated geometry (BL02B1, BL22XU).

SPECTROSCOPY
Electronic and Magnetic Properties

** Probing bulk states of correlated electron systems by high-resolution resonance photoemission*

Selected as one of Outstanding achievements, the high-resolution photoelectron spectroscopy using much higher photon energy than conventionally employed, probed successfully the bulk nature of electronic states and demonstrated this in the 4f electron systems in weakly hybridized Ce compounds (BL25SU).

** X-ray emission spectroscopy of 5f heavy Fermion systems*

Careful experiments on $UPd_2Al_3$ have clearly shown the dual character of the f electrons going from an itinerant to a localized behaviour depending on the temperature (BL23SU).

** Phonon measurements in superconductors by meV-resolution inelastic scattering*

Forefront high-resolution inelastic scattering experiments on the phonon structures characteristic of a series of superconductors, namely $MgB_2$ and its carbon-doped compounds and boron-doped diamonds, demonstrated the significant contribution of electronic excitations and electron-phonon coupling to their superconductivity. Phonon anomalies observed in high Tc superconductors are vital benchmarks for theoretical calculations. (BL11XU, BL35XU).

** Orbital excitations in manganite by eV-resolution resonant inelastic X-ray scattering (RIXS)*

RIXS tuned near the Mn K-absorption edge in the orbitally ordered $LaMnO_3$ revealed distinct features of spectra resulting from a particle-hole excitation across the Mott gap and thus agreed well with theoretical calculations. Thus RIXS demonstrated an important tool to probe orbital dynamics (BL11XU).

** Localized magnetic moments in Au nano-particles .*

Extremely sensitive XMCD experiments evidenced localized magnetic moments on the surface of gold nano-particles. This is a forefront result which should lead to new applications in nano-sciences (BL39XU).

** d-d transition in NiO :*

High resolution accurate non-resonant meV resolved X-ray scattering clearly identified d-d transition and its fine structure in NiO (20meV scale); this is a frontier experimental result which opens a new experimental way for studying electronic correlations at the atomic scale (BL12XU).

** Supramolecular systems*

Structural transition upon mixing pDNA with a cationic micelle was rationalized using SPring-8 SAXS measurements combined with fluorescence, CD and microcalorimetry techniques (BL40B2).

*Recommendations*

** High resolution inelastic X-ray Scattering*

The proposed long beamline for non-resonant meV resolved Inelastic X-ray Scattering should be developed in the future in order to investigate atomic scale correlations in lattice and electronic excitations. This requires the construction of a new beamline which will have more than an order of magnitude higher brilliance and flux in comparison with present generation of inelastic X-ray scattering instruments in the world, and will certainly enable important higher resolution measurements, in particular electronic excitations in strongly correlated electron systems.

** Theoretical modeling*

Due to their quality, the experimental results sometimes deserve a more thorough theoretical approach, as for example the pioneering work on metallofullerenes and myoglobin. Similarly, combined with MEM, systematic use of multipolar analysis of electron density would allow better description of interatomic interactions and bonding. Also the forefront experimental description of the 5f localized / itinerant electrons and the d – d observed transitions are a challenge for the theory.

** Time resolved experiments*

The beam stability and flux of SPring-8 allow the preparation of world leading time-resolved experiments at the pico to femto second time scale; this should be the driving force of the quickly developing ultra fast physics.

** Nano single crystal and amorphous structure determinations*

The world leading measurements on the structure of 100nm $BaTiO_3$ single crystal are impressive; therefore SPring-8 scientists should pursue this work and develop tools to handle nanomaterials. New crystal structure determination methods focusing on the Atomic Probability Density Function should also be used and developed.

[Earth and Planetary Sciences]

*General Statements*

The Japanese high-pressure group has maintained the long-standing strong cooperation between facility staff and outside users since synchrotron X-rays became available in 1982 at Photon Factory, Institute of High Energy Physics (KEK). They have developed the state-of-the-art high-pressure X-ray diffraction techniques and carried out cutting-edge research cooperatively. Such a traditional cooperation has become stronger and wider at SPring-8 where the Earth and Planetary Science (EPS) Forum was established recently among researchers not only in earth and planetary sciences but also in solid state physics and environmental sciences.

*Highlights*

** High-pressure phase transitions in mantle minerals*

High brilliant synchrotron X-rays at SPring-8 incorporated with the highly-sophisticated high pressure technology such as a large multianvil-type apparatus and a laser-heated diamond anvil cell, made possible a reliable in-situ measurement under high-pressure (P) and high-temperature (T) conditions corresponding to the deep interior of the Earth. Such an excellent combination revealed a series of structural phase transitions of minerals at the upper-to-lower mantles and the mantle-to-core boundaries.

The P-T condition at the major seismic discontinuity at a 660km depth in the mantle was successfully determined as 21.1GPa at 1600C through the spinel to post-spinel transition in $Mg_2SiO_4$. (BL04B1)

As selected as one of Outstanding achievements, the crystal structure of the post-perovskite phase of $MgSiO_3$ was successfully determined under the conditions (125GPa, 2,500K) corresponding to a 2,700km depth at the mantle-core boundary where the D" seismic wave velocity discontinuity was observed. This newly-solved crystal structure has a striking high-density layered-structure. This can successfully solve the long-standing mystery of discontinuous seismic changes and seismic anisotropy in the D" layer. (BL10XU)

A stable structure of silica $SiO_2$, one of the most important oxide components not only in the Earth's crust and mantle but also in other planets, was found to be a pyrite-type above 268GPa and 1800K, denser than other known silica phases. This fact implies that it is an important constituent of the core of giant planets such as Uranus and Neptune as theoretically predicted. (BL10XU)

A combination of ultrasonic measurements and in-situ synchrotron X-ray observation (both imaging and diffraction) in a large multianvil apparatus made it possible to accurately determine the elastic wave velocity in the samples of pyrolite and piclogite under high-P/T conditions corresponding to a 660km depth where the mantle transition region (MTR) is observed. A large disagreement between the seismic data and the measured velocities leads to a possible presence of the different material at MTR which may result from the subsided oceanic plate. (BL04B1)

**** Higher-pressure generation using advanced materials***

A significant effort to develop a new hard material to be used as anvils of a high pressure apparatus is inevitable to reach higher pressure for the exploration of the interior of the Earth and other Planets. In Japan such a systematic development has been made by universities and industries. This fact in combination with the development of advanced X-ray optics, has led to high-pressure studies at SPring-8 being at the cutting-edge internationally.

One of the most striking developments is a successful synthesis of a nano-polycrystalline diamond, named "HIME-DIA", with a special capability of hardness exceeding diamond and low thermal conductivity. A high-pressure cell assembled with it has a potential to go beyond the state-of-the-art in the pressure-temperature range accessible to the center of the Earth (364GPa, 5,500K). Also it will benefit not only earth and planetary science but also other fields such as materials and environmental sciences.

***Recommendations***

The following are proposed for future directions:

* Higher P and T accessible to the center of the Earth,
* From static to dynamic experiments for earthquakes, mantle convection, plate tectonics,
* In-situ measurements (sound velocity, electrical/thermal conductivities, viscosity etc.) for chemical composition, differentiation, evolution of the Earth.

These are challenging directions to maintain the international leadership in the filed of earth and planetary sciences. We recommend that SPring-8 will support these directions by providing higher quality beams and enough infra-structures. We also hope that the newly-established Earth and Planetary Science (EPS) Forum will play an important role in creating new science and technology in this subfield.

[Environmental Science]

### *General Statements*

Environmental science program at the SPring-8 is an emergent research area. However, it holds great promise since environmental science has become a very important research field globally in the 21st century, and is also one of four main fields with high priority in Basic Program for Science and Technology determined by Japanese Government. Furthermore, synchrotron radiation has become indispensible for environmental research.

Currently, activities in this field in Japan are behind US and Europe. However, environmental science and technology is a growing field in Japan and there is great potential to attract this large research community to SPring-8.

The overall goal present at the review, namely to link atomic scale structural and chemical information to macroscopic environmental phenomena, is sound and promising. The program effectively uses the micro- XAFS and micro- XRF for speciation, in particular high energy part of the spectrum, to study the effect of toxicity of high Z elements.

### *Highlights*

There are many high quality environmental science research done at SPring-8. However due to the diverse nature of environmental science it is difficult to select a few highlights, and we will highlight only one of them; the work of phytoremediation, which is unique and interesting. There is a special plant, 'fern' which absorbs As ions selectively. By using the micro-XRF method, they studied how As ions get into the plant and found that they move up to leaves and concentrates at an edge of the leaves. This work is still in a preliminary stage, but demonstrates to show how effective micro XRF in SPring-8 works for environmental science.

*Recommendation*

To stimulate the growth of environmental science at SPring-8, additional micro- and nano- XAFS and XRF beamlines are needed. The brilliance of the source and the latest development in focusing optics technology at SPring-8 will give this program a competitive edge.

[Industrial Application]

*General Statements*

The outreach to Japanese industries by SPring-8 staff and management has clearly been a very successful endeavor. This pro-active approach has resulted in that a 20% of the General User beamtime was allocated to over 150 different companies in 2007. This level of industrial use is world-leading among the 3 third-generation hard X-ray sources (Advanced Photon Source, European Synchrotron Radiation Facility, and SPring-8), coming in at 3 to 4 times the usage levels at these other facilities. Below are several examples of industry-related research carried out at SPring-8 that takes advantage of the unique properties of the SPring-8 source.

*Highlights*

**Studies of Ceria Zirconia – a 3-Way Automotive Exhaust Catalyst*

Researchers from Toyota are advancing their understanding of Ceria Zirconia – a 3-Way automotive exhaust catalyst. Automotive three-way catalysts can simultaneously convert the three main pollutants on exhaust gases, CO, HC, and $NO_x$ to $CO_2$, $H_2O$ and $N_2$ respectively. Work at SPring-8 focused on the relationship between the compound's oxygen storage/release capacity (OSC) and its molecular structure. Extended X-ray absorption fine structure (EXAFS) measurements were made on the Ce K-edge (40.45 kev) and Zr K edge (18 keV) to understand the local structure around these atoms and to develop a clearer relationship between the OSC and the local structure. Progress has been impressive and through the end of 2006, over 30 million Toyota vehicles have been fitted with this type of exhaust catalyst. This (and other work) clearly has made an impact on Toyota as they are now in the process of constructing an insertion device beamline (BL33XU) at the SPring-8 facility.

** Development of High-Performance Exhaust-gas Catalysts*

Scientists from Daihatsu are using BL14B1 to further their understanding of so-called intelligent catalysts with the goal of developing a more durable exhaust gas catalyst. Using EXAFS, they are examining the local structure around the palladium atoms and found that precious metal ions entered and exited the ceramic crystals repeatedly, as if they had "intelligence", and the precious metal maintained their catalytic activity during the redox cycle. This information has allowed Daihatsu to achieve a substantial reduction of palladium in the automotive catalysts.

**** Interfacial Magnetism Between FM/AFM Bilayers in Magnetic Sensor Heads***

It is the goal of many hard disk drive manufacturers to reach a recording density of 1 Tb/in$^2$. With this increase in density, instabilities in the exchange coupling between the ferromagnetic (FM)/antiferromagnetic (AFM) bilayers have been observed where the magnetisation in the ferromagnetic layer has changed unexpectedly. Higher robustness is required in the fidelity of the data on hard drives and so work was performed at SPring-8 by researchers from Hitachi to better understand the mechanism of exchange coupling and control of magnetic structures at FM/AFM interfaces. Previously, the existence of pinned interfacial AFM spins had been reported but the mechanism that stabilizes this process was unclear. This work verified the existence of pinned interfacial spins in the antiferromagnetic layer.

**** Monitoring in Real-time the Electrochemical Reaction Inside a Fuel Cell***

Fuel cells have the potential to offer a clean and highly efficient energy conversion system. However more work needs to be carried out before fuel cells can become commercially viable, for example, exploring the durability and reliability of the electro-catalysts that promote the electrochemical reactions on the cells. Time-resolved *in situ* X-ray diffraction was performed at SPring-8 by researchers from NEC to help understand the electrochemical oxidation process of platinum electro-catalysts and how such oxides affect the performance of the cell. Using 30 keV X-rays, diffraction patterns were performed at 0.5 second intervals to study the time-evolution of the system. The researchers found that the surface of platinum nanoparticles was gradually transformed to amorphous-like platinum oxides. These changes in structure of the nanoparticles should correlate with the corrosion phenomena of Pt catalysts and provide a guide for improved performance in the future.

***Recommendations***

Continued outreach will be important to effectively engage the industrial community and maintain the high percentage of industrial usage. More user-friendly equipment, as well as enhanced support to data analysis, will keep industrial users coming back. Regular assessments should be made by the SPring-8 scientists and management to ensure that industry has access to the beamlines and techniques it needs to advance their technologies.

We believe it would be advantageous for SPring-8 management to require that industries provide a summary of their work at SPring-8 and how that work impacted the company. The impact could be patents, internal technical memos, prototypes, products, etc. Even proprietary users can provide such a report, albeit with less technical details. These types of data will be invaluable to assist in the evaluation of the productivity/impact to society of this program.

### *4. Relationship to society, especially Educational Program*

It is important for a facility like SPring-8, which has unique and particular capabilities and at the same time has responsibility in international communities, to have strong ties to society. To have educational programs on a steady basis is one of the most effective activities in this direction.

The Open House held every year in spring is becoming an important event in the area. In addition, there are various activities including, Science Adventure School which consist of talks and demonstrating experiments in elementary schools nearby 6 times a year, Science summer camp for high school students, Summer School for senior undergraduate and master course students. These activities will be highly acknowledged, and should be further encouraged, even though they require a lot of effort of SPring-8 staff. Not only these interactions with domestic communities, but also the international Cheiron School for graduate students, post-docs, young scientists and engineers in the Asia-Oceania region, which started in 2007, will have important implications in years to come on the international scene.

# Appendix

## 1. Members of committee

Prof. Hidetoshi Fukuyama（Tokyo University of Science, Japan）（Chair）

Prof. Gerhard Materlik (Diamond Light Source, UK) (Co-Chair)

Dr. Chi-Chang Kao (BNL, USA)

Prof. Janos Kirz（Advanced Light Source, USA）

Prof. Sine Larsen (ESRF, France)

Dr. D. M. Mills (APS, Argonne National Laboratory, USA)

Prof. Claude Lecomte (Nancy University, France)

Prof. Judith A. K. Howard (Durham University, England)

Prof. Toshiaki Ohta (Ritsumeikan University, Japan)

Dr. Yasuhiko Fujii (Japan Atomic Energy Agency, Japan)

Prof. Kenji Suzuki (Tohoku University, Japan)

Prof. So Iwata (Imperial College London, England)

## 2. Agenda of the committee meeting

**Welcome Dinner (Sunday, November 16)**

| | |
|---|---|
| 18:00 | Welcome Dinner at SPring-8 |
| 20:00 | Brief Meeting (Closed) |

**Day 1 (Monday, November 17)**

08:00 - 08:45 Breakfast Meeting

Session 1: **Opening**

| | | |
|---|---|---|
| 09:00 - 09:10 | Welcome Address | A. Kira / Director General, JASRI |
| 09:10 - 09:20 | Opening Remarks | H. Fukuyama / Chair of SPARC |
| 09:20 - 09:50 | General Introduction | H. Ohno / JASRI |

Session 2: **Instrumentation and Methodology**

| | | |
|---|---|---|
| 10:00 - 10:30 | Overview | SPring-8's Impacts on Synchrotron Radiation Instrumentation<br>T. Ishikawa / RIKEN SPring-8 Center |
| 10:30 - 10:40 | Q&A | |

***** Coffee Break (10:40 - 11:00) *****

Session 3: **Life Science (Structural Biology)**

| | | |
|---|---|---|
| 11:00 - 11:30 | Overview | Structural Biology at SPring-8<br>T. Kumasaka / JASRI |
| 11:30 - 11:40 | Q&A | |
| 11:40 - 12:00 | Topics 1 | Model to Real Target: Lipid Structural Biology as an Applied Science<br>M. Miyano / RIKEN SPring-8 Center |
| 12:00 - 12:05 | Q&A | |
| 12:05 - 12:25 | Topics 2 | Structure of a Biological Macromolecular Nanomachine, the Bacterial Flagellum<br>K. Imada / Osaka University |
| 12:25 - 12:30 | Q&A | |

***** Lunch (12:40 - 14:00) *****

Session 4: **Life Science (Medical Biology)**

| | | |
|---|---|---|
| 14:10 - 14:40 | Overview | Imaging and Diffraction Studies in Medical and Biological |

| | | |
|---|---|---|
| | | Sciences<br>N. Yagi / JASRI |
| 14:40 - 14:50 | Q&A | |

Session 5: **Chemical Science**

| | | |
|---|---|---|
| 14:50 - 15:20 | Overview | Structural Chemistry in Synchrotron Radiation Science & Technology<br>M. Takata / JASRI ・ RIKEN SPring-8 Center |
| 15:20 - 15:30 | Q&A | |
| 15:30 - 15:50 | Topics 1 | Chemistry of Nanoporous Materials<br>S. Kitagawa / Kyoto University |
| 15:50 - 15:55 | Q&A | |

***** Coffee Break (16:00 - 16:20) *****

| | | |
|---|---|---|
| 16:20 - 16:40 | Topics 2 | In-Situ Time-Resolved Dynamic Surface Events on the Pt/C Cathode in a Fuel Cell under the Operating Conditions<br>Y. Iwasawa / The University of Tokyo |
| 16:40 - 16:45 | Q&A | |
| 16:45 - 17:05 | Topics 3 | Soft X-ray Photochemistry at BL27SU<br>K. Ueda / Tohoku University |
| 17:05 - 17:10 | Q&A | |

Session 6: **Closed Session**

| | |
|---|---|
| 17:10 - 18:00 | Discussion |

***** Dinner (18:30 - 20:00) *****

| | |
|---|---|
| 20:30 - 22:00 | Discussion |

**Day 2 (Tuesday, November 18)**

Session 7: **Materials Science (Structure)**

| | | |
|---|---|---|
| 09:00 - 09:30 | Overview | Structural Materials Science Research<br>M. Takata / JASRI・RIKEN SPring-8 Center |
| 09:30 - 09:40 | Q&A | |
| 09:40 - 10:00 | Topics 1 | Structural Studies by Powder Diffraction at SPring-8<br>E. Nishibori / Nagoya University |
| 10:00 - 10:05 | Q&A | |
| 10:05 - 10:25 | Topics 2 | Structure Science of Strongly-Correlated Electron Systems<br>T. Arima / Tohoku University・RIKEN SPring-8 Center |
| 10:25 - 10:30 | Q&A | |
| 10:30 - 10:50 | Topics 3 | Recent Progress in Polymer Science at SPring-8<br>A. Takahara / Kyushu University |
| 10:50 - 10:55 | Q&A | |

***** Coffee Break (10:55 - 11:15) *****

Session 8: **Materials Science (Electronic and Magnetic Properties)**

| | | |
|---|---|---|
| 11:15 - 11:45 | Overview | Spectroscopy for Investigating Properties and Functions in Materials Science<br>J. Mizuki / Japan Atomic Energy Agency |
| 11:45 - 11:55 | Q&A | |
| 11:55 - 12:15 | Topics 1 | High Resolution Inelastic X-ray Scattering<br>A. Baron / JASRI・RIKEN SPring-8 Center |
| 12:15 - 12:20 | Q&A | |

***** Lunch (12:30 - 13:30) *****

| | | |
|---|---|---|
| 13:40 - 14:00 | Topics 2 | Electronic Structure of Soft Materials by Means of Soft X-ray Emission Spectroscopy<br>S. Shin / RIKEN SPring-8 Center |
| 14:00 - 14:05 | Q&A | |
| 14:05 - 14:25 | Topics 3 | Magnetic Materials<br>M. Suzuki / JASRI |
| 14:25 - 14:30 | Q&A | |

Session 9: **Earth and Planetary Science**

| | | |
|---|---|---|
| 14:30 - 15:00 | Overview | Recent Advances in Earth and Planetary Sciences<br>T. Irifune / Ehime University |
| 15:00 - 15:10 | Q&A | |

Session 10: **Environmental Science**

| | | |
|---|---|---|
| 15:10 - 15:40 | Overview | Environmental Studies at SPring-8<br>Y. Takahashi / Hiroshima University |
| 15:40 - 15:50 | Q&A | |

Session 11: **Industrial Application**

| | | |
|---|---|---|
| 15:50 - 16:20 | Overview | Industrial Research at SPring-8<br>Y. Watanabe / JASRI |
| 16:20 - 16:30 | Q&A | |

***** Coffee Break (16:30 - 16:50) *****

Session 12: **Closed Session**

16:50 - 18:00 Discussion and Drafting

***** Dinner (18:30 - 20:00) *****

20:30 - 22:00 Discussion and Drafting (cont'd)

## Day 3 (Wednesday, November 19)

Session 13: **Closed Session**

| | | |
|---|---|---|
| 09:00 – 14:15 | Discussion and Drafting (cont'd) | |

Session 14: **Closing Session**

| | | |
|---|---|---|
| 14:15 - 14:45 | Brief Review Announcement | H. Fukuyama / Chair of SPARC |
| 14:45 – 15:00 | Reciprocal Address | N. Fujishima / Director,<br>Harima RIKEN Institute |
| 15:00 | Adjourn | |

## 3. Terms of SPARC

(1) To measure or evaluate the peak height of academic outputs.
(2) To explain their scientific values in a manner that can convince the public community.
(3) To advise on the future plans.