Special Research Projects

IMS has special research projects supported by national funds. Six projects in progress are:

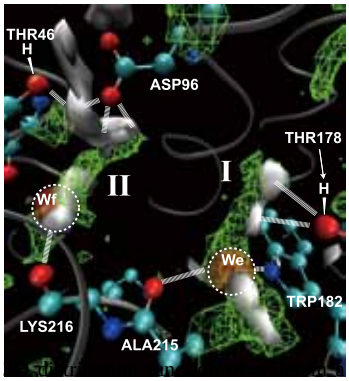
(a) The Ministry of Education, Culture, Sports, Science and Technology
HPCI Strategic Program "The Strategic Program for Innovation Research (SPIRE)"
Field 2 "New Materials and Energy Creation"
"Construction of Innovative High Performance Computing Infrastructure (HPCI)"
(b) Extreme Photonics
(c) MEXT Nanotechnology Platform Program
Platform of Molecule and Material Synthesis
(d) Inter-University Network for Efficient Utilization of Research Equipments
(e) Consortium for Photon Science and Technology (C-PhoST)
(f) Quantum Beam Technology Program

These six projects are being carried out with close collaboration between research divisions and facilities. Collaborations from outside also make important contributions. Research fellows join these projects.

(a) The Ministry of Education, Culture, Sports, Science and Technology HPCI Strategic Program "The Strategic Program for Innovation Research (SPIRE)" Field 2 "New Materials and Energy Creation" "Construction of Innovative High Performance Computing Infrastructure (HPCI)"

HPCI strategy programs "SPIRE" aims to promote scientific research using "K-computer" at RIKEN Advanced Institute for Computational Science. In the strategic filed 2 of SPIRE, the Institute for Solid State Physics (ISSP) of the University of Tokyo, Institute for Molecular Science (IMS), and Institute for Material Research (IMR) of Tohoku University were selected as strategic organizations. The project started in September 2010 for "Computational Material Science: Turning the Headwaters of Basic Science into a Torrent of Innovations in Functional Materials and Energy Conversion" as a strategic target. To promote the activities of the strategic organizations, a new community "Computational Materials Science Initiative (CMSI)" consisting of research fields of condensed matter physics, molecular science and materials science was launched.

Theoretical and Computational Chemistry Initiative (TCCI) at IMS completed the activities of the 2012 fiscal year: (1) TCCI contributed on making "Road-Map for Computational Science" to clarify the requests for post-K computers, such as computing speed, memory size, and other specifications, (2) TCCI organized the third TCCI workshop, the second symposium for communicating with experimental chemists, and the other one for industry–academic partnership, (3)TCCI also sponsored the sixteenth summer school of Molecular Simulations, 52nd Summer School of Young Molecular Scientist's Association, two TCCI winter colleges (molecular simulations, and quantum chemistry), and one workshop for massively parallel programming, and (4)Research Center for Computational Science (RCCS) provided a part of its computing resources to the SPIRE project as one of the actvities of TCCI, (5)TCCI started to promote several software developed in "Next Generation Integrated Nanoscience Simulation Software Development" project, which had been completed by the end of FY 2011, and (6) TCCI created the department for supporting "the Elements Strategy Initiative for Catalysts and Batteries (ESICB)" which started officially.



protein computed with the MC-MOZ method.

In the following years, TCCI is going to pursue the activities above and promote the research using K-computer and the computational molecular science field.

(b) Extreme Photonics

Institute for Molecular Science has a long-standing tradition of promoting spectroscopy and dynamics of molecules and molecular assemblies. Accordingly, photo-molecular science is one of the major disciplines in molecular science. This field is not confined in the traditional spectroscopy, but makes solid basis for other disciplines including nanoscience and bioscience, *etc*. Therefore, continuing developments in spectroscopy and microscopy are vital to enhance our abilities to elucidate more complex systems in time and spatial domains. In order to achieve full developments of photo-molecular science, we need to pursue three branches in developing: (1) new light source, (2) new spatio-temporally resolved spectroscopy, and (3) new methods to control atomic and molecular dynamics. Since 2005, we have started the program of "Extreme Photonics" in collaboration with the RIKEN institute. Currently 6 groups in IMS are involved in this program, and the specific research titles are as follows:

(1) Development of new light sources

TAIRA, Takunori	Micro Solid-State Photonics
FUJI, Takao	Coherent Synthesis of Femtosecond Pulses over the UV-IR Range
KATOH, Masahiro	Coherent Synchrotron Radiation

(2) Development of new spatio-temporally resolved spectroscopy

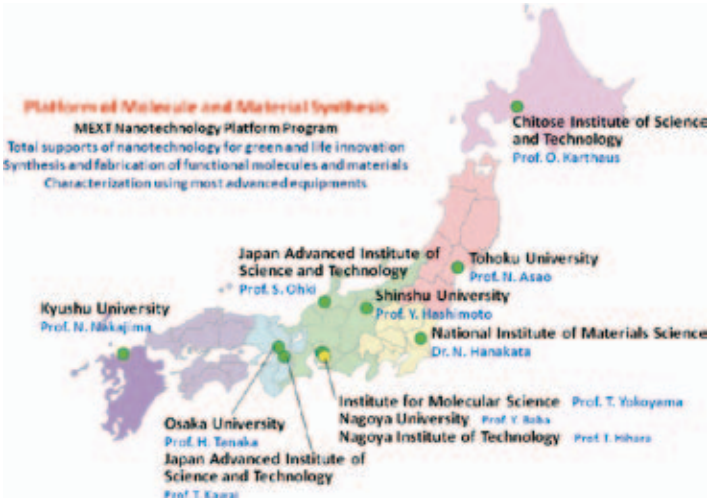
OKAMOTO, Hiromi	Development of Extreme Time-Resolved Near-Field Spectroscopy

(3) Development of new methods to control atomic and molecular dynamics

OHMORI, Kenji	Development of Attosecond Coherent Control and Its Applications
OHSHIMA, Yasuhiro	Quantum-State Manipulation of Molecular Motions by Intense Coherent Laser Pulses

(c) MEXT Nanotechnology Platform Program Platform of Molecule and Material Synthesis

Since July 2012, Nanotechnology Platform Program supported by Ministry of Education, Culture, Sports, Science and Technology has been conducted in order to promote public usage of various nanotechnology facilities. This program will continue until March 2022 and consists of three platforms of nanostructure analysis, nanoprocessing, and molecule and material synthesis, together with the management center of the platforms. Each platform constitutes of about ten organizations all over Japan. IMS conducts a representative core organization of the Molecule and Material Synthesis Platform. All the organizations in this platform are shown in Figure. In this platform, to promote green and life innovation researches using nanotechnology related techniques not only for universities and government institutes but also for private companies, we will open various kinds of our facilities with total supports including molecular synthesis, materials fabrications, characterization, data analysis and scientific discussion. We will encourage applications not only to each element, but to combined usage of several supporting elements for biotechnology and green chemistry. In IMS, the number of accepted proposals amounted 119 (excluding applications from IMS) and the total number of days used for the supports is 731.



List of Supports in IMS

Supporting Element		Responsible Persons		Charging Persons	Remarks
Platform Management		T. Yokoyama Y. Kaneko		Y. Funaki Y. Toyama	
Organization Management in IMS		T. Yokoyama			
Electron Microscopy	300kV Transmission Electron Microscopy	Y. Ohshima		M. Saito	
	Field Emission Scanning Electron Microscopy Focus Ion Beam Processing			S. Nakao	
UVSOR Synchrotron Radiation	Scanning Transmission X-Ray Microscopy	M. Katoh	N. Kosugi	T. Ohigashi	From Apr. 2013
	X-Ray Magnetic Circular Dichroism		T. Yokoyama	T. Nakagawa Y. Takagi	From Apr. 2013
Molecular Properties	Electron Spectroscopy for Chemical Analysis	Y. Ohshima	N. Kosugi	M. Sakai	
	Electron Spin Resonance		T. Nakamura	K. Furukawa M. Fujiwara	
	Superconducting Quantum Interference Device		Y. Ohshima	M. Fujiwara	From Apr. 2013
	Microscopic Raman Spectroscopy		H. Yamamoto	K. Yamamoto M. Uruichi	
	Fourier Transform Far Infrared Spectroscopy				
920 MHz NMR	Solutions	Y. Ohshima	K. Kato	T. Yamaguchi M. Nakano	800 and 600MHz NMR will be supplied in 2013
	Solids		K. Nishimura	M. Nakano	
Functional Molecular Synthesis and Molecular Device Fabrication	Organic Thin Film Solar Cells	T. Yokoyama	M. Hiramoto	T. Kaji	
	Organic Field Effect Transistors		H. Yamamoto	K. Yamamoto M. Uruichi	
	Molecular Catalysts		M. Tada		
	Functional Organic Synthesis		H. Sakurai		
	Functional Metal Complex Synthesis		T. Nagata		
	Large Scale Quantum Mechanical Calculations		M. Ehara		

(d) Inter-University Network for Efficient Utilization of Research Equipments

It is highly important to improve the supporting environment for research and education in the field of science and engineering. Nowadays, advanced research instruments are indispensable for conducting research and education in high standard. To install such sophisticated instruments, significant amount of budgets is necessary. In 2007, for constructing a national-wide network to provide the easy access to high-level equipments to researchers and students in universities all over Japan, the 5 year project “Functioning of Inter-University Network for Efficient Utilization of Chemical Research Equipments,” was launched. The network maintains an internet machine-time reservation and charging system by the help of equipment managers and accounting sections in each university. More than 50 universities all over Japan have been participating to the network. They are grouped into 12 regions and in each region the regional committee discusses and determines the operation of regional network system with the hub university chairing. There is no barrier for every user to access to any universities beyond his/her regional group. From 2009, the registered equipments are open to the researchers and students of every public and private universities. Since 2010, the project name has been changed as “Inter-University Network for Efficient Utilization of Research Equipments,” still keeping the original strategy and stable functioning. In July 2013, the number of user registrants amounts to more than 9000 in 113 universities/institutions covering more than 2000 laboratories in Japan. Usage of the network reaches to a few thousands per month since April 2010, and keeps growing in numbers.

(e) Consortium for Photon Science and Technology (C-PhoST)

In order to establish strong bases in the research and education in optical science, a new 10-year program "Photon Frontier Network" has been started in 2008 by the Ministry of Education, Culture, Sports, Science and Technology (MEXT). Consortium for Photon Science and Technology (C-PhoST) is the one of two research consortia of Photon Frontier Network. It is composed of 4 Core Organizations headed by Principal Investigators (written in parentheses): Osaka University (R. Kodama), JAEA (A. Sugiyama), Kyoto University (S. Noda) and Institute for Molecular Science (K. Ohmori). The major strength of this Consortium is the collaboration between the specialists in three fields: High power lasers, semiconductor lasers, and coherent control. Emphasis is placed in the education to foster young researchers capable of taking leaderships in scientific projects through participation to the forefront researches taking place at C-PhoST and also participation to international collaboration activities.

(f) Quantum Beam Technology Program

Quantum Beam Technology Program of MEXT/JST is aimed to develop technologies and applications of quantum beams such as photon beam, electron/positron beam, neutron beam, ion beam and so on produced by particle accelerators. This program is also aimed to train and educate young researchers and students in this research field. We proposed a development study using the UVSOR accelerators, "Light source development study using electron storage ring and laser" in collaboration with Nagoya University and Kyoto University. Graduate students of SOKENDAI and Nagoya University and a few postdoctoral fellows would be involved in this study. This proposal was approved in 2008 as a five year program.

Under the support of this program, we have developed technologies to produce coherent light beam in the terahertz and the vacuum ultra-violet ranges using the UVSOR-III electron storage ring and lasers. By injecting a laser beam into the UVSOR-III electron storage ring, a density modulation at the radiation wavelength on the electron beam circulating in the storage ring can be produced. Such an electron beam emits coherent synchrotron radiation at the wavelength and its harmonics.

We have modified the configuration of the storage ring to produce a space for this development. We have constructed a new optical klystron type undulator system and two new beam-lines to extract the terahertz light and the VUV light. We have reinforced the laser system which is synchronized with the electron acceleration. These developments and constructions were completed. Some application experiments using these coherent light beams were tested. We continue developments towards users facility.

During these five years, 5 post-doctoral fellows and 6 graduate students joined this research. Two of the students got PhD and both of them have started working in the field of quantum beam technology as researchers.

Okazaki Conference

The 72nd Okazaki Conference
Ultimate Control of Coherence

(January 8–10, 2013)

Organizers: K. Ohmori (*IMS*), Y. Ohshima (*IMS*)

Invited Oversea Lecturers: W. C. Campbell (*UCLA*), G. Pupillo (*Univ. Strasbourg*), S. Jochim (*Univ. Heidelberg*), P. Hommelhoff (*MPI, Garching*), G. Engel (*Univ. Chicago*)

The 72nd Okazaki Conference, designated as "Ultimate Control of Coherence," was held on January 8–10, 2013 at the Okazaki Conference Center. Following the celebrated tradition of the preceding Okazaki Conferences, of which origin dated back to just after the foundation of IMS, the conference focused on the topic that is emerging as a fundamental issue in the field of molecular science and related research area. This time, 20 invited lectures (including those given by 5 oversea lecturers) represented cutting-edge researches addressing the essential questions:

1) How far can we push the limit of control over quantum mechanical systems?
2) What is the possible impact of such an unprecedented control, *e.g.*, onto fundamental physics, quantum computation, and other application?
3) What is the strategy to share a unified aspect in control of coherence between diverse systems and disciplines, *e.g.*, ultracold physics and ultrafast chemistry?
4) How far can we extend the boundary for implication of coherence to complex systems?

Fifty-nine participants contributed to and enjoyed with extensive discussions on the questions.

It was to be most notable that all the oversea lecturers are still in the age of thirties yet have already made outstanding achievements in the field of research. The abroad frameworks that enable to foster such young bright "stars" will be a good model for improving the Japanese research community. It was recognized by most of the precipitants that the conference was unique as promoting concentrated discussions on creation, observation, and manipulation of coherence in the diverged research areas, and it surely provided us a unified concept that overpasses the various disciplines. At the conference dinner held in the Okazaki New Grand Hotel, many addressed a notion that new friendship among people working in diverse fields will be the driving force to lead to innovative researches. We are very much confident that the present conference was the platform to ignite such friendship.

Joint Studies Programs

As one of the important functions of an inter-university research institute, IMS facilitates joint studies programs for which funds are available to cover the costs of research expenses as well as the travel and accommodation expenses of individuals. Proposals from domestic scientists are reviewed and selected by an interuniversity committee.

(1) Special Projects

A. Development of Polarized Quantum Beam Sources and their Applications to Molecular Science

KATOH, Masahiro *(IMS)*
KOBAYASHI, Kensei (*Yokohama Natl. Univ.*)
YAMAMOTO, Naoto (*Nagoya Univ.*)
SODA, Kazuo (*Nagoya Univ.*)
AKITSU, Takashiro (*Tokyo Univ. Sci.*)
KIMURA, Shin-ichi *(IMS)*

By using particle accelerator technologies, polarized quantum beams of various kinds can be produced. At the UVSOR facility, circular polarized coherent synchrotron radiation ranging from visible to deep UV can be produced by using resonator free electron laser.[1)] We have demonstrated that such polarized radiation is a powerful tool for molecular science.[2,3)] In this joint study program, we are developing techniques to produce polarized quantum beams of various kinds and explore their applications.

It was successfully demonstrated at UVSOR to produce circular VUV light beam by using a technique called Coherent Harmonic Generation (CHG).[4)] Towards higher intensity, a new undulator system called optical klystron was developed and installed in the ring. The generation of CHG was already confirmed. The ordinary undulator radiation itself is also useful for experiments that requires wide tunability of the wavelength from UV to VUV but does not require very high intensity. Some experiments utilizing these polarized lights have started.

It was also successfully demonstrated at UVSOR to produce a polarized gamma-ray source by using a technique called Laser Compton Scattering (LCS). Laser photons are injected to the electron beam and are scattered off, and they are converted to gamma-rays via inverse Compton scattering process.[5)] The polarity of the gamma-rays can be changed by changing that of the laser photons. The possible applications are now being explored.

In Nagoya University, a polarized electron source has been developed based on an electron gun technology using GaAs photocathode. The spin polarization higher than 90% has been demonstrated.[6)] In collaboration with Nagoya University, a spin polarized electron source is now under commissioning at UVSOR. Some experiments on bio-molecular science and on inverse photoelectron spectroscopy are under preparation.

Figure 1. Spin polarized electron gun under commissioning at UVSOR.

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2) J. Takahashi, H. Shinojima, M. Seyama, Y. Ueno, T. Kaneko, K. Kobayashi, H. Mita, M. Adachi, M. Hosaka and M. Katoh, *Int. J. Mol. Sci.* **10**, 3044–3064 (2009).
3) T. Nakagawa, T. Yokoyama, M. Hosaka and M. Katoh, *Rev. Sci. Instrum.* **78**, 023907 (2007).
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6) N. Yamamoto, X. G. Jin, A. Mano, T. Ujihara, Y. Takeda, S. Okumi, T. Nakanishi, T. Yasue, T. Koshikawa, T. Ohshima, T. Saka and H. Horinaka, *J. Phys.: Conf. Series* **298**, 012017 (2011).

B. Development of Wavelength Selective Organic Solar Cells

TANAKA, Motohiko (*Chubu Univ.*)
HIRAMOTO, Masahiro (*IMS*)
SATO, Motoyasu (*Chubu Univ.*)
MIYAMOTO, Jun-ichi (*Chubu Univ.*)
KATO, Akira (*Chubu Univ.*)
KAJI, Toshihiko (*IMS*)

Silicon solar cell shades the vast area of lands eliminating the plants. The present project aims at new solar cell system symbiotic with plants, *i.e.*, agriculture (Figure 1). In this system, green-yellow wavelength region for which the photosynthesis of plants does not use is selected by the diffraction grating and focused to the array of several tens microns-wide stripe-type organic solar cells (OSC). Thus, total system has transparent characteristics for plants.

Three research elements are required to construct the present system. (1) Development of wavelength selective (green-yellow region) OSC. (2) Optimization of arrangement of solar cell devices having branch structure similar to the plants. (3) Development of the photocurrent extraction system with a small loss from circuit network connecting the vast number of cells. Research elements (1) and (3) relating to development of OSC and trial manufacture of circuit connecting many OSCs are studied by the present special project.

Trial manufacture of circuit connecting many OSCs is now in progress. Since each cell can generate only small photovoltage and output power is strongly dependent on the irradiated solar light conditions which are easily changed in the system structure (Figure 1), power loss is very large in the simply connected circuit. To overcome this problem, new type of circuit of theoretically zero loss, which utilizes flash memory, is now under designing based on the photovoltaic characteristics of OSC fabricated in IMS (Hiramoto G).

Next year, in order to utilize the green-yellow light, the system combining the micro diffraction grating array with stripe-type OSCs will be designed. On the other hand, OSC which selectively absorbs only green-yellow solar light will be developed.

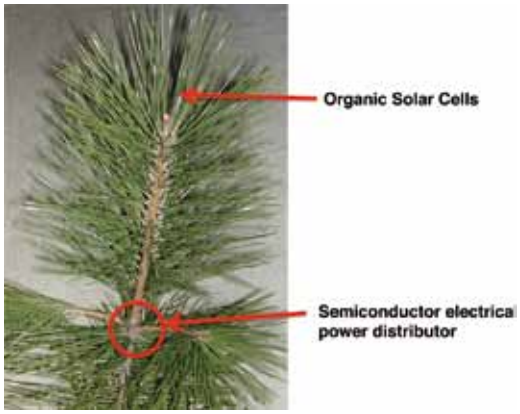

Figure 1. Concept of new plant-like organic solar cell system symbiotic with plants. A vast number of stripe-type organic solar cells only absorb green-yellow wavelength region was connected. Semiconductor power distributor extracts and a small photocurrent from each cell elements and accumulates the electricity. This system has transparent characteristics for the photosynthesis, namely, symbiotic with of natural plants and agriculture.

(2) Research Symposia

(From Oct. 2012 to Sep. 2013)

Dates	Theme	Chair
Oct. 11–12, 2012	Novel Light Generation and Materials Science —Development of Precise Measurement and Manipulation	**ASHIDA, Masaaki** **KATOH, Masahiro**
Nov. 24–26, 2012	Workshop of Quantum Dynamics and Quantum Walks	**SHIKANO, Yutaka** **SEGAWA, Etsuo**
Jan. 10–11, 2013	Prospects for Bio-Meterial Science	**KATO, Reizo** **FUJII, Hiroshi**
Jan. 17–19, 2013	The Present and the Future of Inorganic Chemistry: New Fields of Science Pioneered by Young Scientists	**KITAGAWA, Susumu** **MASAOKA, Shigeyuki**
Jan. 18–21, 2013	The 6-th Japan-China Joint Symposium on Functional Supramolecular Architectures	**MAEDA, Hiromitsu** **JIANG, Donglin**
Feb. 5– 6, 2013	The Frontiers and Perspective of Biological Coordination Chemistry	**AONO, Shigetoshi** **HAYASHI, Takashi** **ITOH, Shinobu**

Feb. 12–13, 2013	Advanced Laser Spectroscopy for Expanding Molecular Science	**OHSHIMA, Yasuhiro**
Mar. 13–14, 2013	Functions of Metal Complexes Derived from Novel Structural Changes	**MURAHASHI, Tetsuro**
Apr. 4– 6, 2013	Fundamentals and Applications of Laser Filaments	**TERASAKI, Akira** **WÖSTE, Ludger** **FUJI, Takao**
May. 25–26, 2013	Hierarchical Molecular Dynamics: From Ultrafast Spectroscopy to Single Molecule Measurements	**TAHARA, Tahei** **SAITO, Shinji**
Jun. 13–15, 2013	Japan-China Joint Coordination Chemistry Symposium for Young Scientists on Advanced Coordination Materials	**UENO, Takafumi** **MURAHASHI, Tetsuro**
Aug. 2– 4, 2013	IMS Workshop on Advanced Spectroscopy of Correlated Materials (ASCM 13)	**MIYAZAKI, Hidetoshi** **KIMURA, Shin-ichi**

(3) Numbers of Joint Studies Programs

Categories		Oct. 2012–Mar. 2013	Apr. 2013–Sep. 2013	Total
Special Projects		0	2	2
Research Symposia		8	4	12
Research Symposia for Young Researchers		0	1	1
Cooperative Research		72	32	104
Use of Facility	Instrument Center	47	14	61
	Equipment Development Center	9	4	13
Use of UVSOR Facility		80	71	151
Use of Facility Program of the Computer Center				190*

* from April 2012 to March 2013

Collaboration Programs

(a) International Inter-Institutional Collaboration Program

We have several inter-institutional collaboration programs in molecular science with leading universities and institutes in foreign countries as follows:

Institution	Period	Main Programs
Institute of Chemistry Chinese Academy of Sciences (ICCAS)	2013. 9–2018. 9	IMS Asian CORE Program
Korea Advanced Institute of Science and Technology (KAIST)	2012. 9–2016. 9	IMS Asian CORE Program
Institute of Atomic and Molecular Sciences (IAMS), Taiwan	2011. 2–2014. 2	IMS Asian CORE Program
Freie Universität Berlin (FUB), Germany	2013. 7–2016. 7	International Collaboration Programs
École Nationale Supérieure de Chimie de Paris (ENSCP)	2009.10–2014.10	IMS-IIP-L
The Korean Chemical Society, Physical Chemistry Division	2010.11–2014.11	Workshop
Indian Association for the Cultivation of Science (IACS)	2013. 3–2017. 3	IMS-IIP
Joint Institute for Laboratory Astrophysics, Colorado (JILA)	2008.10–2013.10	International Collaboration Programs

(b) IMS-Asian Core Program “Molecular Science in East Asian Region toward Post-Nano-Science”

In 2006, Institute for Molecular Science (IMS) started Asian Core Program on “Frontiers of material, photo- and theoretical molecular sciences” (2006–2011). This program, which was sponsored by Japan Society for the Promotion of Science (JSPS), aimed to develop a new frontier in the molecular sciences and to foster the next generation of leading researchers through the collaboration and exchange among IMS and core Asian institutions: Institute of Chemistry, Chinese Academy of Science (ICCAS, China); The College of Natural Science, Korea Advanced Institute of Science and Technology (KAIST, Korea); and Institute of Atomic and Molecular Sciences, Academia Sinica (AIMS, Taiwan). After this JSPS Asian Core Program was successfully completed in March 2011, we have launched IMS Asian Core Program on “Molecular Science in East Asian Region toward Post-Nano-Science” to further promote collaborations with these four key institutes. Within the framework of this IMS Asian Core Program, an educational program, Asian Winter School, with three key institutes are planned within JFY 2013. In addition, several international seminars and collaborations which were spun off from the previous JSPS Asian Core Program are also in progress within the frame work of IMS International Collaboration and so on.

(c) Exchange Program for East Asian Young Researchers “Improvement of Fundamental Research Base for Environmental and Energy Problems”

At the Second East Asia Summit (EAS), held in January 2007, Mr. Shinzo Abe, Prime Minister of Japan, announced a plan to invite about 6,000 young people to Japan mainly from the EAS member states every year for the next five years. Based on this plan, the Government of Japan has launched the Japan-East Asia Network of Exchange for Students and Youths (JENESYS) Programme, under which it is conducting a variety of exchange activities. As a part of the JENESYS Programme, the Japan Society for the Promotion of Science (JSPS) and Japan Student Services Organization (JASSO) have launched the “Exchange Program for East Asian Young Researchers.” Aimed at promoting researcher exchanges with East Asian

countries, this program supports initiatives by Japanese universities and research institutions to invite young researchers (JSPS) and graduate students (JASSO) from those countries. By supporting exchange programs implemented by Japanese universities and research institutions, the “Exchange Program for East Asian Young Researchers” works to establish and expand networks with researchers mainly from Asian countries. It also helps to develop high-caliber human resources and to create a regional science and technology community. IMS is a center of the basic research of physical/chemistry fields in Japan and has a role for the center of both domestic and international collaboration. From 2008, IMS has organized the JENESYS program for chemistry/physics fields. IMS provides the opportunity for young researchers from Asian countries to stay in the laboratories related to the basic research for environmental and energy problem. Through the experience, we encourage them to continue the basic research in their own countries as well as to build up the future collaboration. IMS welcomed totally 15 young researchers in 2012 season from Thailand, Indonesia, Malaysia, Vietnam, Philippines, and India.