# **Special Research Projects**

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

- (a) Next Generation Integrated Nanoscience Simulation Software Development & Application of Advanced High-Performance Supercomputer Project
- (b) The Ministry of Education, Culture, Sports, Science and Technology "Construction of Innovative High Performance Computing Infrastructure (HPCI)" HPCI Strategy Program Field 2 "—New Materials and Energy Creation—"
- (c) Extreme Photonics
- (d) MEXT Nanotechnology Network Program and Nanotechnology Platform Program Platform of Molecule and Material Synthesis
- (e) Inter-University Network for Efficient Utilization of Research Equipments
- (f) Consortium for Photon Science and Technology (C-PhoST)
- (g) Quantum Beam Technology Program

These seven 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.

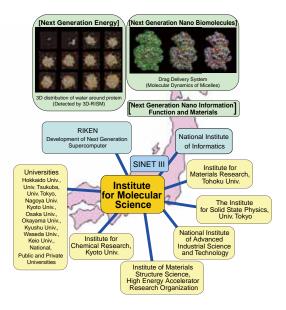
### (a) Next Generation Integrated Nanoscience Simulation Software Development & Application of Advanced High-Performance Supercomputer Project

A national project entitled, "Next Generation Integrated Nanoscience Simulation Software" was initiated on April 1, 2006 at Institute for Molecular Science (IMS). The project was a part of the "Development & Application of Advanced High-Performance Supercomputer Project" of MEXT, which aimed to develop a next generation supercomputer and application software to meet the need in the computational science nation-wide.

The primary mission of our project was to resolve following three fundamental problems in the field of nanoscience, all of which were crucial to support society's future scientific and technological demands: (1) "Next Generation Energy" (*e.g.*, effective utilization of the solar energy), (2) "Next Generation Nano Biomolecules" (*e.g.*, scientific contributions toward overcoming obstinate diseases), and (3), "Next Generation Nano Information Function and Materials" (*e.g.*, molecular devices). In these fields, new computational methodologies and programs were to be developed to clarify the properties of nanoscale substances such as catalysts (enzymes), bio-materials, molecular devises, and so forth, by making the best use of the next generation supercomputer.

Among many application programs developed in the project, we selected six programs, three from the molecular science and three from the solid state physics, as "core applications" in the nano-science, and concentrating our effort to tune those programs to the next generation machine, Kcomputer. The programs in molecular science are concerned with molecular dynamics simulation, quantum chemistry, and statistical mechanics of liquids.

This project was completed successfully as of the end of March, 2012. 46 programs have been released to the public via Portal site for Application Software Library (PAL). Over 1800 science papers have been submitted during the project.

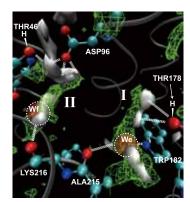


#### (b) The Ministry of Education, Culture, Sports, Science and Technology "Construction of Innovative High Performance Computing Infrastructure (HPCI)" HPCI Strategy Program Field 2 "New Materials and Energy Creation"

HPCI strategy programs aim to promote scientific research using "K-computer," the next-generation supercomputer at RIKEN Advanced Institute for Computational Science. In the strategic filed 2, 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 fiscal year 2011: (1)TCCI established its organization for research and promotion in the field of computational molecular science, (2)TCCI recruited 14 researchers and 2 professors, (3)TCCI organized the second

TCCI workshop, one symposium for interactions with experimental chemistry, and the other one for industry-academic partnership, and (4)TCCI also sponsored the fifteenth summer school of Molecular Simulations, two TCCI winter colleges (molecular simulations, and quantum chemistry), and one workshop for massively parallel programming.



3D distribution function of water in a 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.

### (c) 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:

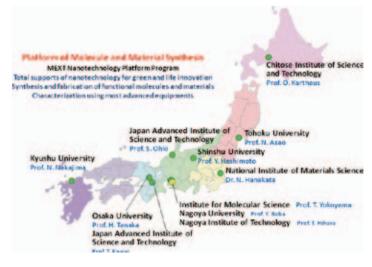
(1) Development of new light sources		
TAIRA, Takunori FUJI, Takao KATOH, Masahiro	Micro Solid-State Photonics Coherent Synthesis of Femtosecond Pulses over the UV-IR Range Coherent Synchrotron Radiation	
(2) Development of new spatio-temporally resolved spectroscopy		
OKAMOTO, Hiromi	Development of Extreme Time-Resolved Near-Field Spectroscopy	
(3) Development of new method	ds 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	

### (d) MEXT Nanotechnology Network Program and Nanotechnology Platform Program Platform of Molecule and Material Synthesis

The Nanotechnology Network Project of the Ministry of Education, Culture, Sports, Science and Technology (MEXT) was completed in March 2012. IMS participated in this project as a core organization (project leader: YOKOYAMA, Toshihiko, Prof. & Director of Research Center for Molecular Scale Nanoscience) with Nagoya University (representative: BABA, Yoshinobu, Prof.), Nagoya Institute of Technology (representative: HIHARA, Takehiko, Prof.) and Toyota Technological Institute (representative: SAKAKI, Hiroyuki, Prof. & Vice President of TTI), and established a nanotechnology support center in central Japan area in 2007–2012. In 2011 Apr.–2012 Mar., the number of accepted projects applied to IMS amounted 138 including 63 in-house applications and the total number of days is 989 including 387 days for in-house use.

In July 2012, a new program started, which is named Nanotechnology Platform Program supported by MEXT and will continue for ten years. This program has three platforms of nanostructure analysis, nanoprocessing, and molecule and material synthesis, together with the center of the platforms. Each platform consist of about ten organizations all over Japan. IMS conducts a representative organization of the platform of Molecule and Material Synthesis, and Research Center for Molecular Scale Nanoscience is a steering center of this project. All the organizations in this platform are shown in Figure.

In order to support Japanese nanotechnology researches not only for universities and government institutes but also for private companies, we will open various kinds of our equipments with total supports including data analysis. The list of the supporting elements is given in Table. We will promote applications not only to each element, but to combined usage of several supporting elements such as nanobiotechnology and green nanotechnology.



Supporting Element		Responsible Persons		Charging Persons	Remarks
Platform Management		T. Yokoyama Y. Kaneko		Y. Funaki	
Organization Management in IMS		T. Yokoyama		Y. Toyama	
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	_	M. Hiramoto	T. Kaji	
	Organic Field Effect Transistors		H. Yamamoto	K. Yamamoto M. Uruichi	
	Molecular Catalysts		M. Tada		
	Functional Organic Synthesis	T. Yokoyama	H. Sakurai		
	Functional Metal Complex Synthesis	-	T. Nagata		
	Large Scale Quantum Mechanical Calculations	-	M. Ehara		

List of Supports in IMS (Nanotechnology Platform Program)

# (e) 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 2012, the number of user registrants amounts to more than 7500 in 92 universities/institutions covering more than 1800 laboratories in Japan. Usage of the network reaches to a few thousands per month since April 2010, and keeps growing in numbers.

#### (f) 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): JAEA (R. Kodama, supported by A. Sugiyama), Osaka University (R. Kodama),

### (g) 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 been developing technologies to produce coherent light beam in the terahertz and the vacuum ultra-violet ranges using the UVSOR-II electron storage ring and lasers. By injecting a laser beam into 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 will be 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.

the UVSOR-II 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 until the end of 2011. First demonstration on producing the coherent terahertz radiation was successful. Some users experiments using these coherent light beam will be tried during the fiscal year 2012.

# Okazaki Conference

### The 71<sup>st</sup> Okazaki Conference

New Perspectives on Molecular Science of Glycoconjugates

(October 12–14, 2011)

**Organizers:** S. Wakatsuki (*KEK*), K. Kato (*IMS*), R. Kato (*KEK*), Y. Yamaguchi (*RIKEN*), T. Satoh (*Nagoya City Univ.*), Y. Kamiya (*IMS*)

Invited Overseas Speakers: M. von Itzstein (*Griffith Univ.*), K.-H. Khoo (*Academia Sinica*), J. C. Paulson (*Scripps Res. Inst.*), T. Peters (*Univ. Lübeck*), R. J. Woods (*Univ. Georgia*)

The 71<sup>st</sup> Okazaki Conference "New perspectives on molecular science of glycoconjugates" was held on October 12–14, 2011. We had 73 participants including 24 invited speakers and 18 poster presenters. The purpose of this conference was to provide a forum where researchers from various fields related to glycoscience come together and exchange their idea.

Carbohydrate chain is called "third life chain" along with nucleic acid and protein and its biological importance has been widely recognized in recent years. However, molecular science of glycoconjugates has remarkably lagged behind those of other biomolecules. This is because carbohydrate chain structures are not directly encoded in the genome and exhibit microheterogeneities along with significant degrees of freedom in internal motion. Moreover, biological functions of the carbohydrate chains are promoted through their cluster formation mediated by weak intermolecular interactions. Thus, decoding processes of *glycocodes* involves a lot of important issues that remain to be addressed in fields of molecular science.

The conference opened with an introductory lecture by Prof. Paulson (Scripps Res. Inst.), which was followed by a variety of topics delivered by researchers from different disciplines including leading glycoscientists. Every talk elicited active discussion with naïve and pertinent questions and comments, which made the conference exciting, enjoyable, and memorable, opening up the possibilities of new collaborations among the participants. Finally, we discussed perspectives on novel molecular science approaches towards understanding of the mechanisms underlying glycoconjugate functions. The conference was so successful that invited overseas speakers remarked that it was one of the best conferences they had ever participated in. We anticipated that the exciting three-day event would be a prelude to new wave of molecular science for providing atomic views of dynamic glycoconjugate functions.



The 71st Okazaki Conference "New Perspectives on Molecular Science of Glycoconjugates," October 12-14, 2011.

# **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.*) YABUTA, Hikaru (*Osaka Univ.*) 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.<sup>1)</sup> We have demonstrated that such polarized radiation is a powerful tool for molecular science.<sup>2,3)</sup> In this joint study program, we are going to develop 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).<sup>4)</sup> Towards higher intensity, a new undulator system called optical klystron was developed and installed in the ring (Figure 1). Its basic performance has been confirmed by observing the spontaneous synchrotron radiation spectra. A first CHG experiment will be done in autumn, 2012.

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.<sup>5)</sup> 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.<sup>6)</sup> In collaboration with Nagoya University, a spin polarized electron source is now under commissioning at UVSOR. The first experiment on bio-molecular science will be carried out in autumn 2012. The application in the field of inverse photoelectron spectroscopy is now under preparation.



Figure 1. Variable Polarization Optical Klystron at UVSOR-III.

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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).

# (2) Research Symposia

		(From Oct. 2011 to Sep. 2012)
Dates	Theme	Chair
Nov. 1– 2, 2011	Molecular Science for Supra-Functional Molecular Systems by Using Experimental and Theoretical Methods	SEKIYA, Hiroshi FURUTANI, Yuji
Mar. 13, 2012	Synposium for Young Inorganic Chemsts Aiming at the Innovation	MIZUTA, Tsutomu MASAOKA, Shigeyuki
Mar. 15–16, 2012	Symposium on Integral Researches toward the Next Generation of Molecular Science	MATSUMOTO, Yoshiteru FURUTANI, Yuji
Jun. 1– 2, 2012	Recent Development of Experimental and Theoretical Methodology on Liquids and Soft Matters: Basic Properties and Applications to Novel Devices	NISHIYAMA, Katsura OKUMURA, Hisashi
Jul. 30–31, 2012	New Avenue for Investigating Molecular Structure via Laser Spectroscopy and Magnetic Measurements	BABA, Masaaki OHSHIMA, Yasuhiro
Jun. 16–17, 2012	Preparatory Meeting for the 52 <sup>nd</sup> Molecular Science Summer School & the 1 <sup>st</sup> Symposium for Young Molecular Scientists	YAMAZAKI, Kaoru FURUTANI, Yuji

# (3) Numbers of Joint Studies Programs

Categories		Oct. 2011–Mar. 2012	Apr. 2012–Sep. 2012	Total
Special Projects		0	1	1
Research Symposia		3	2	5
Research Symposia for Young Researchers		0	1	1
Cooperative Research		55	51	106
Use of Facility	Instrument Center	41	51	92
	Equipment Development Center	7	7	14
Use of UVSOR Facility		78	56	134
Use of Facility Program of the Computer Center				179*

\* from April 2011 to March 2012

# **Collaboration Programs**

## (a) IMS International Program

IMS has accepted many foreign scientists and hosted numerous international conferences since its establishment and is now universally recognized as an institute that is open to foreign countries. In 2004, IMS initiated a program to further promote international collaborations. As a part of this program, IMS faculty members can (1) nominate senior foreign scientists for short-term visits, (2) invite young scientists for long-term stays, and (3) undertake visits overseas to conduct international collaborations.

Leader	Title	Partner
UOZUMI, Yasuhiro	Development of Novel Polymer-Supported Transition Metal Catalysts and Their Application to Selective Organic Transformations	Korea: HAN, Jinwook and group members
YOKOYAMA, Toshihiko	A Development of Uniaxial Magnetic Anisotropy in $Fe_{1-x}Co_x$ Films Grown on Vicinal Surfaces	Germany: PRZYBYLSKI, Marek and group members Turkey: YILDIZ, Fikret
OKAMOTO, Hiromi	Plasmon Characteristics of Hybrid Metal Nanorods	Korea: LIM, Jong Kuk and group members
TAIRA, Takunori	Study of the Coupling between Angular-Quasi-Phase- Matching, Pockels Effect and Bragg Diffraction: Application to the Modulation of Parametric Processes	France: BOULANGER, Benoît and group members
SHIGEMASA, Eiji	Deexcitation Dynamics of Core Excited States Studied by High-Resolution Electron Spectroscopy	France: SIMON, Marc and group members
KATO, Koichi	Ultra High-Field NMR Study of Post-Translational Modifications of Proteins	Korea: LEE, Weontae and group members
SAKURAI, Hidehiro	Synthesis and Properties of Functionalized Buckybowls	Germany: LENTZ, Dieter and group members Korea: KAWANO, Masaki and group members India: SASTR, G. Narahari Thailand: SOMSOOK, Ekasith and group members
KATOH, Masahiro	Beam Dynamics in Free Electron Laser Oscillator	France: BIELAWSKI, Serge and group members
JIANG, Donglin	Synthesis and Fucntions of Two-Dimensional Polymers	China: DONG, Yuping and group members
KIMURA, Shin-ichi	Optical and Photoelectrical Studies on Electronic Structure of Strongly Correlated 3d and 4f Electron Systems	Korea: KWON, Yong-Seung and group members

KOSUGI, Nobuhiro

Research and Development of Scanning Transmission X-Ray Microscopy (STXM)

Canada: HITCHCOCK, Adam P. Germany: RUEHL, Eckart U. S. A.: TYLISZCZAK, Tolek

### (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 2012. 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 2011 season from Thailand, Indonesia, Malaysia, Vietnam, Philippines, and India.

