Special Research Projects

IMS has special research projects supported by national funds. Five 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
Nanotechnology Support Project in Central Japan: Synthesis, Nanoprocessing and Advanced Instrumental Analysis

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

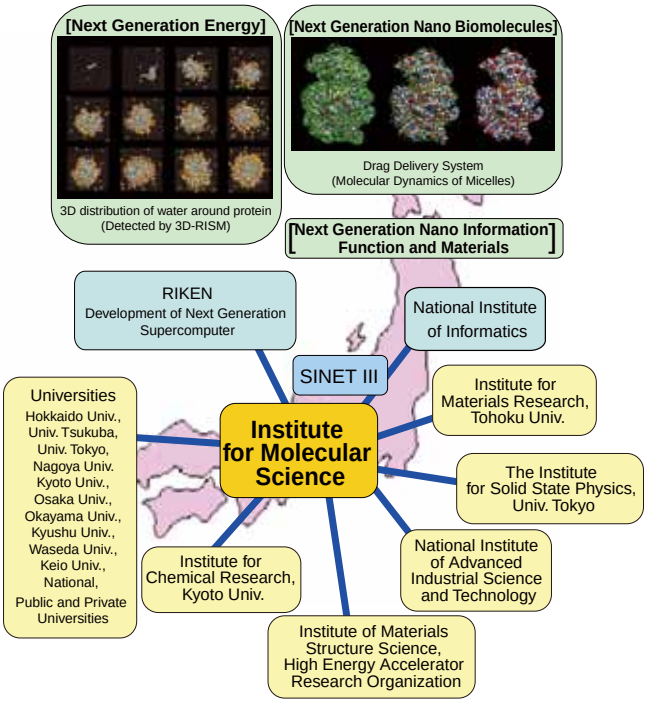
These five projects are being carried out with close collaboration between research divisions and facilities. Collaborations from outside also make important contributions. Research fellows join these projects.

(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 is a part of the "Development & Application of Advanced High-Performance Supercomputer Project" of MEXT, which aims 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 is to resolve following three fundamental problems in the field of nanoscience, all of which are 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 are to be developed to clarify the properties of nanoscale substances such as catalysts (enzymes), biomaterials, molecular devises, and so forth, by making the best use of the next generation supercomputer.

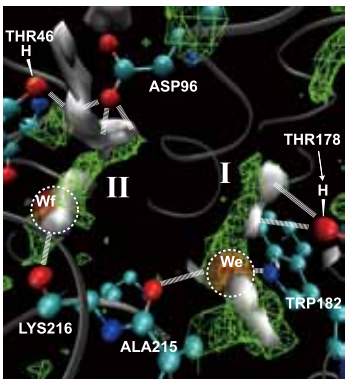
Among many application programs developed in the project, we have selected six programs, three from the molecular science and three from the solid state physics, as "core applications" in the nano-science, and concentrating our effort to tune those programs to the next generation machine. The programs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



(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.

IMS organized "Theoretical and Computational Chemistry Initiative (TCCI)" with the aim of advancing molecular science in close cooperation with the other two institutes and will conduct the activities in research promotion, research support, personnel training, and promotion of utilizing supercomputers in the related fields. The feasibility study on the program was completed in FY 2010 and the full-scale research activities have been currently performing since FY2011.



3D distribution function of water in a protein computed with the MC-MOZ method.

(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 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

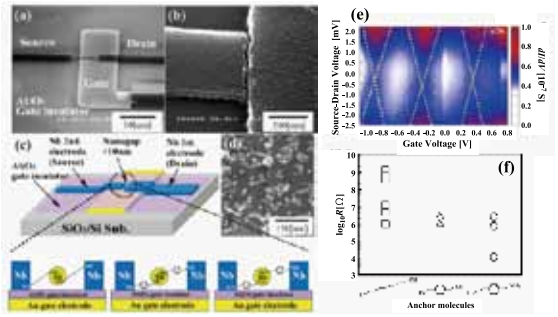
OHMORI, Kenji	Development of Attosecond Coherent Control and Its Applications
OHSHIMA, Yasuhiro	Quantum-State Manipulation of Molecular Motions by Intense Coherent Laser Pulses

(d) MEXT Nanotechnology Network
Nanotechnology Support Project in Central Japan: Synthesis, Nanoprocessing and Advanced Instrumental Analysis

The Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan started the Nanotechnology Network Project in April 2007 in order to support Japanese nanotechnology researches not only for university and government institutes but also for private companies. IMS participates 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 establishes a nanotechnology support center in central Japan area for these five years. We will support

1) Public usage of various advanced nanotechnology instruments such as ultrahigh magnetic field NMR (920 MHz), advanced transmission electron microscopes, and so forth
2) Design, synthesis and characterization of organic, inorganic and biological molecules and materials,
3) Semiconductor nanoprocessing using advanced facilities and technologies.

We will promote applications not only to each supporting element, but to combined usage of several supporting elements such as a nanobiotechnology field that is highly efficient in this joint project. In 2010 Apr.–2011 Mar., the number of accepted projects applied to IMS amounted 136 including 75 in-house applications and the total number of days is 807 including 435 days for in-house use.



Example of the recent research achievement by Y. Negishi (Osaka University) *et al.* (a) SEM image of the superconducting single-electron transistor, (b) SEM image of the nanogap electrodes before deposition of Au nanoparticles, (c) schematic views of the superconducting single-electron transistor, (d) SEM image of the nanogap electrodes after deposition of Au nanoparticles, (e) Coulomb diamond observed in the superconducting single-electron transistor, (f) Resistance of the superconducting single-electron transistor at room temperature. The transistor consists of Au nanoparticle quantum dots connected by three kinds of ligand molecules of alkanedithiol, benzenethiol and xylenediamine. From Y. Negishi, T. Iwai and M. Ide, *Chem. Commun.* **46**, 4713–4715 (2010) and T. Nishino, R. Negishi, M. Kawao, T. Nagata, H. Ozawa and K. Ishibashi, *Nanotechnology* **21**, 225301 (2010).

List of Supports in IMS

Person in Charge	Support Element
OKAMOTO, Hiromi	Space- and Time-Resolved Near-Field Microspectroscopy
YOKOYAMA, Toshihiko	Magneto-Optical Characterization of Surface Nanomagnetism
YOKOYAMA, Toshihiko	Electron Spectroscopy for Chemical Analysis
NISHI, Nobuyuki	Tunable Picosecond Raman Spectroscopy
HIRAMOTO, Masahiro	Fabrication and Characterization of Organic Semiconductor Devices
NISHI, Nobuyuki; YOKOYAMA, Toshihiko	300kV Transmission Analytical Electron Microscopy
YOKOYAMA, Toshihiko	Focus Ion Beam Processing & Field Emission Scanning Electron Microscopy
NAGAYAMA, Kuniaki	Phase Contrast Transmission Electron Microscopy for Nanobiological Materials
TADA, Mizuki	Design and Structural Analysis of Molecular Catalysts
YOKOYAMA, Toshihiko; KATO, Koichi	920 MHz NMR Spectrometer
NAGASE, Shigeru	Quantum Chemical Calculation for Molecular Design
SUZUKI, Toshiyasu; NAGATA, Toshi; SAKURAI, Hidehiro	Synthesis & Design of Functional Organic Nanomaterials

(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 2011, the number of user registrants amounts to more than 6900 in 83 universities/institutions covering more than 1500 laboratories in Japan. Usage of the network reaches to a few thousands per month in the last two fiscal years (April 2010–) and keeps growing in numbers.

Okazaki Conference

The 70th Okazaki Conference
Molecular Mechanism of Photosynthetic Energy Conversion: The Present Research and Future Prospects

(December 4–6, 2010)

Organizers: M. Sugiura (*Ehime Univ.*), T. Nagata (*IMS*), H. Ishikita (*Kyoto Univ.*), Y. Kato (*Univ. Tokyo*), H. Mino (*Nagoya Univ.*)

Invited Overseas Speakers: J. Murray (*Imperial College*), A. Boussac (*CEA Saclay*), J. Messinger (*Umea Univ.*) R. Debus (*UC Riverside*), A. Holzwarth (*Max-Planck Inst.*), E.-W. Knapp (*Free Univ. Berlin*), F. Rappaport (*Inst. Biol. Phys. Chim.*), G. Fleming (*UC Berkeley*), W. Hillier (*Aust. Natl. Univ.*)

The 70th Okazaki Conference was held on Dec. 4–6, 2010 in Okazaki Conference Center. We had about 100 participants including 25 invited speakers and 27 poster presenters. The purpose of this conference was to provide a forum where researchers from various fields related to photosynthesis come together and exchange their idea.

Photosynthesis has been the focus of interest of many researchers since the emergence of modern science. During the last two decades, remarkable progress has been made. Many of the key proteins in photosynthesis have their structures unveiled by X-ray crystallography, and also the dynamic aspects of these biomolecules are revealed by various other techniques such as ultrafast spectroscopy and magnetic resonance. On the other hand, from the view point of chemistry, we are still far from being able to reconstruct photosynthesis in our hands. Nevertheless, building up artificial photosynthetic systems on the basis of our knowledge about natural system is a worthwhile goal.

In this conference, hot debates were held on topics at the forefront of photosynthesis research, not only by the experts in the particular field, but also involving researchers from other fields. Such kind of crossover discussion should be extremely important in our deeper understanding complex systems like photosynthesis. We hope, in the near future, the new knowledge and friendship shared by the participants of this conference will lead to emergency of new approach in photosynthesis research.

The 70th Okazaki Conference "Molecular Mechanism of Photosynthetic Energy Conversion:The Present Research and Future Prospects", 4-6 Dec 2010, Okazaki, Japan.

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 (Figure 1).[1] We have demonstrated that such polarized radiation is a powerful tool for molecular science.[2,3] In this joint study program, we are going to develop techniques to produce polarized quantum beams of various kinds and explore their applications.

We are developing a technique called coherent harmonic generation to produce coherent synchrotron radiation with circular polarization in the VUV range. By using an external laser source, we can produce micro-bunching on electron bunches circulating in the storage ring. Such electron bunches can radiate coherently at the laser harmonics and we can control its polarity by using a variable polarization undualtor.[4]

We are developing a polarized gamma-ray source based on a technique called laser Compton scattering. 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 gamma-rays keep the polarity of the incident laser photons. Thus, we can control the polarity of the gamma-rays by controlling that of the laser photons. In addition, the gamma-rays are quasi-monochromatic, energy tunable and ultra-short in pulse length.

We are developing polarized electron source based on an electron gun technology, which has been developed in Nagoya University (Figure 2). By using GaAs photocathode, spin polarization higher than 90% has been demonstrated.[6] By using a laser source synchronized with the RF acceleration of the storage ring, the polarized electron pulses are synchronized in time with other quantum beams described above.

We are going to apply these unique quantum beams to biomolecular science and materials science. An interesting point is that all these quantum beam sources are synchronized. We will explore combined use of these beams.

Figure 1. UVSOR Free Electron Laser.

Figure 2. Photocathode Electron Gun to produce spin polarized electron beam.

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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).
4) M. Labat, M. Hosaka, M. Shimada, M. Katoh and M. E. Couprie, *Phys. Rev. Lett.* **101**, 164803 (2008).
5) Y. Taira, M. Adachi, H. Zen, T. Tanikawa, M. Hosaka, Y. Takashima, N. Yamamoto, K. Soda and M. Katoh, *Nucl. Instrum. Methods Phys. Res., Sect. A* **637**, 5116–5119 (2011).
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. 2010 to Sep. 2011)

Dates	Theme	Chair
Jan. 7– 8, 2011	Recent Progress and Prospects of Cluster Science and Functional Nano-Structure Science	**NISHI, Nobuyuki**
Oct. 5– 6, 2010	Surafce and Interface Chemistry for Green Innovation	**MATSUMOTO, Yoshiyasu** **YOKOYAMA, Toshihiko**
Jan. 14, 2011	Generation and Applications of Intense THz Radiation	**KIMURA, Shin-ichi**
Jan. 8– 9, 2011	Currents Status and Future Prospects of Coordination Chemistry	**TANAKA, Koji**
Mar. 1, 2011	Progress and Strategy in Physical Chemistry and Biophysical Chemistry	**KITAGAWA, Teizo** **KOSUGI, Nobuhiro**
Jun. 28–29, 2011	The 5th Symposium of Japan Society for Molecular Science	**NAKAI, Hiromi** **SAITO, Shinji**
Jul. 9, 2011	Preparatory Meeting for Molecular Science Summer School	**AKASE, Dai** **FURUTANI, Yuji**

(3) Numbers of Joint Studies Programs

Categories		Oct. 2010–Mar. 2011	Apr. 2011–Sep. 2011	Total
Special Projects		0	1	1
Research Symposia		5	1	6
Research Symposia for Young Researchers		1	0	1
Cooperative Research		63	53	116
Use of Facility	Instrument Center	32	42	74
	Equipment Development Center	5	8	13
Use of UVSOR Facility		77	61	138
Use of Facility Program of the Computer Center				171*

* from April 2010 to March 2011

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
MITSUKE, Koichiro	Observation of Long-Term Change in the Dye-Sensitized TiO_2 or ZnO Photovoltaic Electrodes by XPS, XAFS and UPS	Thailand: VAILIKHIT, Veeramol and group members
EHARA, Masahiro	Theoretical Studies on the Interaction between Antiviral Drugs and Proteins: Adamantines	Australia: ARULMOZHIRAJA, Sundaram and group members
UOZUMI, Yasuhiro	Development of Novel Polymer-Supported Transition Metal Catalysts and Their Application to Selective Organic Transformations	Korea: HAN, Jinwook and group members
TADA, Mizuki	Synthesis of New Oxide-Supported Metal Complex Catalysts	Singapore: HOR TZI SUM, Andy 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
OKUMURA, Hisashi	Generalized-Ensemble Molecular Dynamics Simulations of Peptide Aggregation	Taiwan: HU, Chin Kun and group members
SAKURAI, Hidehiro	Studies on the Metal Cluster Catalysts Directed toward the Utilization of Biomasses	Thailand: SOMSOOK, Ekasith 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
KATOH, Masahiro	Beam Dynamics in Free Electron Laser Oscillator	France: BIELAWSKI, Serge and group members
KOSUGI, Nobuhiro	Study of Weak Intermolecular Interaction by Resonant Soft X-Ray Photoelectron Spectroscopy	France: MIRON, Catalin 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
JIANG, Donglin	Studies on the Synthesis of Two-Dimensional Polymers	China: DONG, Yuping and group members
SHIGEMASA, Eiji	Deexcitation Dynamics of Core Excited States Studied by High-Resolution Electron Spectroscopy	France: SIMON, Marc and group members

(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, two joint seminars (bilateral) and one educational program, Asian Winter School, with three key institutes are planned within JFY 2011. 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 7 graduate students in 2010–2011 season by JASSO-JENESYS program from Thailand, Singapore, Malaysia, Vietnam, Philippines, and India.

After the successful three seasons of the JSPS-JENESYS Programme, IMS would like to launch a new *post*-JENESYS program named *EXODASS* (EXchange prOgram for the Development of Asian Scientific Society) Program. We opened the first season of EXODASS program in the spring semester of 2011. Although several candidates had cancelled the invitation due to the earthquake, we finally welcomed 8 young researchers/graduate students from Thailand, Singapore, and Vietnam.