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) Formation of Interdisciplinary and International Bases for Natural Sciences, NINS
"Development of New Computational Methods for Large-Scale Systems and Establishment of Advanced Simulation Center for Molecules and Materials"

(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

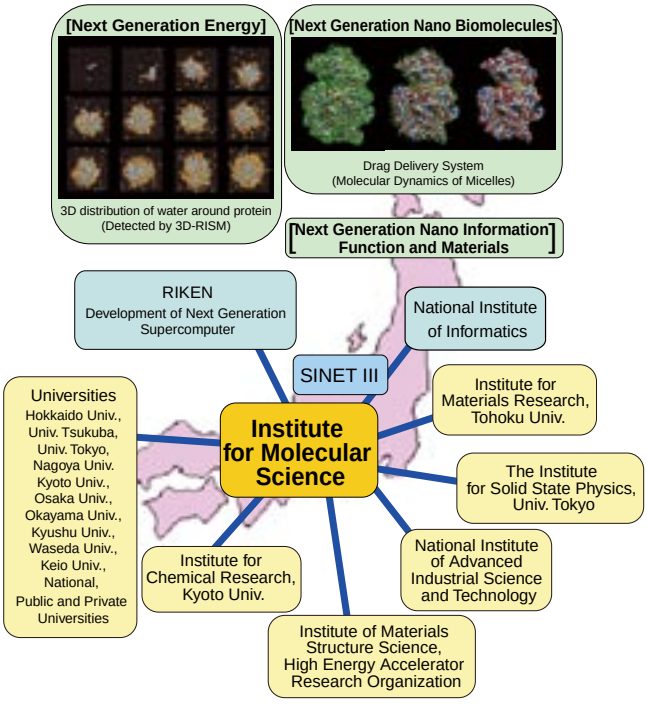
These five projects are being carried out with close collaboration between research divisions and facilities. Collaborations from outside also make important contributions. Research fellows join these projects.

(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), 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 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.

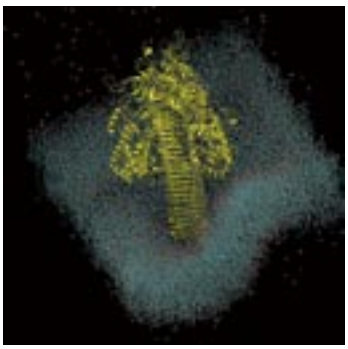


(b) Formation of Interdisciplinary and International Bases for Natural Sciences, NINS "Development of New Computational Methods for Large-Scale Systems and Establishment of Advanced Simulation Center for Molecules and Materials"

This project has aimed to develop advanced methodologies for large-scale calculations and has been organized by five institutes of the National Institutes of Natural Sciences, *i.e.* Institute for Molecular Science, National Astronomical Observatory of Japan, National Institute for Fusion Science, National Institute for Basic Biology, and National Institute for Physiological Sciences, and other universities and research institutes.

In this project, we integrated the different views and methodologies in each field that belongs to a different hierarchy of natural sciences. In addition, we developed new methodologies in their own fields. Structures and dynamics of large-scale complex systems, *e.g.* biological systems, have been investigated with a variety of sophisticated computational methods based on theories of quantum and statistical mechanics. Seminars and workshops for the development of human resources have been also conducted by this project.

The followings were the research titles of groups participating from IMS:



Massive molecular dynamics to simulate puncture of lipid bilayer by gp5.

EHARA, Masahiro	Theoretical Studies of Molecular Excited States and Chemical Reactions
HIRATA, Fumio	Theoretical Study of Molecular Recognition Based on the 3D-RISM Theory
NAGASE, Shigeru	Quantum Chemistry Calculations of Nanomolecules
NOBUSADA, Katsuyuki	Theoretical Calculations for Electron Dynamics Strongly Coupled to the Electromagnetic Field
OKUMURA, Hisashi	Development of New Algorithms for Molecular Dynamics Simulation and its Application to Biomolecular Systems
SAITO, Shinji	Theoretical Studies of Condensed Phase Dynamics by Using Molecular Simulation
YONEMITSU, Kenji	Theory for Nonequilibrium Control of Collective Dynamics in Quantum-Classical Hybrid Many-Particle Systems
YANAI, Takeshi	Theory Development for Multireference Electronic Structures with *ab initio* Quantum Chemical Methods

(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:

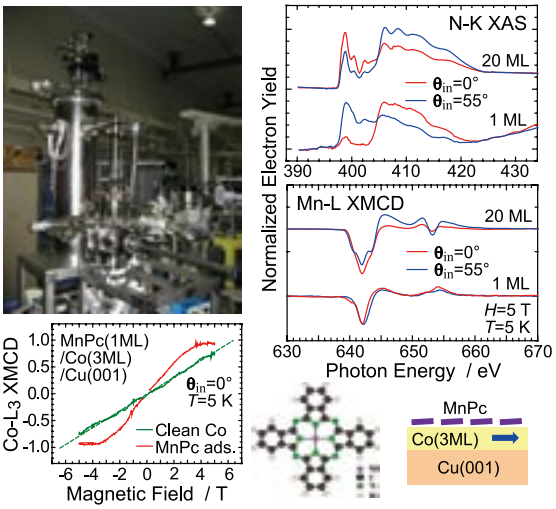
(1) Development of new light sources	
TAIRA, Takunori	Micro Solid-State Photonics
FUJI, Takao	Coherent Synthesis of Femtosecond Pulses over the UV-IR Range
KATOH, Masahiro	Coherent Synchrotron Radiation
(2) Development of new spatio-temporally resolved spectroscopy	
OKAMOTO, Hiromi	Development of Extreme 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 researchers 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 2009 Apr.–2010 Mar., the number of accepted projects applied to IMS amounted 131 including 58 in-house applications and the total number of days is 1033 including 332 days for in-house use.



A photo of the measurement system of high magnetic field (±7 T) and low temperature (5 K) X-ray magnetic circular dichroism installed at UVSOR-II and some data examples concerning a Mn-phthalocyanine molecular magnet layer on a 3-monolayer Co film grown epitaxially on a Cu(001) single crystal.

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	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

Academic and industrial activities in Chemistry in Japan have been world-leading over the past 30 years. Needless to say, it is highly important to improve the supporting environment for research and education in science and engineering. In particular, research equipments advance all the time to more intelligent and expensive ones, making measurement time shorter with higher reliability. It would be economic and efficient for the researchers and students of all national and private universities to share such equipments for performing high level research and education.

From 2007, we started the 5 year project "Functioning of Inter-University Network for Efficient Utilization of Chemical Research Equipments." This network is operated through an internet machine-time reservation and charging system by the help of equipment managers and accounting sections in each university. All the universities are grouped into 12 regions and in each region the hub university organizes the regional committee for the operation of regional network system. 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.

Although the financial condition of the government is now extremely hard, the government decided to start this project in the end of 2006. In 2007, some starting budget was appropriated for preparing the new system and we started a trial network operation with 119 equipments offered by 55 universities and IMS. In 2008 and 2009, the budget increased more than ten times and has been used for preparing a full-scale operation system of machine reservation/charging, and for repairing/upgrading of 19 and 25 instruments, respectively. In the 2009 fiscal year, the 36 advanced instruments were newly introduced into the network, such as transmission electron microscopes, high-resolution mass-spectrometers, nuclear magnetic resonance imaging systems, a surface Plasmon resonance spectrometer, high resolution nuclear magnetic resonance spectrometers for solid samples, a highly sensitive high-resolution electron spin resonance spectrometer, a highly sensitive small angle X-ray diffraction spectrometer, et al. These most advanced instruments can encourage the users in outer universities. Since 2010, the annual budget for operating this network is added into the ordinary revenue of the institute for stable functioning. For example, 25 cooperative research projects have been selected for activation of the use of the advanced instruments registered. In August 2010, the number of user registrants amounts to 6430 in 73 universities and IMS covering 1418 laboratories in Japan. Now the registered equipment increases to 336.

We believe that this innovative system can motivate and stimulate researchers and students to carry out new researches, and make chemistry research in Japan far more successful and active.

Okazaki Conference

The 69th Okazaki Conference
New Frontier in Quantum Chemical Dynamics
(February 21–23, 2010)

Organizers: S. Nanbu (*Sophia Univ.*), T. Ishida (*Kyoto Univ.*), A. D. Kondorskiy (*Lebdev Phys. Inst.*), N. Kosugi (*IMS*), K. Nobusada (*IMS*)

Invited Overseas Speakers: V. Aquilanti (*Univ. Perugia*), PKe-Li Han (*Dalian Inst. Chem. Phys.*), A. D. Kondorskiy (*Lebdev Phys. Inst.*), L. Bonnet (*Univ. Bordeaux I*), Y. Zhao (*Xiamen Univ.*), N. Doltsinis (*King's College London*)

The 69th Okazaki Conference was held on February 21–23, 2010 in Okazaki Conference Center. We had more than 100 participants including 33 invited speakers. The scope of the conference is as follows. Quantum effects play crucial roles in a variety of physical, chemical, and biological dynamics, providing specific properties and uniqueness in material and nano-scale molecular system. Since wide abilities of the modern technology to modify the objects at atomic scale, operate with different parts of proteins and DNA, controllable synthesize of complicated molecules opens an exciting perspectives to place the quantum effects in the service. In this outlook of the modern chemistry, the persistent effort of theoreticians would provide us the new insight into the future science. The purpose of the conference is that cutting-edge researchers working on molecular dynamics get together to discuss the most recent results, approaches and tendencies in the area of treating and control of the quantum effects.

Topics of the conference:

(1) Quantum Effects in Chemical Dynamics and Non-Adiabatic transition
  (a) Basic theory and semiclassical theory of non-adiabatic transition
  (b) Tunneling phenomena of many degrees of freedom
(2) Reaction (molecular) dynamics with many degrees of freedom
  (a) Quantum interference in semiclassical theory of many degrees of freedom
  (b) Ab initio MD simulations
  (c) Quantum effects in solution reactions
(3) Molecular design and control of molecular function
  (a) Control of photoreaction by laser
  (b) Molecular design including quantum effects.

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. Developments of New Methodology for the Research of Biomolecular Sensing System

URISU, Tsuneo *(IMS)*
TERO, Ryugo *(IMS)*
ASANO, Toshifumi *(SOKENDAI)*
UNO, Hidetaka *(SOKENDAI)*
WANG, Zhihong *(IMS, JST-CREST)*
TAKADA, Noriko *(IMS)*
MIZUTANI, Nobuo *(IMS)*
AOYAMA, Masaki *(IMS)*
SUZUI, Mitsukazu *(IMS)*

Investigation of signal transduction in the *in vitro* 2D neural networks using dissociated cultured neurons is valuable for understanding the cell biology of neurons and synapses and also important for development of treatment methods with intractable diseases such as neurodegenerative diseases and muscular dystrophy and related drag developments. In the previous reports, the action potential, the long-term synaptic potentiation (LTP) was induced by the stimulation using pipette patchclamp, and the corresponding excitatory post synaptic currents (EPSCs) were measured by another pipette with a whole cell arrangement. Although pipette patch clamp is an established highly reliable method of electrophysiology, it has such weak points as simultaneous multi-point measurements and long term monitoring are difficult. To overcome these weak points of pipette patch clamp, planer patch clamp has been recently proposed. Furthermore, to apply planer patch clamp method to neural cells, we have proposed and been developing incubation type planer patch clamp method. Concerning the stimulation of electrically excitable cells, photostimulation provides a versatile alternative to electrode stimulation, which has several challenges, such as difficult simultaneous multi-point measurements in intracellular electrodes and limited spatial resolution in extracellular electrodes. Laser beam stimulation has several advantages such as high spatial and time resolutions, not so strong requirement for the mechanical stability and easy simultaneous multi-point stimulations.

In this project, we have successfully developed the incubation type planer patch clamp biosensor (Figure 1) and observed the light gated ion channel current of ChR2 expressed C2C12 cells (Figure 2) using this biosensor. Furthermore, we are now developing the multi channel devices using plastic substrates. The unique structure of this device is that microfluidics are formed upper side of the substrate and the electrode structures, which correspond to the pipette of the pipette patch clamp, are formed at the lower side, and these structures are formed by the both side embossing technique. Recently we have succeeded in the cell positioning at the micropore region by the single cell manipulations (Figure 3).

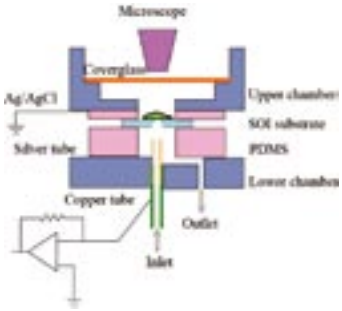


Figure 1. Schematic structure of the incubation type planer patch clamp biosensor.

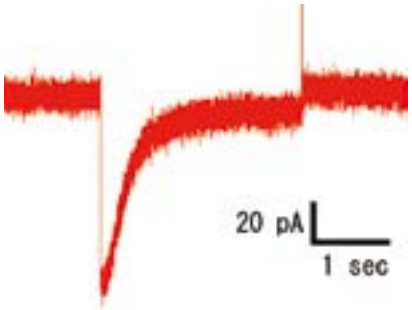


Figure 2. Observed light gated ion channel current of ChR2 expressed C2C12 cell using incubation type planer patch clamp biosensor.

Figure 3. Single cell manipulations on the microfluidic circuits. Single cell is positioned on the microfluidic area.

(2) Research Symposia

(From Oct. 2009 to Sep. 2010)

Dates	Theme	Chair
Nov. 6, 2009	Molecular Imaging for System Biology	**OZAWA, Takeaki** **URISU, Tsuneo**
Oct. 30–31, 2009	Progressive Research on Unconventional Dielectrics —Electron and Ferroelectricity—	**IKEDA, Naoshi** **ISHIHARA, Sumio** **YAKUSHI, Kyuya** **YAMAMOTO, Kaoru**
Mar. 23–24, 2010	What Can We "Learn" or "Get" from a Growing Rhodopsin Family?	**SUDO, Yuki** **FURUTANI, Yuji**
Feb. 19–20, 2010	Control of Potential Spaces in Molecular Assemblies —Approaches from Coordination Chemistry—	**CHANG, Ho-Chol** **TANAKA, Koji**
Feb. 19–20, 2010	Status and Prospects of Synchrotron Light Source Technologies	**KATOH, Masahiro**
Jun. 18–19, 2010	Plasmon-Enhanced Optical Field and Its Development into Molecular Science	**IMURA, Kohei** **OKAMOTO, Hiromi**
Jul. 2, 2010	Preparatory Meeting for Molecular Science Summer School	**OTAKI, Hiroki** **FURUTANI, Yuji**

(3) Numbers of Joint Studies Programs

Categories		Oct. 2009–Mar. 2010	Apr. 2010–Sep. 2010	Total
Special Projects		1	0	1
Research Symposia		5	1	6
Research Symposia for Young Researchers		0	1	1
Cooperative Research		59	59	118
Use of Facility	Instrument Center	34	27	61
	Equipment Development Center	4	1	5
Use of UVSOR Facility		77	63	140
Use of Facility Program of the Computer Center				171*

* from April 2009 to March 2010

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
SHIGEMASA, Eiji	Deexcitation Dynamics of Core Excited Molecules Studied by Electron Spectroscopy	France: Dr. SIMON, Marc and group members
KATOH, Masahiro	Generation of Coherent Radiation by Using Laser and Electron Beam	France: Dr. COUPRIE, Marie Emmanuelle Dr. BIELAWSKI, Serge and their group members
KIMURA, Shin-ichi	Optical and Photoelectrical Studies on the Local to Itinerant Electronic Structure of Strongly Correlated Electron Systems	Korea: Prof. KWON, Yong-Seung and group members Germany: Dr. SICHELSHMIDT, Jorg
KOSUGI, Nobuhiro	Intermolecular Interaction Revealed by Resonant Soft X-Ray Spectroscopies	Germany: Prof. RUEHL, Eckart and group members France: Dr. MIRON, Catalin and group members Korea: Prof. YEOM, Han Woong and group members
UOZUMI, Yasuhiro	Development of Novel Polymer-Supported Transition Metal Catalysts and Their Application to Selective Organic Transformations	Korea: Prof. HAN, Jin Wook and group members
SAKURAI, Hidehiro	Development of Novel Gold Cluster Catalyst Supported by Polymers	Thailand: Prof. CHAVASIRI, Warinthorn and group members
SAKURAI, Hidehiro	Design of Novel Buckybowls: An Interplay between Experiment and Theory	India: Dr. SASTRY, G. Narahari and group members
JIANG, Donglin	Studies on the Synthesis of Two-Dimensional Polymers	China: Prof. WANG, Changchun and group members
TAIRA, Takunori	Study of the Coupling between Angular-Quasi-Phase-Matching and Pockels Effect: Application to the Modulation of Parametric Processes	France: Prof. BOULANGER, Benoît Prof. SEGONDS, Patricia Prof. AKA, Gerard Philippe and their group members
YOKOYAMA, Toshihiko	A Competition between Magnetic Anisotropy and Interlayer Coupling in the Multilayer Systems of Alternating In-Plane and Perpendicular Anisotropy	Germany: Prof. PRSYBYLSKI, Marek and group members

URISU, Tsuneo	Construction of Neural Network for Molecular Signal Transduction System and Development of Molecular Science New Field	Bangladesh: Prof. RAHMAN, Mashiur
OKAMOTO, Hiromi	Studies on Electric-Field Enhancement in Self-Assembled Nanostructures of Metal Particles	Korea: Prof. JEONG, Dae Hong and group members
OHSHIMA, Yasuhiro	Excited-State Dynamics Explored by High-Resolution Laser Spectroscopy	Korea: Prof. KIM, Sang Kyu and group members

(b) Asian Core Program "Frontiers of Material, Photo- and Theoretical Molecular Sciences"

Asian Core Program is a multilateral international collaboration program carried our by JSPS (Japan Society for the Promotion of Science). It is designed to create world-class research hubs in selected fields within the Asian region, while fostering the next generation of leading researchers. The program is based on a principle of equal partnership among core institutions in Japan and other Asian countries, so that each institution is expected to secure its own matching fund. Institute for Molecular Science has launched a collaboration project "material, photo- and theoretical molecular sciences" (2006–2011) within the framework of this Asian Core Program with three key institutes in east Asian countries: Institute of Chemistry, Chinese Academy of Science (China); The College of Natural Science, Korea Advanced Institute of Science and Technology (Korea); and Institute of Atomic and Molecular Sciences, Academia Sinica (Taiwan). At present, ten joint researches are in progress, and eight joint seminars are planned within JFY 2010.

(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) has 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 (*e.g.*, master's and doctoral students and post-doctoral researchers) 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 for 14–90 days. 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 13 young researchers in 2009–2010 season from Thailand, Singapore, Malaysia, Vietnam, and India.