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.

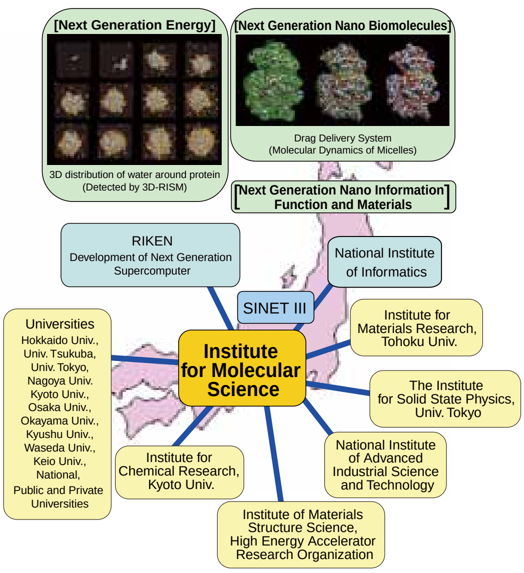
(a) Next Generation Integrated Nanoscience Simulation Software Development & Application of Advanced High-Performance Supercomputer Project

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, K-computer. The programs in molecular science are concerned with molecular dynamics simulation, quantum chemistry, and statistical mechanics of liquids.

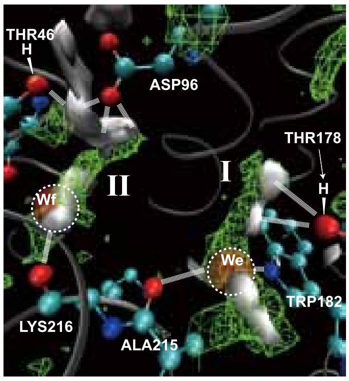
This project was completed successfully as of the end of March, 2012. 46 programs have been released to the public via Portal site for Application Software Library (PAL). Over 1800 science papers have been submitted during the project.



(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	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

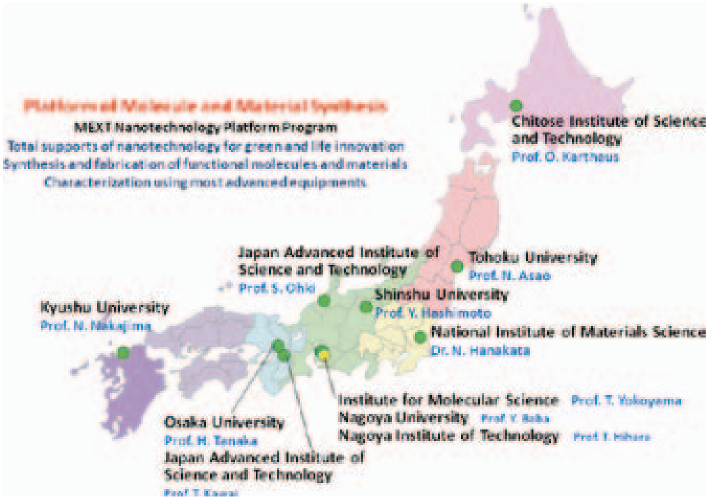
OHMORI, Kenji	Development of Attosecond Coherent Control and Its Applications
OHSHIMA, Yasuhiro	Quantum-State Manipulation of Molecular Motions by Intense Coherent Laser Pulses

(d) MEXT Nanotechnology Network 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.



List of Supports in IMS (Nanotechnology Platform Program)

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		

(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), 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.

(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 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.