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

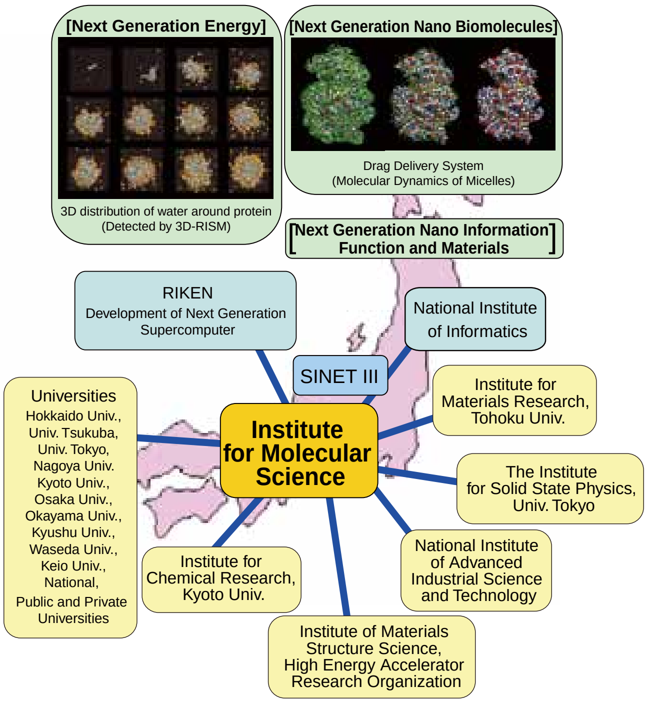
These five projects are being carried out with close collaboration between research divisions and facilities. Collaborations from outside also make important contributions. Research fellows join these projects.

(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), bio-materials, molecular devises, and so forth, by making the best use of the next generation supercomputer.

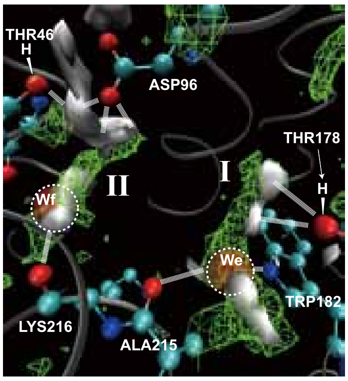
Among many application programs developed in the project, we have selected six programs, three from the molecular science and three from the solid state physics, as "core applications" in the nano-science, and concentrating our effort to tune those programs to the next generation machine. The programs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



(b) 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

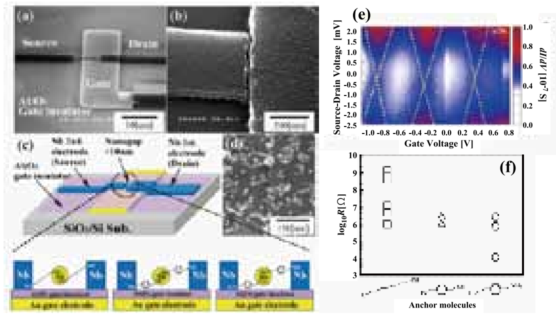
OHMORI, Kenji	Development of Attosecond Coherent Control and Its Applications
OHSHIMA, Yasuhiro	Quantum-State Manipulation of Molecular Motions by Intense Coherent Laser Pulses

(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.