SPECIAL RESEARCH PROJECTS

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

(a) —Grand Challenge in Nanoscience— 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"

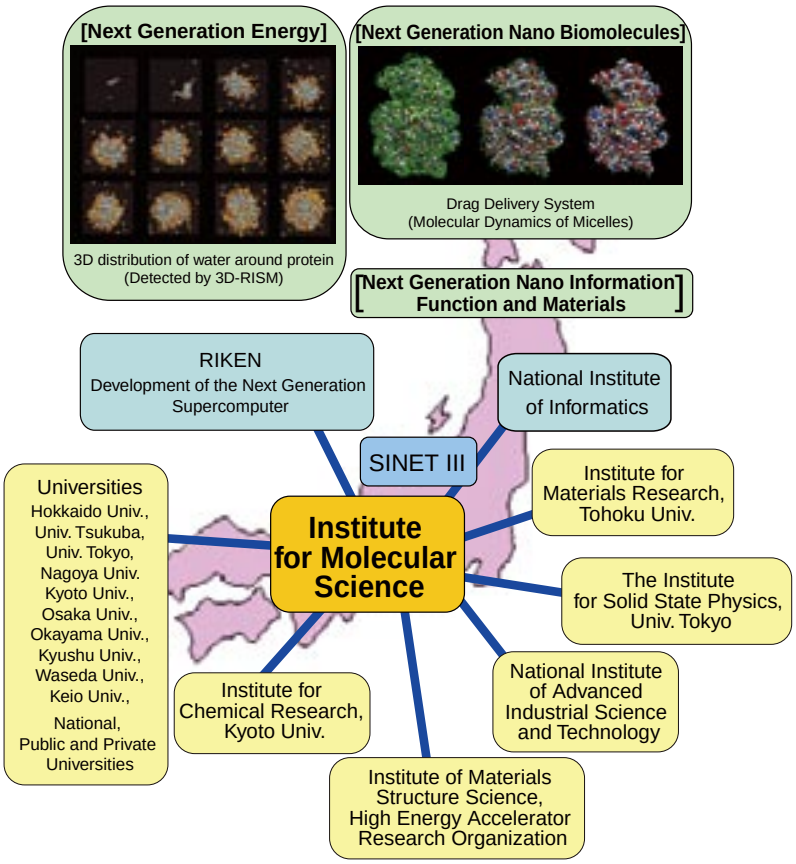
(c) Nanotechnology Support Project: Molecular Synthesis and Analysis Group

(d) Extreme Photonics

These four 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) —Grand Challenge in Nanoscience— Next Generation Integrated Nanoscience Simulation Software Development & Application of Advanced High-Performance Supercomputer Project

A national project named, "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 nation's computational science needs. The primary mission of our project is to resolve following three fundamental problems in the field of nanoscience, all of which are crucial to supporting society's future scientific and technological needs: (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.



(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 aims to establish a core computational science center for molecular and material systems and to develop advanced methodologies for large-scale calculations. The project 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. We are trying to create a new interdisciplinary field by integrating the different views and methodologies traditionally associated with each field that belongs to a different hierarchy of natural sciences. Structures and dynamics of large-scale complex systems, such as nanomaterials and biological systems, are investigated by using a variety of sophisticated computational methods based on theories of electronic structure, molecular dynamics method, statistical mechanics, and so on. The development of new computational methods utilizing parallel computation has also been furthered organizing the members having different scientific backgrounds. Seminars and workshops for the advanced calculations and for the development of human resources are also conducted by this project.

OKAZAKI, Susumu	Large-Scale Molecular Dynamics Calculations for Aqueous Solution of Amphiphilic Molecules
HIRATA, Fumio	Theoretical Study of Molecular Recognition Based on the 3D-RISM Theory
NAGASE, Shigeru	Quantum Chemistry Calculations of Nanomolecules
SAITO, Shinji	Theoretical Analyses of Condensed Phase Dynamics by Using Molecular Dynamics Simulation
YONEMITSU, Kenji	Theory for Nonequilibrium Control of Collective Dynamics in Quantum-Classical Hybrid Many-Particle Systems
MORITA, Akihiro	Theory and Computation of Interfacial Nonlinear Optical Phenomena
NOBUSADA, Katsuyuki	Theoretical Calculations for Electron Dynamics Strongly Coupled to the Electromagnetic Field

(c) Nanotechnology Support Project: Molecular Synthesis and Analysis

The Ministry of Education, Culture, Sports, Science and Technology, Japan (MEXT) started the "Nanotechnology Support Project" from 2002 for the purpose of supporting nanotechnology research initiatives. In order to effectively utilize the large facilities and specialized equipment that is required for this research, all of which are difficult for individual research organizations or projects to maintain, we provide nanotechnology researchers with the opportunity to use these facilities and equipment as well as provide the necessary technical support. We also promote the exchange of ideas and research between different fields or across boundaries, extending beyond the spheres of industry, academia and government research groups in our efforts to encourage developments within nanotechnology.

List of Supports

Preparation of Molecular Electronic Devices and Electric Conductivity Measurements	OGAWA, Takuji; URISU, Tsuneo
Automated Molecular Synthesis for Molecular Electronic Devices	OGAWA, Takuji; SUZUKI, Toshiyasu; NAGATA, Toshi; SAKURAI, Hidehiro
Space- and Time-Resolved Near-Field Microspectroscopy	OKAMOTO, Hiromi
Ultrafast and Raman Spectroscopic Measurement of Nanosystems	NISHI, Nobuyuki
Mass Spectrometric Analysis of Nanoclusters	TSUKUDA, Tastuya
MicroESCA Spectrometer	YOKOYAMA, Toshihiko
920 MHz NMR Spectrometer	UOZUMI, Yasuhiro
High Sensitive Magnetic Measurements	NISHIJO, Jun-ichi
Electron Microscopy (i) 300kV Transmission Analytical Electron Microscope, (ii) Field Emission Scanning Electron Microscope, and (iii) Focus Ion Beam System	NISHI, Nobuyuki; TSUKUDA, Tastuya
Computational Support to Molecular Design	NAGASE, Shigeru
Preparation and Characterization of Organic Electronic Devices	OGAWA, Takuji; TADA, Hirokazu

(d) 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 chemical reactions. Since 2005, we have started the program of "Extreme Photonics" in collaborating with the RIKEN institute. Currently 8 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
SARUKURA, Nobuhiko	New Coherent Vacuum Ultraviolet Light Source

(2) Development of new spatio-temporally resolved spectroscopy

OKAMOTO, Hiromi	Development of Extreme Time-Resolved Near-Field Spectroscopy
MATSUMOTO, Yoshiyasu	Development of Spatio-Temporally Resolved Spectroscopy for Surfaces and Interfaces
OZAWA, Takeaki	Developments of Luminescent Probes based on Protein Structures and Analysis System of Biological Functions

(3) Development of new methods to control chemical reactions

OHMORI, Kenji	Development of Attosecond Coherent Control and Its Applications
HISHIKAWA, Akiyoshi	Reaction Imaging and Control with Extremely Short Laser Pulses
OHSHIMA, Yasuhiro	Quantum-State Manipulation of Molecular Motions by Intense Coherent Laser Pulses