

Special Research Projects

IMS has special research projects supported by national funds. Four 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

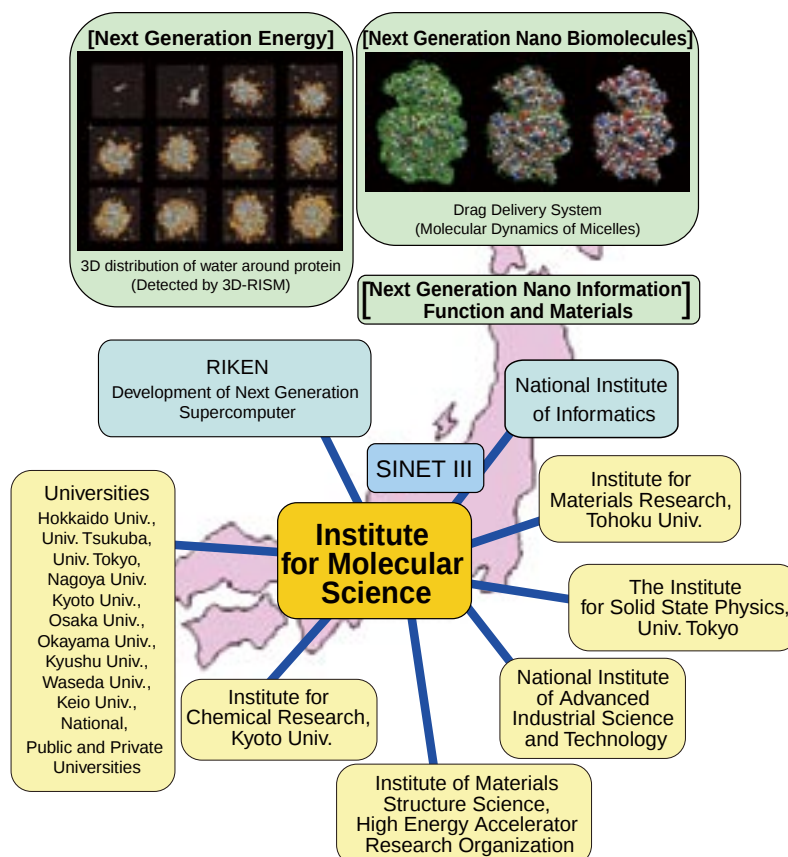
These four projects are being carried out with close collaboration between research divisions and facilities. Collaborations from outside also make important contributions. Research fellows join these projects.

(a) 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

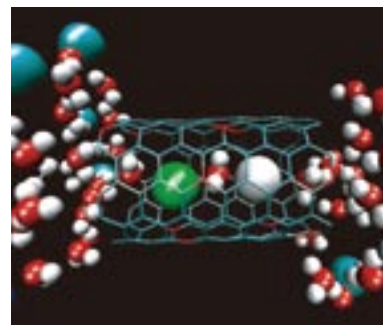
technological demands: (1) “Next Generation Energy” (*e.g.*, effective utilization of the solar energy), (2) “Next Generation Nano Biomolecules” (*e.g.*, scientific contributions toward overcoming obstinate diseases), and (3), “Next Generation Nano Information Function and Materials” (*e.g.*, molecular 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 devices, 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.



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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
NOBUSADA, Katsuyuki	Theoretical Calculations for Electron Dynamics Strongly Coupled to the Electromagnetic Field
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 <i>ab initio</i> 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 chemical reactions. Since 2005, we have started the program of “Extreme Photonics” in collaborating with the RIKEN institute. Currently 7 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

(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

(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: SUMIYAMA, Kenji, 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 2007 Apr.–2007 Spt., the number of accepted projects applied to IMS amounted 39.



300kV Transmission Electron Microscopy and Some Typical Examples.

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
NISHI, Nobuyuki	300kV Transmission Analytical Electron Microscopy
TSUKUDA, Tatsuya	Focus Ion Beam Processing & Field Emission Scanning Electron Microscopy
NAGAYAMA, Kuniaki	Phase Contrast Transmission Electron Microscopy for Nanobiological materials
UOZUMI, Yasuhiro	920 MHz NMR Spectrometer
OGAWA, Takuji	Preparation of Molecular Electronic Devices and Electric Conductivity Measurements
NAGASE, Shigeru	Quantum Chemical Calculation for Molecular Design
TSUKUDA, Tatsuya; SUZUKI, Toshiyasu; NAGATA, Toshi; SAKURAI, Hidehiro	Synthesis & Design of Functional Organic Nanomaterials