

# 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.

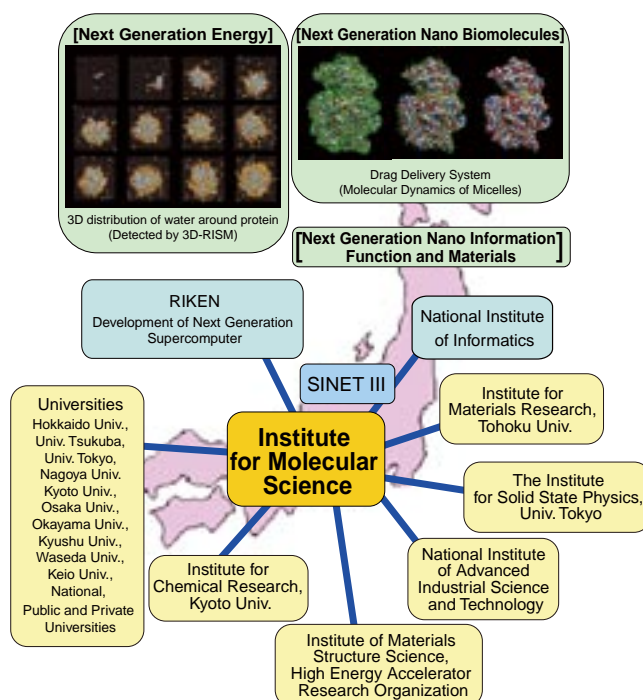
## (a) Next Generation Integrated Nanoscience Simulation Software Development & Application of Advanced High-Performance Supercomputer Project

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), biomaterials, molecular devices, 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.



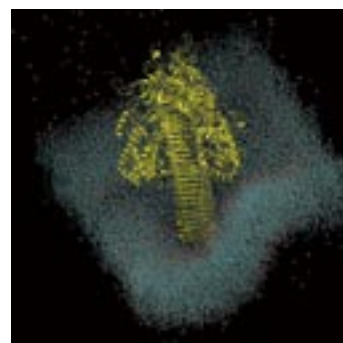
## (b) Formation of Interdisciplinary and International Bases for Natural Sciences, NINS “Development of New Computational Methods for Large-Scale Systems and Establishment of Advanced Simulation Center for Molecules and Materials”

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 <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 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
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### (3) Development of new methods to control atomic and molecular dynamics

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

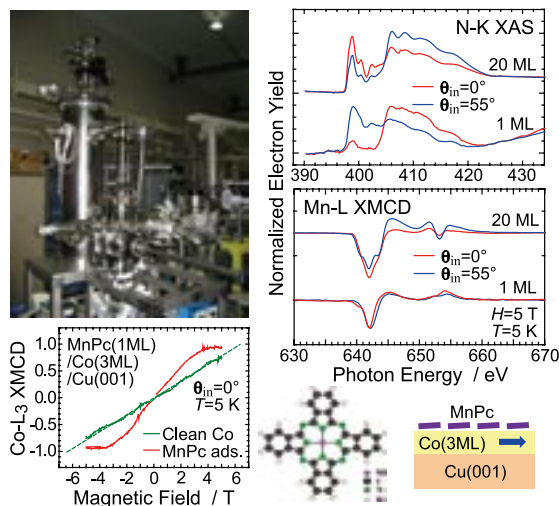
### (d) MEXT Nanotechnology Network Nanotechnology Support Project in Central Japan: Synthesis, Nanoprocessing and Advanced Instrumental Analysis

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 ( $\pm 7$  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.

