Institute for Molecular Science

annual review

2007

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

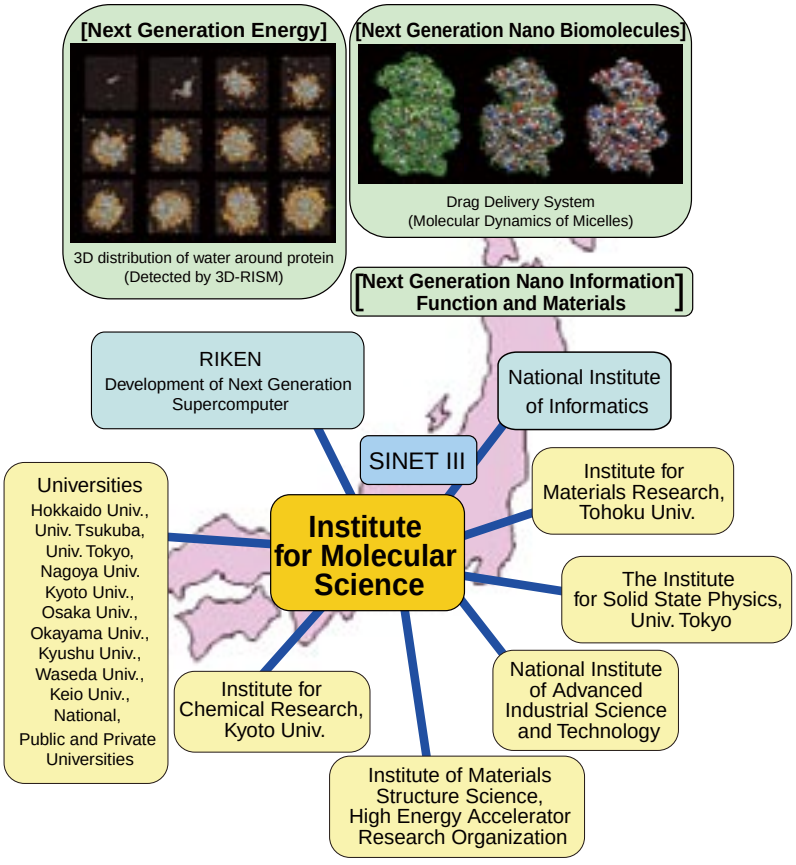
(d) MEXT Nanotechnology Network
Nanotechnology Support Project in Central Japan: Synthesis, Nanoprocessing and Advanced Instrumental Analysis

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

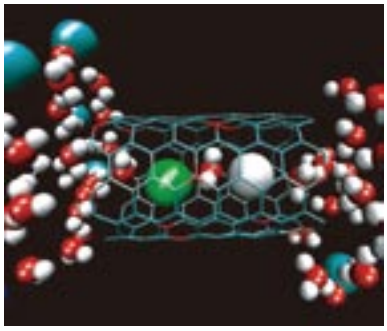
A national project entitled, "Next Generation Integrated Nanoscience Simulation Software" was initiated on April 1, 2006 at Institute for Molecular Science (IMS). The project is a part of the "Development & Application of Advanced High-Performance Supercomputer Project" of MEXT, which aims to develop 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), 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.



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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 ab initio 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

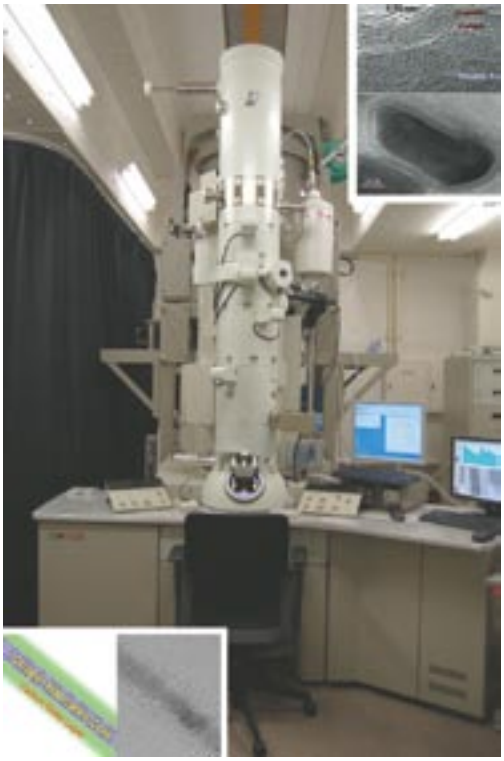
OHMORI, Kenji	Development of Attosecond Coherent Control and Its Applications
HISHIKAWA, Akiyoshi	Reaction Imaging and Control with Extremely Short Laser Pulses
OHSHIMA, Yasuhiro	Quantum-State Manipulation of Molecular Motions by Intense Coherent Laser Pulses

(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, Tastuya	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

Joint Study Programs

As one of the important functions of an inter-university research institute, IMS facilitates joint study programs for which funds are available to cover the costs of research expenses as well as the travel and accommodation expenses of individuals. Proposals from domestic scientists are reviewed and selected by an interuniversity committee.

(1) Special Projects

A. New Developments in Spin Science Using Pulsed and High-Frequency ESR

KATO, Tatsuhisa *(Josai Univ.)*
MIZOGUCHI, Kenji *(Tokyo Metropolitan Univ.)*
SAKAMOTO, Hirokazu *(Tokyo Metropolitan Univ.)*
NAKAMURA, Toshikazu *(IMS)*
FURUKAWA, Ko *(IMS)*

In order to develop advanced ESR (electron spin resonance) spectroscopy for materials science, we performed functional materials studies, both on isolated molecules and on molecular assemblies. The following two topics were investigated: 1) We determined the molecular structure of novel systems such as Gd@C_{82} and their spin interaction using ESR spectroscopy, and explored the functionality of the complicated molecule system. 2) We carried out an analysis of spin dynamics for functional molecular assemblies, including molecular conductors and magnetic materials. We searched for cooperative phenomena involved in intra-molecule freedom, and new functional physical-properties originating in molecular assemblies.

A-1 ESR Spectra of Bingel Monoadducts of Gd@C_{82}

Two kinds of Bingel monoadducts of Gd@C_{82} exhibited a sharp contrast in the ESR spectra. The reaction of La@C_{82} with diethyl bromomalonate in the presence of a base (the Bingel reaction) generated five mono-adducts. Akasaka and coworkers recently synthesized two monoadducts of Gd@C_{82}, mono-A and mono-E, at high purity. ESR spectra of the adducts were obtained using a high-field (W-band) ESR spectrometer at low temperature in solution, which showed remarkable contrast between mono-A and mono-E. The ESR spectrum of mono-A was unambiguously assigned to the spin state of S = 7/2, and that of mono-E to S = 3.

A-2 Peculiar Ground State of β"-(BEDT-TTF)-TCNQ Revealed by ESR

One of the two segregated stack isomers of (BEDT-TTF)-TCNQ (abbreviated as ET-TCNQ), β"-ET-TCNQ, has been studied. Since the unit cell of β"-ET-TCNQ has one ET and one TCNQ molecule with a charge transfer of 0.5 electrons, a quarter-filled band with strong on-site Coulomb correlation determines the electronic states.

It is known that (1) the β"-form has metallic characteristics at low temperatures with definite Fermi surfaces, (2) the charge separation within the ET layer melts away below 170 K, and (3) the 1D TCNQ stack has weak dimerization at all temperatures. However, several open questions still remain for this system, including anomalies in the electrical resistivity at 80 K and 20 K, and heat capacity anomalies at 10 K and 20 K.

Here, on the basis of ESR and ^{1}H NMR spectra, and spin susceptibility for each of the ET and TCNQ stacks deduced from the ESR g-shift, we propose a model with partial CDW nesting in ET sheets below 80 K, spin-Peierls transition at 20 K within the TCNQ 1D stacks, and the RKKY broadening of the ESR spectra of the TCNQ soliton-like spins via conduction electrons of the ET layer with a Kondo temperature of 10 K.

A-3 Spin-Dynamics Investigation by Pulsed ESR for Spin-Peierls Phases in Conventional Systems and Charge-Ordered TMTTF Salts

TMTTF-based salts undergo charge-ordering (CO) transitions in the intermediate paramagnetic states between the resistivity minimum temperature and the phase-transition temperature towards the ground state. In our previous report, the charge configuration patterns of the charge-ordering phases in the intermediate paramagnetic states were determined to be –O–o–O–o– ($4k_F$) along the stacking axes for $(TMTTF)_2MF_6$ salts (M = P, As, Sb) by ESR linewidth anisotropy analysis. However, the charge configuration of the ground state (for example, $(TMTTF)_2PF_6$ (spin-Peierls)) has not yet been clarified. Moreover, the co-existence of the CO ($4k_F$) and spin-Peierls ($2k_F$) phases seems unlikely.

To determine spin dynamics in the proximity of the spin-Peierls phase, pulsed ESR investigations were carried out for one-dimensional organic conductors, $(TMTTF)_2X$, compared to a conventional spin-Peierls system, $MEM(TCNQ)_2$. While the ESR spin-lattice relaxation rate, ESR-T_1^{-1}, of $MEM(TCNQ)_2$ shows ordinal spin-gap behavior at around the spin-Peierls phase transition temperature, T_{sP}, the ESR-T_1^{-1} of $(TMTTF)_2PF_6$ cannot be explained within the framework of simple spin-gap formation in the proximity of T_{sP}. Possible reorientation of charge configuration is likely. We discuss the electronic properties from a microscopic point of view.

B. Construction of the Research Methodology for Biomolecular Sensing System

URISU, Tsuneo *(IMS)*
TOMINAGA, Makoto *(OIIB)*
MORIGAKI, Kennichi *(AIST)*
ISOBE, Hiroko *(Univ. Tsukuba)*
ISHII, Kiyoshi *(Chubu Univ.)*

The target of this project is the development of a kind of neural cell chips as shown in Figure 1, in which a couple of cells is combined by synapse and the detection of action potential, fluorescence or FRET signal and neurotransmitter molecules.

Figure 2 is shown the first device which we have developed last year.[1)] Transient receptor potential V1 (TRPV1) transfected HEK293 cell is positioned on the micropore of the Si chip. The chip is integrated into the microfluidic circuit. Channel current triggered by capsaicin was successfully observed. The desensitization unique to the TRPV1 channel was observed.

Figure 1. Schematic image of the target neural cell chip in this project.

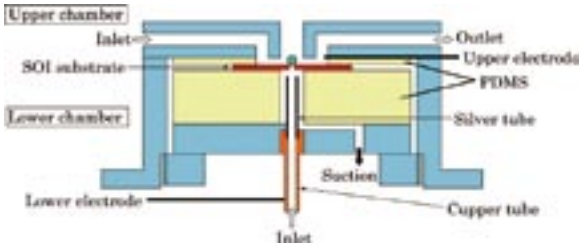


Figure 2. Planer patch clamp device fabricated in this project using Si-SOI substrate.

Reference

1) Z. L. Zhang *et al.*, *Thin Solid Film* (2007) in press.

(2) Research Symposia

(From 2006 Oct. to 2007 Sep.)

Dates	Theme	Chair
Nov. 7– 8, 2006	Approach from Interstellar and Molecular Sciences to the Origin of Homochirality	**KAWAGUCHI, Kentaro** **OHSHIMA, Yasuhiro**
Nov. 17–18, 2006	Workshop on Research for VUV Luminescence	**ITOH, Minoru** **SHIGEMASA, Eiji**
Nov. 29–30, 2006	Large-Amplitude Vibration by High-Resolution Molecular Spectroscopy	**BABA, Masaaki** **OHSHIMA, Yasuhiro**
Dec. 5– 6, 2006	Recent Advances in Molecular Science via Sum Frequency Generation Spectroscopy	**OUCHI, Yukio** **MORITA, Akihiro**
Dec. 21–22, 2006	Hierarchy of Molecular Interactions in Complicated Systems: A Basis for Understanding of Biological Functions	**TAHARA, Tahei** **NISHI, Nobuyuki**
Mar. 11–12, 2007	New Development of Materials Molecular Science	**KATO, Reizo** **YAKUSHI, Kyuya**
Mar. 14–15, 2007	Functions and Properties of Nano-Structure Controlled Hybrid Inorganic-Organic Composites	**OHBA, Masaaki** **TANAKA, Koji**
Mar. 19–20, 2007	Progress in Science of Nanoclusters and Nanoparticles —Reactivity, Structure, and Dynamics	**MAFUNE, Fumitaka** **TSUKUDA, Tatsuya**
Mar. 19–20, 2007	Molecular Science of Enzymes Relating to Heme Degradation	**FUJII, Hiroshi**

May 22–23, 2007	Molecular Science for Living Cells	**OHTA, Nobuhiro** **OZAWA, Takeaki**
Jun. 1– 3, 2007	Metals and Molecular Assemblies —The Way to Frontier of Supramolecular Science—	**UENO, Takashi** **KAWAGUCHI, Hiroyuki**
Jun. 23, 2007	Physical Chemistry Symposium for Young Scientists in Molecular Science	**HAMAGUCHI, Hiroo** **HISHIKAWA, Akiyoshi**
Aug. 29–31, 2007	Coupled Simulation in Molecular Science: Theories and Applications	**AOYAGI, Mutsumi** **SAITO, Shinji**
Sep. 10–11, 2007	Synchrotron Radiation and Surface Electron Emission Microscopy: Recent Progress in Microscopic Techniques for Nanomaterials Science	**ASAKURA, Kiyotaka** **YOKOYAMA, Toshihiko**
Sep. 28–29, 2007	Scientific Basis of New Field “Molecular Communication”	**URISU, Tsuneo**

(3) Numbers of Joint Study Programs

Categories		2006 Oct.–2007 Mar.	2007 Apr.–2007 Sep.	Total
Special Projects		0	2	2
Research Symposia		9	6	15
Cooperative Research		39	44	83
Use of Facility	Laser Research Center for Molecular Science	1	–	1
	Research Center for Molecular Scale Nanoscience	21	–	21
	Instrument Center	–	23	23
	Equipment Development Center	5	2	7
Use of UVSOR Facility		62	70	132
Use of Facility Program of the Computer Center				141

Collaboration Programs

(a) IMS International Program

IMS has accepted many foreign scientists and hosted numerous international conferences since its establishment and is now universally recognized as an institute that is open to foreign countries. In 2004, IMS initiated a new program to further promote international collaborations. As a part of this new program, IMS faculty members can (1) nominate senior foreign scientists for short-term visits, (2) invite young scientists for long-term stays, and (3) undertake visits overseas to conduct international collaborations.

Leader	Title	Partner
OHMORI, Kenji	Quantum Control of Atoms and Molecules with Amplitude- and Phase-Shaped Optical Pulses	France: Prof. GIRARD, Bertrand and his group members U.S.A.: Prof. LEVIS, Robert J. and his group members
SHIGEMASA, Eiji	Dynamics in Resonant Auger Decay Studied by Electron-Ion Coincidence Spectroscopy	France: Dr. SIMON, Marc Dr. GUILLEMIN, Renaud Dr. JOURNEL, Loic U.K.: Dr. ELAND, John H. D.
KIMURA, Shin-ichi	Optical and Photoelectrical Studies on the Local to Itinerant Electronic Structure of Strongly Correlated Electron Systems	Korea: Prof. KWON, Yong-Seung Dr. IM, Hojun Dr. KIM, Hyeong-do and group members
TAIRA, Takunori	Passively Q-Switched Nd-Lasers with YCOB Doubler	France: Prof. AKA, Gerard Philippe Dr. LOISEAU, Pascal Dr. XU, Ke
KATOH, Masahiro	Beam Dynamics in Free Electron Laser	France: Dr. COUPRIE, Marie Emmanuelle and group member Dr. BIELAWSKI, Serge and group member
KOSUGI, Nobuhiro	Resonant Soft X-Ray Spectroscopic Study at UVSOR BL3U	Germany: Prof. RUEHL, Eckart and group members Sweden: Prof. AGREN, Hans Prof. PETTERSSON, Lars G. M. Prof. NORDGREN, Joseph and group members U.S.A.: Dr. GUO, Jinghua
TANAKA, Koji	Photochemical Water Oxidation and Multi-Electron Reduction of Carbon Dioxide	U.S.A.: Dr. FUJITA, Etsuko Dr. MUCKERMAN, James T.
JIANG, Donglin	Studies on Molecular Design and Self-Assembly of Light-Harvesting Antennae	China: Prof. WANG, Changchun and group members

SAKURAI, Hidehiro	Studies on Columnar Structure of Buckybowl Supramolecules	India: Dr. SASTRY, Narahari G. and group members
NAGASE, Shigeru	Theoretical Study on Chemical Modification and Functionalization of Single-Walled Carbon Nanotubes	China: Prof. LU, Jing and group memberes

(b) Asian Core Program "Frontiers of Material, Photo- and Theoretical Molecular Sciences"

Asian Core Program is a multilateral international collaboration program carried our by JSPS (Japan Society for the Promotion of Science). It is designed to create world-class research hubs in selected fields within the Asian region, while fostering the next generation of leading researchers. The program is based on a principle of equal partnership among core institutions in Japan and other Asian countries, so that each institution is expected to secure its own matching fund. Institute for Molecular Science has launched a new collaboration project "material, photo- and theoretical molecular sciences" (2006–2011) within the framework of this Asian Core Program with three key institutes in east Asian countries: Institute of Chemistry, Chinese Academy of Science (China); The College of Natural Science, Korea Advanced Institute of Science and Technology (Korea); and Institute of Atomic and Molecular Sciences, Academia Sinica (Taiwan). At present, nine joint researches are in progress, three joint seminars have so far been carried out, and another seven seminars are planned.