

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 Chemical 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.

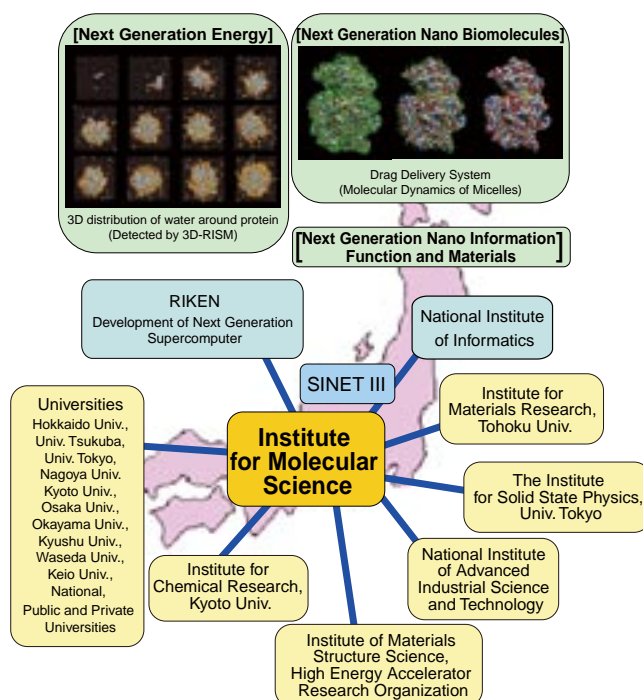
(a) Next Generation Integrated Nanoscience Simulation Software Development & Application of Advanced High-Performance Supercomputer Project

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 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.

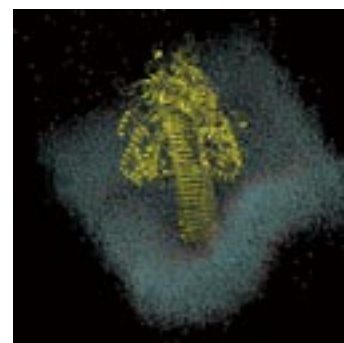


(b) Formation of Interdisciplinary and International Bases for Natural Sciences, NINS “Development of New Computational Methods for Large-Scale Systems and Establishment of Advanced Simulation Center for Molecules and Materials”

This project aims to establish a core computational science center for molecular and material systems and to develop advanced methodologies for large-scale calculations. We are trying to create a new interdisciplinary field by integrating the different views and methodologies in each field that belongs to a different hierarchy of natural sciences. Structures and dynamics of large-scale complex systems, *e.g.* nanomaterials and biological systems, are investigated with a variety of sophisticated computational methods based on theories of quantum and statistical mechanics, and so on. Seminars and workshops for the advanced calculations and for the development of human resources are also conducted by this project.

The project is 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. The followings are 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

(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

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

OHMORI, Kenji Development of Attosecond Coherent Control and Its Applications

HISHIKAWA, Akiyoshi Reaction Imaging and Control with Extremely Short Laser Pulses

OHSIMA, Yasuhiro Quantum-State Manipulation of Molecular Motions by Intense Coherent Laser Pulses

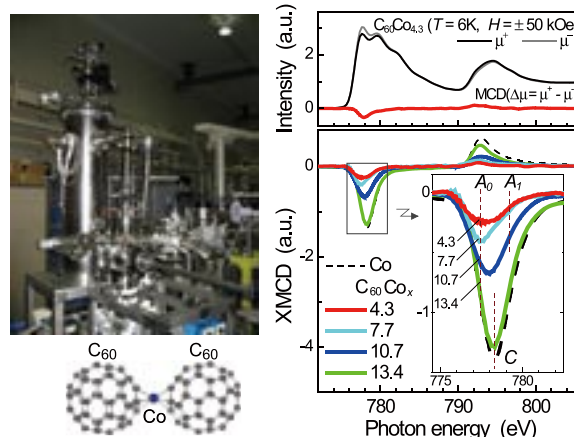
(d) MEXT Nanotechnology Network Nanotechnology Support Project in Central Japan: Synthesis, Nanoprocessing and Advanced Instrumental Analysis

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 company researchers. 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 2008 Apr.–2009 Mar., the number of accepted projects applied to IMS amounted 127 (the total number of days is 897).



(left) Measurement system of high magnetic field (± 7 T) and low temperature (5 K) X-ray magnetic circular dichroism installed at UVSOR-II and (right) examples of the recorded XMCD data by Drs. Y. Matsumoto and S. Sakai in JAERI, published in *Chem. Phys. Lett.* **470**, 244–248 (2009).

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 Chemical 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 are advancing 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 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.

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 appro-

riated 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 June, the number of user registrants amounts to 4563 in 72 universities and IMS covering 1299 laboratories in Japan. Now the registered equipment increases to 206. With the supplementary budget in 2009, the government decided to introduce the 36 advanced instruments, 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.* into the network. These most advanced instruments can encourage the users in outer universities.

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.



Okazaki Conference

The 68th Okazaki Conference From Aromatic Molecules to Graphene; Chemistry, Physics and Device Applications

Organizers: T. Enoki (*Tokyo Tech.*), T. Yokoyama (*IMS*), K. Tsukagoshi (*NIMS*), T. Kubo (*Osaka Univ.*), K. Kusakaba (*Osaka Univ.*)

Invited Overseas Speakers: P. W. de Heer (*Georgia Tech.*), P. Esquinazi (*Univ. Leipzig*), F. Guinea (*Inst. Ciencia de Mater., Madrid*), R. Haddon (*Univ. California, Riverside*), S. G. Louie (*Univ. California, Berkeley*), A. F. Morpurgo (*Univ. Geneva*), K. Novoselov (*Univ. Manchester*), A. Sood (*Indian Inst. Sci., Bangalore*)

The 68th Okazaki Conference was held on Jan. 21–23, 2009 in Okazaki Conference Center, in which we had about 90 of attendees including 38 invited speakers. The discovery of single sheet of graphite, which is called graphene, has triggered intensive studies on graphene and related materials. The electronic structure of graphene is described in terms of massless Dirac fermion, which makes it distinguished from traditional electronic systems. The interesting unconventional

electronic feature of graphene is stimulating also in building electronic/spintronics device applications. Nanosized graphene called nanographene provides another intriguing issue due to the presence of edges. Indeed the electronic structure of nanographene is strongly dependent on the shape of the edges. The creating of nonbonding π -electron state (edge state) around the zigzag edges brings about unconventional nanoscopic magnetism and chemical reactivities. This situation is relevant to the issue of non-Kekulé structure with neutral radical state in aromatic hydrocarbon molecules in organic chemistry.

In this conference we were aiming at enriching the aspects of the issues on graphene by discussing comprehensively the physics, chemistry and device applications of graphene, nanographene and aromatic hydrocarbon molecules on the common basis. It was devoted to develop a new interdisciplinary area of graphene-related research by bridging between physics, chemistry and device applications.



Joint Studies Programs

As one of the important functions of an inter-university research institute, IMS facilitates joint studies 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, Tatsuhiisa (*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 investigated the electron-spin coupled states composed of Cu(II) ions in the square-planar coordination with the ligands. 2) We carried out an analysis of spin dynamics for functional molecular assemblies, including²⁾ metal ions inserted in M-DNA and³⁾ dye-sensitized solar cell. We searched for cooperative phenomena involved in intra-molecule freedom, and new functional physical-properties originating in molecular assemblies.

A-1 Spin Coupled State Composed of Cu(II) Ions in Square-Planar Ligand Field

The arrays of spin active metal ions are expected to lead to the coupled spin states. Herein we show two unique approaches to form copper ions' arrays, which exhibited the coupled high spin states. As the first approach, Fujita *et al.* reported a discrete homo Cu(II)–Cu(II)–Cu(II) metal array, as shown in Figure 1., through the intercalation of Cu-aza-porphines into an organic pillared coordination box, which is self assembled from two panels, three pillars and six Pd(II) hinges.¹⁾ We clarified by using an ESR spectrometer that the homo Cu–Cu–Cu array shows unique spin interaction, which is clearly reproduced by a computer simulation as a quartet spin state.²⁾

The other approach is owing to the efficient self-assembly properties of DNA. Shionoya *et al.* showed that upon replacement of hydrogen-bonded base pairing by metal-mediated base pairing in DNA, it is possible to align metal ions within the double helical DNA scaffold.³⁾ They reported the alignment of up to five Cu(II) ions within the DNA scaffold by using a hydroxypyridone-metal base pair, H-MBP in Figure 2. Electron spin transient nutation (ESTN) measurement as well as cw-ESR observation exhibited that the Cu(II) centers were ferro-magnetically coupled to one another, with each Cu(II) center being in a distorted square-planar geometry.⁴⁾ On the other hand Clever and Carell reported the alignment up to ten Cu(II) ions within the DNA double helix using a salicylic aldehyde metal base pair in the presence of an ethylenediamine,

salen ligands metal base pair (S-MBP) in Figure 2. However, no magnetic measurements were reported for the S-MBPs.⁵⁾ Recently Ono *et al.* synthesized the thymidine dimer linked DNA with N4-carboxymethylcytosine metal base pair, CA-MBP in Figure 2, having the alignment up to five Cu(II) ions. The EPR spectrum exhibited the spectra due to the coupled spin state with much smaller dipole interaction than the case of Shionoya's metal-DNA. The comparison among the cases shows that the magnetic interactions in the metal-DNA structures are strongly dependent on the conformation characteristics of the metal base pair. The formation of an extended network in the stacked array of H-MBP favors ferro-magnetic coupling, whereas the ordered pairwise-stacked arrangement of S-MBP suppresses magnetic coupling. In the case of CA-MBP, the Cu(II) array exhibits the small magnetic dipole interaction, indicating the long distance between neighboring Cu(II) ions.

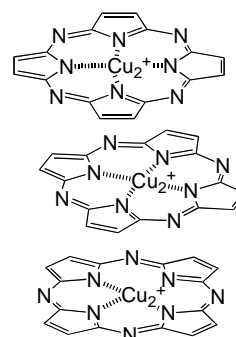


Figure 1. Stacked array of Cu-aza-porphines.

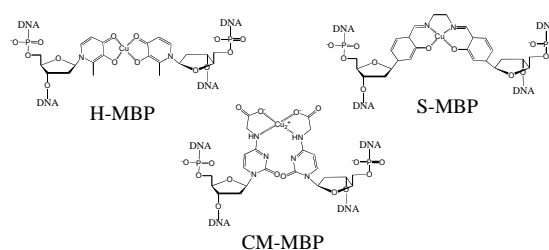


Figure 2. Three metal base pairs, hydroxypyridone MBP (H-MBP), salicylic aldehyde MBP with ethylenediamine (S-MBP), and N4-carboxymethylcytosine MBP (CA-MBP).

A-2 ESR Study of Metal Ions Inserted in M-DNA

In the view point of materials science, DNA shows several interesting properties such as self-organizing nature based on the complementarity of base pairs, arbitrariness of sequence design, and the possibility of π -electron stacking between adjacent bases. However, it has been confirmed that natural

DNA is a semiconductor with a large energy gap more than 5 eV. To introduce charge carriers into the DNA, there are several possibilities: Composite with divalent metal ions, chemical doping, and electric field induction. Here, we report an ESR study on the divalent metal ions of M-DNA.

It has been confirmed that several alkaline earth and transition metal ions, such as Mg, Ca, Mn, Fe, Co, Ni, and Zn, could form composites with DNA, locating in between the bases of a base pair. The magnetic transition metal ions are useful as a probe to investigate the electronic states of metal ions in the M-DNAs. Especially, Mn^{2+} ions are the ideal magnetic probe with $S = 5/2$ which gives ESR signal around the free electron g -value, $g \sim 2$. Analysis of ESR spectra in M^{2+} -DNA has led us to the conclusion that the charge transfer from the metal ions to the DNA base pairs did not occur, keeping DNA semiconducting after M^{2+} introduction. Only the exception has been found in Fe-DNA, where Fe^{2+} ion introduced into DNA base pairs changed to Fe^{3+} , as confirmed by its color and ESR g -value just near $g \sim 2$, corresponding to $S = 5/2$ expected for a high-spin state of Fe^{3+} , as demonstrated in Figure 3. Thus, one could conclude that one electron should transfer to DNA in Fe-DNA. Fe-DNA also shows another curious behaviors in magnetization and ESR spectra, which suggest a mixture of high-spin state, $S = 5/2$ and low-spin state, $S = 1/2$ of Fe^{3+} , especially as a function of Fe concentration.

On the location of metal ions are suggested to be in between the bases of a base pair from several experimental facts. However, the bonding state of the metal ion is still open question. We have succeeded to study the bonding state of Mn in Mn-DNA from the analysis of six hyperfine split spectra of $\text{Mn}_{0.01}\text{Ca}_{0.99}$ -DNA taken at Q-band in Figure 2. It is known that the separation of the central two spectra represents the bonding nature of metal ion. Isolated Mn^{2+} ion in the ionic crystal CaF_2 shows the separation of more than 100 G, but in the crystal, ZnS made of mainly covalent bond indicates the separation of around 70 G. From the separation of 96 G in $\text{Mn}_{0.01}\text{Ca}_{0.99}$ -DNA in Figure 4, we can clearly conclude that the bonding of Mn ion with surrounding bases in Mn-DNA is ionic in character. The present observation of the bonding nature of metal ions in M-DNA strongly supports further investigation and understanding of M-DNA, experimentally and theoretically.

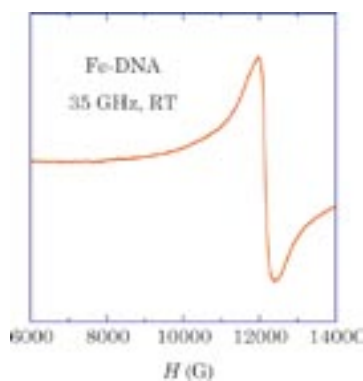


Figure 3. (left) ESR spectrum of Fe-DNA located at about $g = 2$, suggesting that $S = 5/2$ for Fe^{3+} .

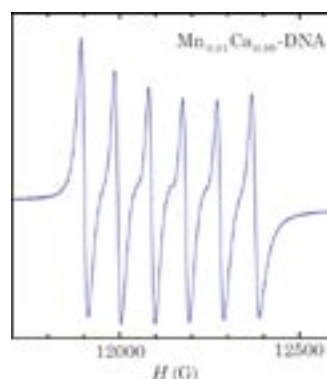


Figure 4. (right) ESR spectra of Mn ion in $\text{Mn}_{0.01}\text{Ca}_{0.99}$ -DNA show the six hyperfine peaks. The separation of the center two spectra could be a measure of bonding nature, ionic or covalent.

A-3 ESR Study of Spin Dynamics for Dye-Sensitized Solar Cell

In dye-sensitized solar cells (DSSC), dye molecules are excited from the ground state S to the excited state S^* by photo energy. The electron transfer from the excited dye molecules to the electrode plays an important role of the photoelectric transfer characteristic in DSSC. A various type of dye molecules were investigated. Time-resolved ESR measurements give us to detailed information of the photoelectric transfer characteristic. The aim of the present study is to reveal the relationship between the photoelectric transfer characteristic and the spin dynamics of electron in DSSC. The spin dynamics of the various organic dye molecules such as the eosin-Y was investigated by time-resolved ESR spectroscopy with laser photolysis (Nd:YAG 2nd harmonics, 532 nm). We discuss the spin dynamics of the various organic dye molecules with TiO_2 .

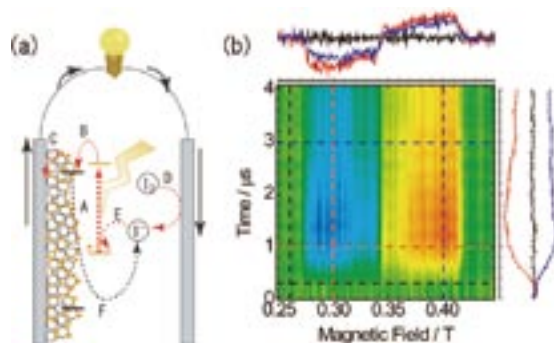


Figure 5. (a) Schematic image of the DSSC and (b) TR-ESR spectra for eosin-Y.

References

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- 2) K. Ono, M. Yoshizawa, T. Kato and M. Fujita, *Chem. Commun.* 2328–2330 (2008).
- 3) K. Tanaka, Y. Yamada and M. Shionoya, *J. Am. Chem. Soc.* **124**, 8802–8803 (2002).
- 4) K. Tanaka, A. Tengeiji, T. Kato and M. Shionoya, *Science* **299**, 1212–1213 (2003).
- 5) G. H. Clever and T. Carell, *Angew. Chem., Int. Ed.* **46**, 250–253 (2007).

B. Construction of the Research Methodology for Biomolecular Sensing System

URISU, Tsuneo (*IMS*)
 TERO, Ryugo (*IMS*)
 ASANO, Toshifumi (*IMS*)
 UNO, Hidetaka (*SOKENDAI*)
 SHIBASAKI, Koji (*OIIB*)
 TOMINAGA, Makoto (*OIIB*)
 SHIGEMOTO, Ryuichi (*NIPS*)
 FUKAZAWA, Yugo (*NIPS*)
 YAWO, Hiromu (*Tohoku Univ.*)
 ISHIZUKA, Toru (*Tohoku Univ.*)

The neurodegenerative diseases are intractable diseases for which neither of the cause and the treatment method is clarified. Statistically, 20% of more than 85 years old persons get dementia. Thus developments of treatment method and clarification of the cause are the urgent problem of human beings. Concerning this point, it is one of the problems to be solved that there is no suitable screening device of neural systems. In this program, we have started the research to develop a screening device which have the function of in vitro neural network analysis.

B-1 Development of Cell Culture Type Planar Ion Channel Biosensor for Nerve Cell Signaling Analysis

Cells growing on SOI substrates with and without the FN coating are compared. The FN coating clearly promoted cell growth. Although we did not control the cell positions, a cell was often positioned on the micropore.

The sequence of steps in the incubation mode recording is as follows. The culture mediums in the upper and lower chambers were exchanged to the extracellular and intracellular solutions, respectively, for the ion channel current measure-

ments. Perforated patch mode recordings were formed by nystatin (100–200 µg/ml). The increase of capacitance (5–10 pF) of the cell membrane was observed 5–10 min after addition of the nystatin solution.

The whole-cell current of the TRPV1 activated by capsaicin stimulation was recorded. The first capsaicin application induced a large current increase, and the current increase induced by the second application was weaker than the first one. The decrease in the sensitivity unique to the capsaicin stimulation of TRPV1 with a Ca²⁺-containing solution was observed.

B-2 Fabrication of Light Gated Ion Channel Biosensor

In the investigation of the electrically excitable cells, photo-stimulation provides a versatile alternative to electrode stimulation. Channel of the excitable cell by the photo-stimulation is especially useful in constructing the neural network analysis device. In the present work, we have expressed *Chlamydomonas reinhardtii* channelrhodopsin 2 (ChR2) on the cell membrane of a kind of excitable cell C2C12, and measured the basic characteristics of the photo-response. ChR2 has a light absorbance peak at 460 nm and forms a non-selective cation channel, the gating of which is triggered by the photo-isomerization of the all-trans retinal to 13-cis configuration. To investigate the photo-response characteristics of ChR2-expressed C2C12 cell, we have constructed the planer-type ion channel biosensor by putting a single C2C12 cell on the micropore of the Si substrate and successfully observed the light-gated whole cell channel current. We are now measuring the basic characteristics of this system such as, effects of cell-cell interaction and coupling of the cell's own characteristics and the chamber's electric characteristics on the time dependence of the whole cell current.

(2) Research Symposia

(From Oct. 2008 to Sep. 2009)

Dates	Theme	Chair
Jan. 22–23, 2009	Plasmonic Materials for Molecular Science	UENO, Kosei IMURA, Kohei
Mar. 5– 6, 2009	Workshop on Biradical Chemistry and Its Future Perspect	ABE, Manabu SAKURAI, Hidehiro
Jul. 23, 2009	Preparatory Meeting for Molecular Science Summer School	TANAKA, Midori HISHIKAWA, Akiyoshi

(3) Numbers of Joint Studies Programs

Categories		Oct. 2008–Mar. 2009	Apr. 2009–Sep. 2009	Total
Special Projects		0	1	1
Research Symposia		2	0	2
Research Symposia for Young Researchers		0	1	1
Cooperative Research		44	60	104
Use of Facility	Instrument Center	36	18	54
	Equipment Development Center	4	9	13
Use of UVSOR Facility		85	70	155
Use of Facility Program of the Computer Center				147*

* from April 2008 to March 2009

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 program to further promote international collaborations. As a part of this 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
SHIGEMASA, Eiji	Deexcitation Dynamics of Core Excited Molecules Studied by Electron Spectroscopy	France: Dr. SIMON, Marc and group members
KATOH, Masahiro	Generation of Coherent Radiation by Using Laser and Electron Beam	France: Dr. COUPRIE, Marie Emmanuelle Dr. BIELAWSKI, Serge and their group members
KIMURA, Shin-ichi	Optical and Photoelectrical Studies on the Local to Itinerant Electronic Structure of Strongly Correlated Electron Systems	Korea: Prof. KWON, Yong-Seung and group members Germany: Dr. SICHELSHMIDT, Jorg
KOSUGI, Nobuhiro	Study of Weak Intermolecular Interaction by Resonant Soft X-Ray Photoelectron Spectroscopy	Germany: Prof. RUEHL, Eckart Dr. WINTER, Bernd and their group members Sweden: Prof. PETTERSSON, Lars G. M. Prof. GEL'MUKANOV, Faris and their group members France: Dr. MIRON, Catalin and group members
UOZUMI, Yasuhiro	Development of Novel Asymmetric Catalysis with Chiral Pincer Complexes	China: Prof. WANG, Hongxing
SAKURAI, Hidehiro	Development of Novel Gold Cluster Catalyst Supported by Polymers	Thailand: Prof. CHAVASIRI, Warinthorn and group members
JIANG, Donglin	Study on the Synthesis of Magnetic Particles with Light-Harvesting Antenna	China: Prof. WANG, Changchun and group members
TAIRA, Takunori	Q-Switched Nd-Microchip Lasers with COB Doubler	France: Prof. AKA, Gerard Philippe Prof. LOISEAU, Pascal and their group members
YOKOYAMA, Toshihiko	Two Photon-Photoemission Magnetic Circular Dichroism in Co Ultrathin Film on Pt(111)	Germany: Prof. SCHONHENSE, Gerd and group members
YOKOYAMA, Toshihiko	A Competition between Magnetic Anisotropy and Interlayer Coupling in the Multilayer Systems of Alternating In-Plane and Perpendicular Anisotropy	Germany: Prof. PRSYBYLSKI, Marek and group members

URISU, Tsuneo

Construction of Neural Cell Molecular Signal
Transmission System and Development of Molecular
Science New Field

China:

Prof. WANG, Chang-Shun
Mr. HE, Tingchao

OHMORI, Kenji

Coherent Control of Ultracold Atoms and Molecules

Canada:

Prof. SHAPIRO, Moshe
and group members

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

Asian Core Program is a multilateral international collaboration program carried out 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 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, and six joint seminars are planned within JFY 2009.

(c) Exchange Program for East Asian Young Researchers “Improvement of Fundamental Research Base for Environmental and Energy Problems”

At the Second East Asia Summit (EAS), held in January 2007, Mr. Shinzo Abe, Prime Minister of Japan, announced a plan to implement a ¥35-billion youth exchange program, inviting about 6,000 young people to Japan mainly from the EAS member states every year for the next five years. Based on this plan, the Government of Japan has launched the Japan-East Asia Network of Exchange for Students and Youths (JENESYS) Programme, under which it is conducting a variety of exchange activities. As a part of the JENESYS Programme, the Japan Society for the Promotion of Science (JSPS) has launched the “Exchange Program for East Asian Young Researchers.” Aimed at promoting researcher exchanges with East Asian countries, this program supports initiatives by Japanese universities and research institutions to invite young researchers (*e.g.*, master’s and doctoral students and post-doctoral researchers) from those countries. By supporting exchange programs implemented by Japanese universities and

research institutions, the “Exchange Program for East Asian Young Researchers” works to establish and expand networks with researchers mainly from Asian countries. It also helps to develop high-caliber human resources and to create a regional science and technology community. IMS is a center of the basic research of physical/chemistry fields in Japan and has a role for the center of both domestic and international collaboration. From 2008, IMS has organized the JENESYS program for chemistry/physics fields. IMS provides the opportunity for young researchers from Asian countries to stay in the laboratories related to the basic research for environmental and energy problem for 14–60 days. Through the experience, we encourage them to continue the basic research in their own countries as well as to build up the future collaboration. IMS welcomed totally 24 young researchers (11 in 2008 autumn and 13 in 2009 spring) from Thailand, Singapore, Malaysia, Indonesia, Vietnam, and India.

