# Special Research Projects

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

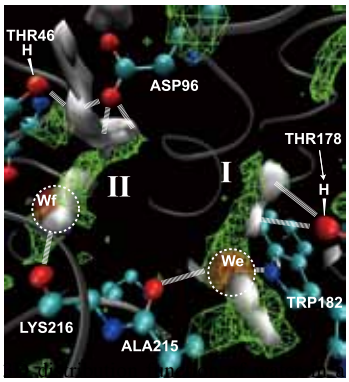
(a) The Ministry of Education, Culture, Sports, Science and Technology
HPCI Strategic Program "The Strategic Program for Innovation Research (SPIRE)"
Field 2 "New Materials and Energy Creation"
"Construction of Innovative High Performance Computing Infrastructure (HPCI)"
(b) Extreme Photonics
(c) MEXT Nanotechnology Platform Program
Platform of Molecule and Material Synthesis
(d) Inter-University Network for Efficient Utilization of Research Equipments
(e) Consortium for Photon Science and Technology (C-PhoST)

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) The Ministry of Education, Culture, Sports, Science and Technology HPCI Strategic Program "The Strategic Program for Innovation Research (SPIRE)" Field 2 "New Materials and Energy Creation" "Construction of Innovative High Performance Computing Infrastructure (HPCI)"

HPCI strategy programs "SPIRE" aims to promote scientific research using "K-computer" at RIKEN Advanced Institute for Computational Science. In the strategic filed 2 of SPIRE, the Institute for Solid State Physics (ISSP) of the University of Tokyo, Institute for Molecular Science (IMS), and Institute for Material Research (IMR) of Tohoku University were selected as strategic organizations. The project started in September 2010 for "Computational Material Science: Turning the Headwaters of Basic Science into a Torrent of Innovations in Functional Materials and Energy Conversion" as a strategic target. To promote the activities of the strategic organizations, a new community "Computational Materials Science Initiative (CMSI)" consisting of research fields of condensed matter physics, molecular science and materials science was launched.

Theoretical and Computational Chemistry Initiative (TCCI) at IMS completed the activities of the 2013 fiscal year: (1) TCCI continued to contribute on making "Road-Map for Computational Science" to clarify the requests for post-K computers, such as computing speed, memory size, and other specifications, (2)TCCI organized the fourth TCCI workshop, the third symposium for communicating with experimental chemists, and the other one for industry–academic partnership, (3)TCCI also sponsored the seventeenth summer school of Molecular Simulations, two TCCI winter colleges (molecular simulations, and quantum chemistry), and one workshop for massively parallel programming, (4)Research Center for Computational Science (RCCS) continued to provide a part of its computing resources to the SPIRE project as one of the actvities of TCCI, and (5)TCCI and RCCS started to promote several software developed in "Next Generation Integrated Nanoscience Simulation Software Development" project, which had been completed by the end of FY 2011.



protein computed with the MC-MOZ method.

In the following years, TCCI is going to pursue the activities above and promote the research using K-computer and the computational molecular science field.

## (b) 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 the 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

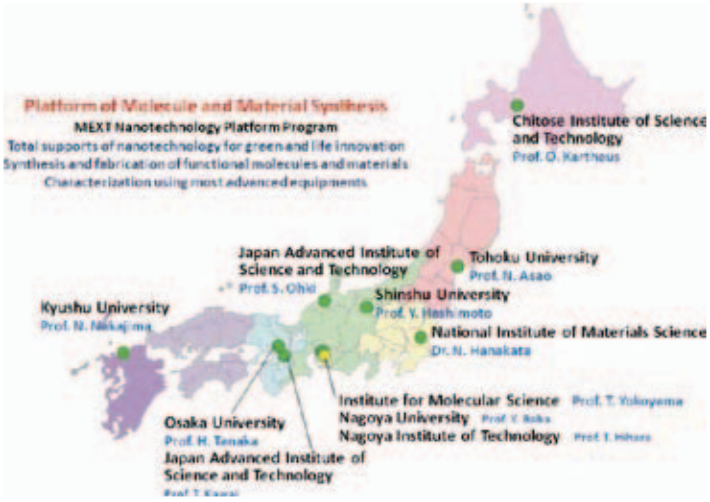
| | |
|---|---|
| OKAMOTO, Hiromi | Development of Extreme Time-Resolved Near-Field Spectroscopy |

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

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

## (c) MEXT Nanotechnology Platform Program Platform of Molecule and Material Synthesis

Since July 2012, Nanotechnology Platform Program supported by Ministry of Education, Culture, Sports, Science and Technology has been conducted in order to promote public usage of various nanotechnology facilities. This program will continue until March 2022 and consists of three platforms of nanostructure analysis, nanoprocessing, and molecule and material synthesis, together with the management center of the platforms. Each platform constitutes of about ten organizations all over Japan. IMS conducts a representative core organization of the Molecule and Material Synthesis Platform. All the organizations in this platform are shown in Figure. In this platform, to promote green and life innovation researches using nanotechnology related techniques not only for universities and government institutes but also for private companies, we will open various kinds of our facilities with total supports including molecular synthesis, materials fabrications, characterization, data analysis and scientific discussion. We will encourage applications not only to each element, but to combined usage of several supporting elements for biotechnology and green chemistry. In IMS, the number of accepted proposals amounted 123 (103 non-proprietary and 20 proprietary proposals, excluding applications from IMS) and the total number of days used for the supports is 2488 (2379 days for non-proprietary proposals and 109 days for proprietary ones).



List of Supports in IMS (FY2013)

| Supporting Element | | Responsible Persons | | Charging Persons |
|---|---|---|---|---|
| Platform Management | | T. Yokoyama, Y. Kaneko, M. Inoue | | Y. Funaki, Y. Toyama, M. Yokota, K. Nakane |
| Organization Management in IMS | | T. Yokoyama | | |
| UVSOR Synchrotron Radiation | Scanning Transmission X-Ray Microscopy | M. Katoh | N. Kosugi | T. Ohigashi, Y. Inagaki |
| | X-Ray Magnetic Circular Dichroism | | T. Yokoyama | Y. Takagi, M. Uozumi, Y. Uemura |
| | Microstructure Fabrication | M. Katoh | M. Suzui, M. Aoyama | N. Takada, T. Kondou |
| Electron Microscopy | 300kV Transmission Electron Microscopy | Y. Ohshima | | T. Ueda |
| | Field Emission Scanning Electron Microscopy | | | S. Nakao |
| | Focus Ion Beam Processing | | | |
| Molecular Properties | Electron Spectroscopy for Chemical Analysis | Y. Ohshima | N. Kosugi | M. Sakai |
| | Electron Spin Resonance | | T. Nakamura | M. Fujiwara |
| | Superconducting Quantum Interference Device | | | |
| | Microscopic Raman Spectroscopy | | H. Yamamoto | M. Uruichi |
| | Fourier Transform Far Infrared Spectroscopy | | | |
| High Field NMR | 920 MHz NMR Solutions & Solids | Y. Ohshima | K. Kato, K. Nishimura | T. Yamaguchi M. Nakano |
| | 800 MHz Solutions, Cryostat Probe | | K. Kato | T. Yamaguchi |
| | 600 MHz Solids | | K. Nishimura | |
| Functional Molecular Synthesis and Molecular Device Fabrication | Organic Thin Film Solar Cells | T. Yokoyama | M. Hiramoto | T. Kaji |
| | Organic Field Effect Transistors | | H. Yamamoto | M. Suda, M. Uruichi |
| | Molecular Catalysts | | M. Tada | S. Muratsugu |
| | Functional Organic Synthesis | | H. Sakurai | S. Higashibayashi |
| | Large Scale Quantum Mechanical Calculations | | M. Ehara | R. Fukuda |
| | Magnetic Thin Films | | T. Yokoyama | Y. Takagi, M. Uozumi, Y. Uemura |

## (d) Inter-University Network for Efficient Utilization of Research Equipments

It is highly important to improve the supporting environment for research and education in the field of science and engineering. Nowadays, advanced research instruments are indispensable for conducting research and education in high standard. To install such sophisticated instruments, significant amount of budgets is necessary. In 2007, for constructing a national-wide network to provide the easy access to high-level equipments to researchers and students in universities all over Japan, the 5 year project "Functioning of Inter-University Network for Efficient Utilization of Chemical Research Equipments," was launched. The network maintains an internet machine-time reservation and charging system by the help of equipment managers and accounting sections in each university. 73 national universities all over Japan have been participating to the network. They are grouped into 12 regions and in each region the regional committee discusses and determines the operation of regional network system with the hub university chairing. 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. Since 2010, the project name has been changed as "Inter-University Network for Efficient Utilization of Research Equipments," still keeping the original strategy and stable functioning. In June 2014, the number of user registrants amounts to more than 9000 in 147 universities/institutions covering more than 2300 laboratories in Japan. Usage of the network reaches to a few thousands per month since April 2010, and keeps growing in numbers.

## (e) Consortium for Photon Science and Technology (C-PhoST)

In order to establish strong bases in the research and education in optical science, a new 10-year program "Photon Frontier Network" has been started in 2008 by the Ministry of Education, Culture, Sports, Science and Technology (MEXT). Consortium for Photon Science and Technology (C-PhoST) is the one of two research consortia of Photon Frontier Network. It is composed of 4 Core Organizations headed by Principal Investigators (written in parentheses): Osaka University (R. Kodama), JAEA (A. Sugiyama), Kyoto University (S. Noda) and Institute for Molecular Science (K. Ohmori). The major strength of this Consortium is the collaboration between the specialists in three fields: High power lasers, semiconductor lasers, and coherent control. Emphasis is placed in the education to foster young researchers capable of taking leaderships in scientific projects through participation to the forefront researches taking place at C-PhoST and also participation to international collaboration activities.