Special Research Projects

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

(a) The Ministry of Education, Culture, Sports, Science and Technology (MEXT)
Flagship Project, Priority Research Issue
"Development of New Fundamental Technologies for High-Efficiency Energy Creation, Conversion/Storage, and Use"

(b) MEXT Nanotechnology Platform Program
Platform of Molecule and Material Synthesis

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

(d) Consortium for Photon Science and Technology (C-PhoST)

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.

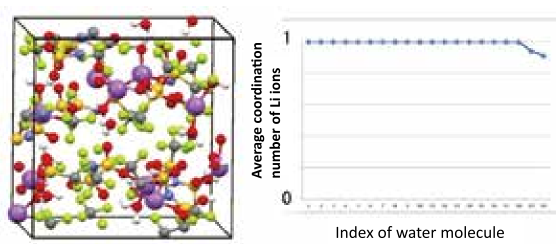
(a) The Ministry of Education, Culture, Sports, Science and Technology (MEXT) Flagship Project, Priority Research Issue, "Development of New Fundamental Technologies for High-Efficiency Energy Creation, Conversion/Storage, and Use"

A new supercomputer, the so-called post-K computer, is being developed by RIKEN as the successor to the K computer and is expected to help to solve various social and scientific problems. Nine priority research issues have been defined by the government, and at the same time, software development is also in progress. IMS leads one of the priority research issues, "Development of New Fundamental Technologies for High-Efficiency Energy Creation, Conversion/Storage, and Use" in collaboration with Kobe University, RIKEN, the University of Tokyo, the National Institute for Materials Science (NIMS), Nagoya University, Okayama University, Hokkaido University, and Waseda University, incorporating 46 institutions including 16 companies.

We propose to perform these state-of-the-art calculations to unravel the following issues. Branch A: Production and storage of alternative energy sources with solar cells and artificial photosynthesis; Branch B: Conversion and storage of energies produced in fuel cells and rechargeable batteries; Branch C: Separation, recovery, and storage of methane and CO_2 and effective use of energies and resources produced by catalytic reactions. We will also collaborate with experimentalists in academia and researchers in industries to establish new energy technologies that are highly efficient, inexpensive, environmentally clean, and sustainable.

Because of the limitation of current computer performance, conventional computational research has typically focused on isolated and/or subtotal systems to obtain partial information about the mechanism of the total system. The highly integrated computer resources of the post-K computer will be powerful enough to make such research obsolete; Post-K will open frontiers to establish a new academic standard in computational chemistry and physics, and will facilitate understanding of complex phenomena in real materials and heterogeneous systems.

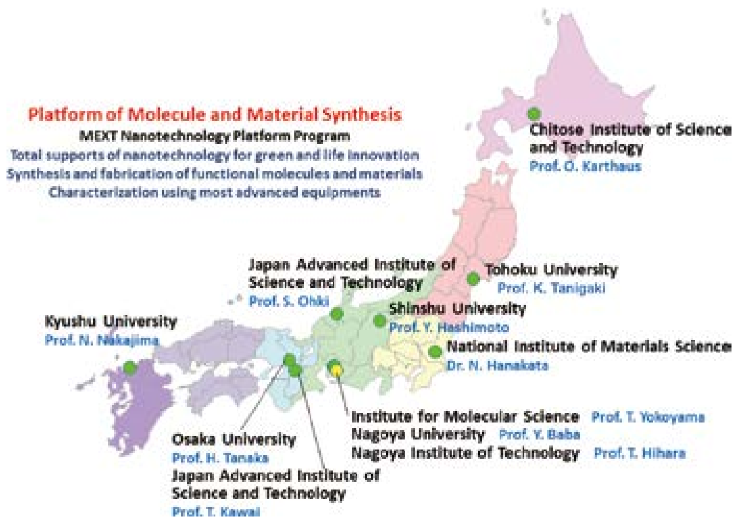
In the 2016 financial year, two symposia to promote collaboration with other national projects were held; *i.e.*, "The third symposium for collaboration of large experimental facilities and supercomputers" on September 1 2016, and "The first workshop for cooperation with the elements strategy initiative" on November 29 and 30. The third annual symposium of this project was also held on December 15 and 16, and more than 100 participants engaged in discussions. Furthermore, the research and development plan for the priority research issue "Development of New Fundamental Technologies for High-Efficiency Energy Creation, Conversion/Storage, and Use" was refined and submitted to MEXT. We plan to maintain similar activities for the duration of the Flagship project.



The mechanism of hydrate-melt electrolytes for high-energy-density aqueous batteries, was found computationally in this project. (Left) schematic picture of equilibrium state of newly-developed hydrate melt, (Right) coordination number of Li ions from each water molecule. *Nat. Energy* **1**, 16129 (2016).

(b) 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 (MEXT) 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 in FY2016 amounted 187 (161 non-proprietary and 25 proprietary proposals, excluding in-house applications from IMS) and the total number of days used for the supports is 3079 (2922 days for non-proprietary proposals and 147 days for proprietary ones).



List of Supports in IMS (FY2016)

Supporting Element		Responsible Persons	Charging Persons
Platform Management		T. Yokoyama	M. Ohara, I. Noda, Y. Toyama, Y. Funaki, M. Yokota, N. Nakagawa, A. Ota, Y. Hyodo
Organization Management in IMS			
UVSOR Synchrotron Radiation	Scanning Transmission X-Ray Microscopy	N. Kosugi	T. Ohigashi, Y. Inagaki
	X-Ray Magnetic Circular Dichroism	T. Yokoyama	Y. Takagi, Y. Uemura
Microstructure Fabrication	Maskless Lithography with Step Gauge	H. Yamamoto	M. Suzui, M. Aoyama, N. Takada, T. Kondou, M. Nakano
	3D Optical Surface Profiler		
Equipment Development	Machine Shop		M. Suzui, M. Aoyama, H. Yoshida, T. Kondou, T. Toyota
Electron Microscopy	Field Emission Scanning Electron Microscopy	S. Kera	S. Nakao
	Low vacuum Analytical Scanning Electron Microscopy		S. Nakao, M. Sakai
	Focus Ion Beam Processing		S. Nakao
X-rays	Single Crystal X-Ray Diffractometer		M. Fujiwara
	Low Temperature Single Crystal X-Ray Diffractometer for Microcrystals		Y. Okano
	Powder X-Ray Diffractometer		M. Fujiwara
	X-Ray Fluorescence Analysis		T. Ueda
	Small Angle X-Ray Scattering for Solutions	S. Akiyama	A. Mukaiyama

<table>
<tr><td rowspan="2">Electron Spectroscopy</td><td>Electron Spectroscopy for Chemical Analysis</td><td>N. Kosugi</td><td>M. Sakai, Y. Inagaki</td></tr>
<tr><td>Angle Resolved Ultraviolet Photoelectron Spectroscopy for Functional Band Structures</td><td>N. Kosugi, S. Kera, K. Tanaka</td><td>H. Yamane, S. Ideta, T. Ueba</td></tr>
<tr><td rowspan="3">Electron Spin Resonance</td><td>Pulsed High Field ESR</td><td>T. Nakamura, S. Kera</td><td>M. Asada, S. Iki, M. Fujiwara</td></tr>
<tr><td>X-Band CW ESR</td><td rowspan="17">S. Kera</td><td rowspan="2">S. Iki, M. Fujiwara</td></tr>
<tr><td>X, Q-Band CW ESR</td></tr>
<tr><td>SQUID</td><td>Superconducting Quantum Interference Device</td><td>S. Iki, M. Fujiwara</td></tr>
<tr><td rowspan="3">Thermal Analysis</td><td>Differential Scanning Calorimeter (Solutions)</td><td rowspan="2">S. Makita, H. Nagao</td></tr>
<tr><td>Isothermal Titration Calorimeter (Solutions)</td></tr>
<tr><td>Calorimeter for solids</td><td>M. Fujiwara</td></tr>
<tr><td>Mass Spectrometer</td><td>Matrix Assisted Laser Desorption/Ionization Time of Flight Mass Spectrometer</td><td>S. Makita</td></tr>
<tr><td rowspan="5">Spectroscopy</td><td>Microscopic Raman Spectroscopy</td><td rowspan="2">M. Uruichi</td></tr>
<tr><td>Fourier Transform Far Infrared Spectroscopy</td></tr>
<tr><td>Fluorescence Spectroscopy</td><td rowspan="2">T. Ueda</td></tr>
<tr><td>Ultraviolet & Visible Absorption Spectroscopy</td></tr>
<tr><td>Circular Dichroism</td><td>S. Makita</td></tr>
<tr><td rowspan="4">Lasers</td><td>Picosecond Laser</td><td>T. Ueda</td></tr>
<tr><td>Nanosecond Excimer/Dye Laser</td><td rowspan="3">T. Yamanaka</td></tr>
<tr><td>Nanosecond Nd:YAG OPO Laser</td></tr>
<tr><td>Nanosecond Fluorinated Excimer Laser</td></tr>
<tr><td rowspan="4">High Field NMR</td><td>920 MHz NMR Solutions & Solids</td><td>K. Kato, K. Nishimura S. Kera</td><td>S. Makita, H. Nagao</td></tr>
<tr><td>800 MHz Solutions, Cryostat Probe</td><td>K. Kato</td><td>M. Yagi, S. Yanaka</td></tr>
<tr><td>600 MHz Solids</td><td>K. Nishimura</td><td></td></tr>
<tr><td>600 MHz Solutions</td><td>S. Kera</td><td>S. Makita, H. Nagao</td></tr>
<tr><td rowspan="7">Functional Molecular Synthesis and Molecular Device Fabrication</td><td>Organic Thin Film Solar Cells</td><td>M. Hiramoto</td><td></td></tr>
<tr><td>Organic Field Effect Transistors</td><td>H. Yamamoto</td><td>M. Suda</td></tr>
<tr><td>Functional Organic Synthesis</td><td>T. Yokoyama</td><td>S. Higashibayashi</td></tr>
<tr><td>Large Scale Quantum Mechanical Calculations</td><td>M. Ehara</td><td></td></tr>
<tr><td>Magnetic Thin Films</td><td>T. Yokoyama</td><td>Y. Takagi, Y. Uemura</td></tr>
<tr><td>Metal Complexes</td><td>S. Masaoka</td><td>M. Kondo</td></tr>
<tr><td>Inorganic Materials</td><td>G. Kobayashi</td><td></td></tr>
</table>

(c) Inter-University Network for Common Utilization of Research Equipments

It is highly important to improve instrumental supporting environments for research and education in the field of science and engineering. Nowadays, advanced research instruments are indispensable for conducting researches and educations with high standard quality. To install such sophisticated instruments, tremendous amount of budgets would be necessary. In 2007, for constructing a national-wide network to provide easy accesses to high-level equipments to researchers and students in universities all over Japan, the five-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. 72 national universities as well as Institute for Molecular Science (total 73 organizations) all over Japan have been participating in the network. They are grouped into 12 local regions and in each region the regional committee discusses and determines the operation of regional network systems 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 all the public (prefectural *etc.*) and private universities. Since 2010, the project has been renamed "Inter-University Network for Common Utilization of Research Equipments" still keeping the original strategy and stable functioning. In July 2017, the number of registered users amounts to 11,500 in 251 universities/institutions/companies covering 2,788 laboratories in Japan. Usage of the network reaches almost 10,000 times per month and keeps growing in numbers. We are now reconstructing a new reservation and charging system that will be more user-friendly, convenient and safe for a long period. Moreover, we will actively provide various opportunities where technical staffs and users can improve their technical skills and frankly communicate with each other.

(d) Consortium for Photon Science and Technology (C-PhoST)

In order to establish strong bases in the research and education in optical science, a 10-year program "Photon Frontier Network" was 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), Kansai Photon Science Institute (K. Kondo), Kyoto University (S. Noda) and Institute for Molecular Science (K. Ohmori). The major strength of this Consortium is the collaboration among the specialists in three fields: High power lasers, photonic crystals, and coherent control.