

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 2020 Project, Priority Research 5
“Development of New Fundamental Technologies for Highly-Efficient 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 2020 Project, Priority Research 5 “Development of New Fundamental Technologies for Highly-Efficient Energy Creation, Conversion, Storage, and Use”

A new supercomputer, post-K computer, is being developed by RIKEN as a successor to the K computer. This will help solve various social and scientific problems. Nine priority research fields were defined by the government and the application software for them is also being developed. Among them, IMS is responsible to the priority research 5, “Development of New Fundamental Technologies for Highly-Efficient Energy Creation, Conversion, Storage, and Use.” IMS organizes a network project group with Kobe University, RIKEN, the University of Tokyo, National Institute for Material Science (NIMS), Nagoya University, Okayama University, Hokkaido University, and Waseda University in corporation with 46 institutions including 14 companies.

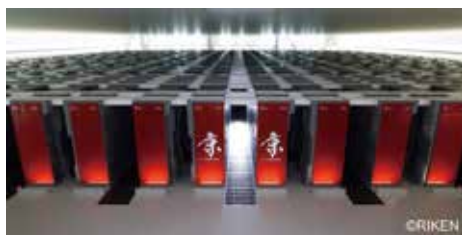
The highly integrated computer resources of the post-K computer will allow us to expand our current research across many disciplines. Realistic simulations will be made possible at the electronic and molecular scales, and will help us gain the details of chemistry and physics in complex compounds that play substantial roles in solar energy reactions and electrochemical processes.

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

CO₂; effective use of energies and resources produced by catalytic reactions. We are also collaborating with experimental researchers and industries to establish new energy technologies that are highly efficient, low cost, environmentally clean, and sustainable.

Due to the restriction in computer resources, computational researches have been typically limited to the investigation of isolated and/or partial systems to provide only one aspect of the entire system. The post-K computer is powerful enough to make such calculations obsolete; it will open new frontiers and establish new academic standard in computational chemistry and physics, enabling the understanding of fully complex physics associated with interfaces of real materials as well as inhomogeneous electrons and molecules.

In FY2015, we organized an advisory committee containing seven members: Three experimental researchers, two computational scientists, one computer scientist, and one senior researcher from industry. Then we held meetings of this committee on October 20, 2015, and January 4, 2016 where we explained and discussed the research plan of the project. The second open symposium of the project was held on March 7, 2016. Many researchers participated in the symposium and joined the discussions. Finally we refined the research and development plan of the project and submitted it to MEXT. We plan to keep similar activities during the project period.

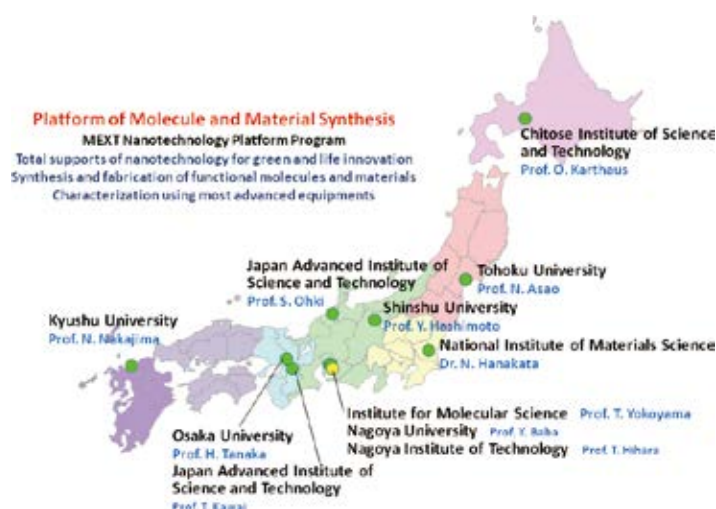


K computer being used by Priority Research 5.

(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 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 univer-

sities 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 FY2015 amounted 170 (161 non-proprietary and 9 proprietary proposals, excluding applications from IMS) and the total number of days used for the supports is 3113 (3065 days for non-proprietary proposals and 48 days for proprietary ones).



List of Supports in IMS (FY2015)

Supporting Element		Responsible Persons	Charging Persons
Platform Management		T. Yokoyama	Y. Kaneko, M. Inoue, Y. Funaki, J. Aoki, M. Yokota, N. Nakagawa, A. Ota
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, M. Uozumi, Y. Uemura
Microstructure Fabrication	Maskless Lithography with Step Gauge	H. Yamamoto	M. Suzui, M. Aoyama, N. Takada, T. Kondou
	3D Optical Surface Profiler		
Equipment Development	Machine Shop		M. Aoyama, H. Yoshida
Electron Microscopy	300kV Transmission Electron Microscopy	T. Yokoyama	T. Ueda, S. Iki
	Field Emission Scanning Electron Microscopy		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
	Single Crystal X-Ray Diffractometer for Microcrystals	Y. Okano	
	Powder X-Ray Diffractometer	M. Fujiwara	
	X-Ray Fluorescence Analysis	T. Ueda, S. Iki	
	Small Angle X-Ray Scattering for Solutions	S. Akiyama	A. Mukaiyama

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

(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 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 in 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 university. 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 August 2016, the number of user registrants amounts to 10,821 in 211 universities/institutions/companies covering 2,594 laboratories in Japan. Usage of the network reaches almost 10,000 times per month and keeps growing in numbers. We are now planning to reconstruct a new reservation and charging system that will be more user-friendly and convenient. 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” 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), 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.