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

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"

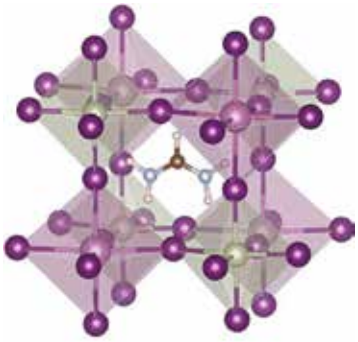
A new supercomputer, the so-called post-K computer, is being developed by RIKEN as the successor to the K computer and is expected to help to solve various social and scientific problems. Nine priority research issues have been defined by the government, and at the same time, software development is 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 47 institutions including 17 companies.

We propose to perform state-of-the-art calculations to unravel the following issues. Branch A: Production and storage of alternative energy sources using 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 which 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.

The midterm evaluation on the project was performed by MEXT in the financial year of 2017. In response to the comments of the evaluation committee, we have introduced a working group to confirm the current status of materials informatics to explore possible application to the subjects in the projects.

"The first collaborative symposium for experimental and industrial researchers" was held focusing on the theme of "Light Energy Conversion" in Kobe on December 11. Four researchers outside the project gave invited lectures and had a panel discussion. The fourth annual symposium of the project was also held in Kobe on December 12. During these symposia, a total 71 participants joined the 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.

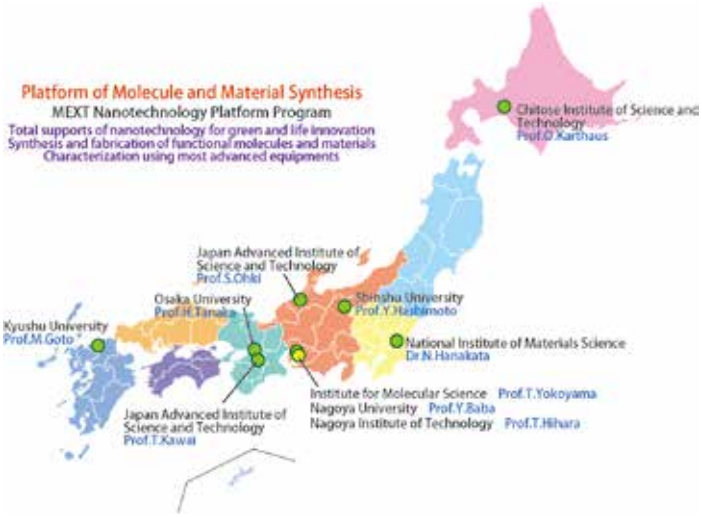


Double Perovskite

New material candidates were found in this project for "non-toxic perovskite solar cells" by searching based on highly efficient material screening using the K computer. Novel 51 low-toxic halide perovskites were discovered, most of which were newly proposed in this study. *J. Phys. Chem. Lett.* **8**, 4826–48319 (2017)

(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 FY2017 amounted 201 (170 non-proprietary and 31 proprietary proposals, excluding in-house applications from IMS) and the total number of days used for the supports is 3362 (3175 days for non-proprietary proposals and 187 days for proprietary ones).



List of Supports in IMS (FY2018)

Supporting Element		Responsible Persons	Charging Persons
Platform Management		T. Yokoyama	M. Ohara, Y. Toyama, Y. Shibata
Organization Management in IMS			Y. Hyodo, Y. Funaki, M. Yokota
UVSOR Synchrotron Radiation	X-Ray Magnetic Circular Dichroism	T. Yokoyama	T. Koitaya
Microstructure Fabrication	Maskless Lithography with Step Gauge	H. Yamamoto	E. Shigemasa, M. Aoyama, N. Takada, T. Kondou
	3D Optical Surface Profiler		
Equipment Development	Machine Shop		E. Shigemasa, M. Aoyama, T. Kondou, T. Toyota
Electron Microscopy	Field Emission Scanning Electron Microscopy	T. Yokoyama	Y. Matsuo
	Low vacuum Analytical Scanning Electron Microscopy		Y. Matsuo, M. Sakai
	Focus Ion Beam Processing		Y. Matsuo
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

Electron Spectroscopy	Electron Spectroscopy for Chemical Analysis	T. Yokoyama	M. Sakai, Y. Inagaki
	Angle Resolved Ultraviolet Photoelectron Spectroscopy for Functional Band Structures	S. Kera, K. Tanaka	S. Ideta
Electron Spin Resonance	Pulsed High Field ESR	T. Yokoyama, T. Nakamura	M. Asada, S. Iki, M. Fujiwara
	X-Band CW ESR	T. Yokoyama	S. Iki, M. Fujiwara
	X, Q-Band CW ESR		
SQUID	Superconducting Quantum Interference Device		S. Iki, M. Fujiwara
Thermal Analysis	Differential Scanning Calorimeter (Solutions)		T. Mizukawa, H. Nagao
	Isothermal Titration Calorimeter (Solutions)		
	Calorimeter for solids		M. Fujiwara
Mass Spectrometer	Matrix Assisted Laser Desorption/Ionization Time of Flight Mass Spectrometer		T. Mizukawa, K. Fujikawa
Spectroscopy	Microscopic Raman Spectroscopy		M. Uruichi
	Fourier Transform Far Infrared Spectroscopy		
	Fluorescence Spectroscopy		T. Ueda
	Ultraviolet & Visible Absorption Spectroscopy		
	Circular Dichroism		T. Mizukawa, K. Fujikawa
Lasers	Picosecond Laser		T. Ueda
High Field NMR	800 MHz Solutions, Cryostat Probe	K. Kato	M. Yagi, S. Yanaka, Y. Isono
	600 MHz Solids	K. Nishimura	
	600 MHz Solutions	T. Yokoyama	T. Mizukawa, 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	N. Momiyama	A. Izumiseki, N. Ohtsuka
	Large Scale Quantum Mechanical Calculations	M. Ehara	S. Ito
	Magnetic Thin Films	T. Yokoyama	T. Koitaya
	Metal Complexes	S. Masaoka	M. Kondo
	Inorganic Materials	G. Kobayashi	
	Biomolecule System	S. Akiyama	A. Mukaiyama, Y. Furuike

(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 this year, we have launched a new reservation and charging system that is more user-friendly, convenient and safe for a long period. The number of registered users amounts to 10,000 in 325 universities/institutions/companies covering over 3,000 laboratories in Japan (August, 2018). Usage of the network reaches almost 11,000 times per month and keeps growing in numbers. Moreover, we have actively provide various opportunities where technical staffs and users can improve their technical skills and frankly communicate with each other.