Computational Materials Science Initiative

Making Concepts Real

The large-scale computing leads the way
to new materials and energy creation

CMSI is a research community promoting Field 2 "New Materials and Energy Creation" within the HPCI Strategy Program (SPIRE) of the Ministry of Education, Culture, Sports, Science and Technology, Japan.

The Path to the Future

Bridging basic science and applied research

CMSI Representative Director

Shinji Tsuneyuki

Professor, Institute for Solid State Physics /
Graduate School of Science,
The University of Tokyo

Theory and experiments have long been the two main methods of scientific research. In the 21st century, however, we have added a third method: simulations that take full advantage of the capabilities of high performance computers. Computational materials science — materials research in which simulations, statistical processing and other calculations are used as essential tools — links theory and experiments to open new doorways in science and technology. This new science targets materials down to a single atom and up to the level of materials for practical use.

The Computational Materials Science Initiative (CMSI) is a network-style research community made up of computational science researchers specializing in condensed matter physics, molecular science and materials science. CMSI was established in order to promote Field 2 "New Materials and Energy Creation" in the High Performance Computing Infrastructure (HPCI) Strategic Program for Innovative Research (SPIRE) of the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan. The Initiative is centered on three core institutes — the Institute for Solid State Physics (The University of Tokyo), the Institute for Molecular Science (National Institutes of Natural Sciences) and the Institute for Materials Research (Tohoku University) — and includes 11 cooperating institutes and personnel from universities, research institutes and companies involved in the field of computational materials science.

The goal of CMSI is to use supercomputers, among which the K computer boasts the world's top performance, to create a new generation of materials science. To this end, four strategic issues have been established: next-generation advanced device science, molecular function and chemical conversion, energy conversion, and basic science of novel quantum states/new materials. CMSI is also strengthening its collaboration with SPring-8/SACLA, J-PARC and other large experiment facilities in order to work on creating materials that do not use rare elements.

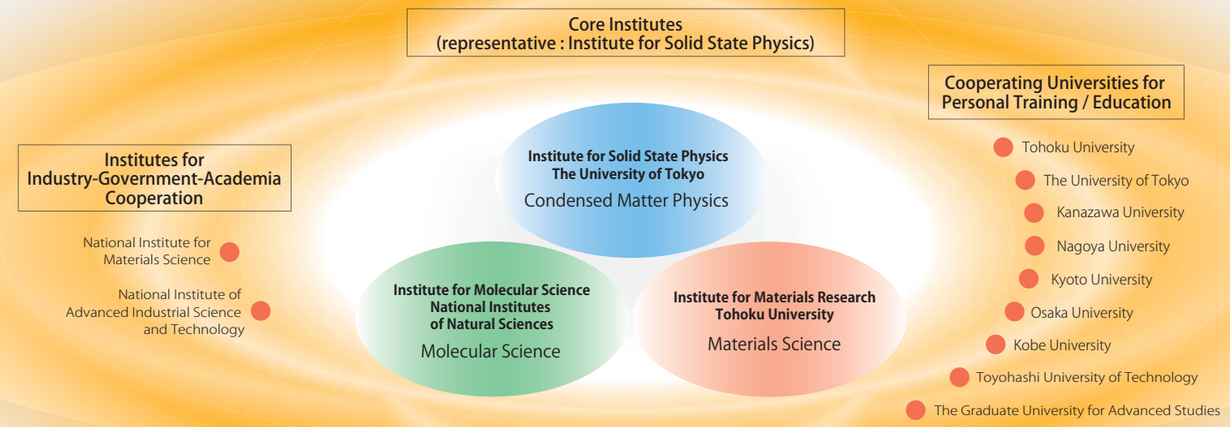
CMSI research is leading the headwaters of basic science into a torrent of applied research.

Next Generation of Nanoscience Integrating Three Fields

Towards reality beyond the imagination

CMSI Network

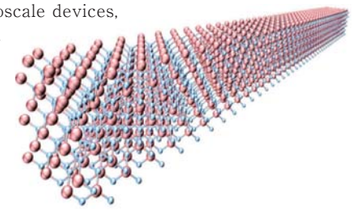
CMSI is an open research community that benefits from the participation of numerous researchers affiliated with 14 institutes and a diverse array of other entities nationwide.



CMSI Research Topics

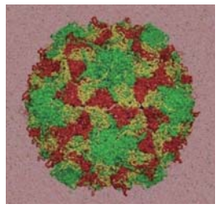
Next-generation advanced device science

As semiconductor devices become smaller and smaller, it will become difficult to design or predict the operation of semiconductor devices using the existing techniques in the very near future. The advanced supercomputers will enable us to achieve simulations of whole practical nanoscale devices, based on electronic theory, and to develop guidelines for designing new devices that incorporate the quantum effects that control nano-level phenomena.



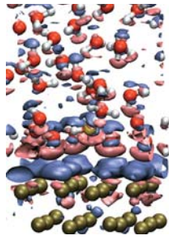
Molecular function and chemical conversion

Electronic states as well as structure and dynamics of nano-scale molecular assembly are investigated based on quantum chemical and molecular dynamics calculations. An example is virus in water. Very large-scale all-atom molecular dynamics simulations of virus using the advanced supercomputers enable investigations of infection and immunity at a molecular level, leading to control of virus and infectious diseases.



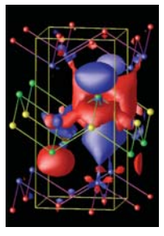
Energy conversion

Finding new materials that will revolutionize the ways in which we convert and store energy is one of the most urgent issues of the day. Simulations on a scale never before seen will identify the basic processes of fuel cells, methane hydrate and so on and locate promising materials. In this way, the computational materials science will build the foundation for next-generation energy technologies.



Basic science of novel quantum states / new materials

Achievements in basic research on material diversity and hierarchies, such as the discovery, elucidation, prediction of new concepts in physics and new quantum functionalities, are the intellectual property of humanity. At the same time, they are also an important source of future applied research. CMSI is pursuing state-of-the-art basic research into condensed matter physics and quantum chemistry, in areas such as the search for novel quantum states in strongly correlated quantum systems, elucidation of the dynamics of electron systems, prediction of the quantum finestructure of molecules, and emergence of new functionalities through fluctuations and dynamics.



Development of Human Network and Resources

Driving supercomputers to reach new heights

The distinctive feature of CMSI activities is that one of their major objectives, in addition to state-of-the-art research and development, is the formation of a basic infrastructure for research and development that will lead to the next generation of computational materials science. For this purpose, CMSI holds seminars, symposiums, workshops, training sessions, collaboration with experimental researchers and company researchers, and other activities to build a network of people with an interest in computational materials science, especially young researchers. CMSI also provides support for organization-building and activities to promote the development and dissemination of computers and computer programs.

In addition, CMSI promotes personnel training and education as well as public relations activities to promote the role of computational materials science in society and encourage understanding and interest.

Tsutomu Kawatsu

CMSI Molecular Science Division Researcher
Fukui Institute for Fundamental Chemistry, Kyoto University

My goal is to establish a sampling simulation method that can treat quantum chemical properties in a statistical manner, while achieving a balance between speed and accuracy.

Kazuhito Shida

CMSI Materials Science Division Researcher
Institute for Materials Research, Tohoku University

I want to optimize programs like TOMBO — a first-principles electronic state calculation program developed by the Institute for Materials Research — on an advanced supercomputer in order to gain new knowledge in the field of materials science.

Tomoko Mizuguchi

CMSI Molecular Science Division Researcher
Institute for Chemical Research, Kyoto University

I want to combine molecular science research and software operation advancement in order to help establish methods for analysis and control of molecular ensemble functions at the atomic and molecular level.

Truong Vinh Truong Duy

CMSI Condensed Matter Physics Division Researcher
Research Center for Simulation Science, Japan Advanced Institute of Science and Technology (JAIST)

My field of study is information science, and I wish to apply information processing technologies to computational materials science and get involved in interdisciplinary research that crosses the traditional boundary between two fields.

Kanako Yoshizawa

CMSI Condensed Matter Physics Division Researcher
Institute for Solid State Physics, The University of Tokyo

I want to develop packages that are convenient, highly expandable and can be used by many researchers, in the hope that this will lead to the discovery of a new type of physics that uses the new generation of advanced supercomputers.

Cover：CMSI researchers draw a sun with any color they like.
Eventually the sun will let the whole society glow with colorful light.

HPCI Strategy Program（SPIRE）Field 2 "New Materials and Energy Creation"
Computational Materials Science Initiative

Office: Institute for Solid State Physics, The University of Tokyo
Kashiwanoha 5-1-5, Kashiwa, Chiba 277-8581, Japan
TEL(+81) 4-7136-3279　FAX(+81) 4-7136-3441　http://cms-initiative.jp