February 2013 NO.7

Torrent

10^{16} Weave New Materials

Special : Research Topics in CMSI

Interview with Priority Research Topic Leaders and Special Support Topic Leaders

Approach of Priority Area Researchers

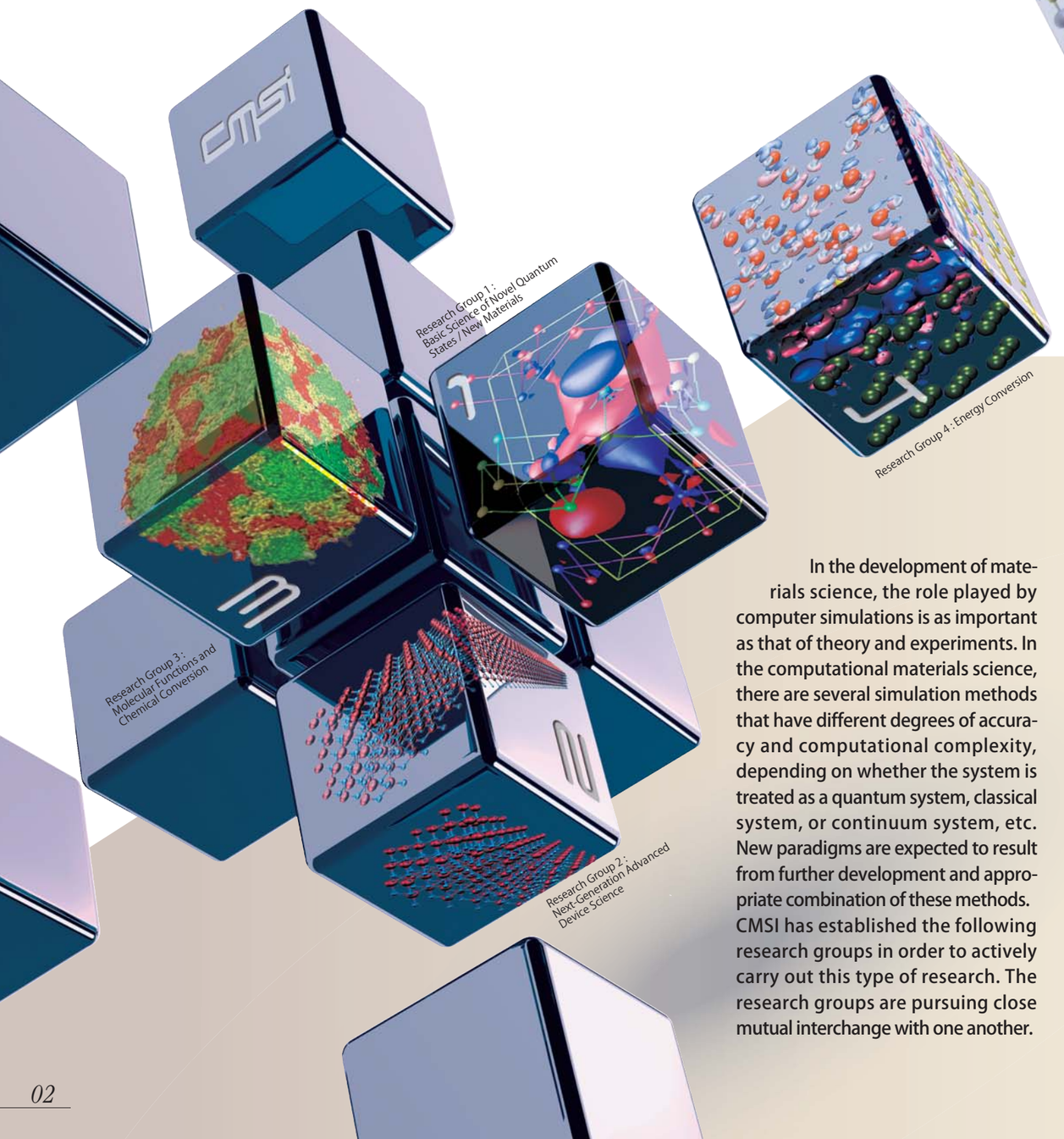
The 3rd CMSI Poster Award

Torrent [tɔ́:rənt]:
The Newsletter of the Computational Materials Science Initiative (CMSI)

Special

Research Topics in CMSI

New paradigm introduced by the K computer



In the development of materials science, the role played by computer simulations is as important as that of theory and experiments. In the computational materials science, there are several simulation methods that have different degrees of accuracy and computational complexity, depending on whether the system is treated as a quantum system, classical system, or continuum system, etc. New paradigms are expected to result from further development and appropriate combination of these methods. CMSI has established the following research groups in order to actively carry out this type of research. The research groups are pursuing close mutual interchange with one another.

Research Group 1 : Basic Science of Novel Quantum States / New Materials

New materials with novel properties have been discovered in recent years, including high-temperature superconductors (materials with zero electrical resistance) produced through iron and copper oxides, topological insulators (insulators in which only the surface exhibits metallic conduction), and fullerene and other nanocarbon materials. This research group will determine the mechanism by which the functions of these new materials are manifested within the context of materials science, and will work to improve and establish more precise calculation methods (the Monte Carlo method, the MP2-F12 method and so on).

Research Group 2 : Next-Generation Advanced Device Science

The thin wire technologies for the semiconductors that control the performance of today's electronic devices are approaching the limit of their effectiveness. This research group will work to achieve a fuller understanding of the behavior of optical devices (components that use light in place of electrical signals), which have attracted considerable attention as a next-generation technology, as well as silicon nanowires (fine silicon wires measuring several nanometers in diameter) in an effort to achieve practical applications for these technologies.

Research Group 3 : Molecular Function and Chemical Conversion

This research group will treat biomolecules as materials in an effort to understand virus propagation/infection and immunological mechanisms on the molecular level. Based on the knowledge achieved through this research, simulations will be conducted for the docking of candidate drug materials and the proteins that make up viruses, in order to help in the discovery of new drugs.

Research Group 4 : Energy Conversion

An understanding of electrode chemical reactions is essential in order to discover materials that can provide increased capacity and longer life to the fuel cells and lithium-ion batteries that are used in electric vehicles and the like. Moreover, in order to efficiently extract methane from methane hydrate (a compound consisting of methane enclosed by water molecules, which is expected to become an ecological energy source), the process by which methane hydrate forms and dissolves must be understood. This research group will work to elucidate these chemical reaction processes using computer simulations.

Research Group 5 : Multiscale Materials Science

To increase the toughness of iron and steel materials, an understanding of not only the microscale behavior of electrons and atoms but also their mesoscale internal structure is essential. Moreover, control of crystal growth is needed since the formation of structures in the coagulation process exerts an effect on the macroscopic properties of the products. This research group will conduct simulations whose goal is smooth linkage on various scales.

CMSI has established "Priority Research Topics" for computational materials science, in which research is needed urgently, as well as "Special Support Topics" that are considered to be candidates to become the next Priority Research Topics. For use of the K computer, computing resources allocated to CMSI are used for Priority Research Topics, while computing resources that have been secured by the researchers themselves (by applying for general use of the K computer) are used for Special Support Topics. Topics will be newly adopted or replaced through a review held in each fiscal year, judged by the parallelization efficiency achieved with respect to the K computer and the scientific importance of the topic in question.

In the following pages, seven CMSI Priority Research Topics and two of the Special Support Topics that have been selected for general use of the K computer will be profiled, based on interviews with representatives of each topic conducted by a CMSI Division Researcher. The Priority Area Researchers active in the study of each Priority Research Topic will also be featured.
(See Torrent No.3 for an explanation of CMSI's unique Division Researcher and Priority Area Researcher programs.)

(Tatsuya Sakashita,CMSI Condensed Matter Physics Division Researcher,Institute for Solid State Physics, The University of Tokyo)

CMSI research topics being carried out by using the K computer

	Research Topics	Page
Research Group 1 : Basic Science of Novel Quantum States / New Materials	Priority Research Topic: Search for new quantum phases in strongly-correlated quantum systems and explanation of dynamics	p. 4
	Priority Research Topic: Electron states and dynamics: new developments in molecular theory and integration of heat fluctuations	p. 6
Research Group 2 : Next-Generation Advanced Device Science	Priority Research Topic: Prediction of electron functions in nanostructures using the density functional approach	p. 8
	Special Support Topic: Photo-induced electron dynamics in nanostructures and development of quantum devices with optical and electronic functionality	p. 18
Research Group 3 : Molecular Functions and Chemical Conversion	Priority Research Topic: Development of the molecular science of viruses through all-atom simulations	p. 10
Research Group 4 : Energy Conversion	Priority Research Topic: Large-scale calculations for basic processes in fuel-cell related materials	p. 12
	Priority Research Topic: Mechanism of hydrogen and methane hydrate formation and dissolution and thermodynamic stability	p. 14
	Special Support Topic: Fundamental study for development of high-performance Li-ion battery	p. 18
Research Group 5 : Multiscale Materials Science	Priority Research Topic: Development of multiscale structural design and assessment techniques to improve the performance of metallic structural materials	p. 16

Interview with Priority Research Topic Leader

Search for new quantum phases in strongly-correlated quantum systems and explanation of dynamics

Interviewee :
Masatoshi Imada
Professor, Graduate School of Engineering, The University of Tokyo

Interviewer :
Tsuyoshi Okubo
CMSI Condensed Matter Physics Division Researcher
Institute for Solid State Physics, The University of Tokyo

What kind of research is being conducted for this Priority Research Topic?

To a considerable degree, the nature of matter is determined by the behavior of electrons. Over the past half-century, considerable progress has been made in the area of electron state calculations that reveal this behavior. For semiconductors (systems that have weak electron interaction) in particular, it has become possible to make quantitative predictions of condensed matter properties to some extent, mainly through the use of the density functional approach. For systems with strong electron interaction, however, it is known that the ordinary density functional approach does not produce reliable results. In the meantime, since around 1980, many intriguing phenomena resulting from strong interaction between electrons have been discovered. Some examples are transition metal compounds that include cuprate high-temperature superconductors, organic conductors made up of molecular crystals, and heavy electron systems known as f-electron systems.

These phenomena have a potential for new applications unlike anything seen in the semiconductor industry that experienced dramatic development during the previous century. As typical quantum many-body problems, they have also attracted considerable attention due to their potential to produce new approaches and concepts. The objective of this Priority Research Topic is to elucidate these phenomena by means of large-scale numerical calculation techniques using supercomputers.

Specifically, the objective is to understand new types of quantum states and as-yet undefined quantum phases that exist in the real world. Examples of new quantum states include high-temperature superconductors that are based on new mechanisms, and various types of quantum-liquid phases that include quantum spin liquids. From the standpoint of phase transition, we are also searching for phase transitions that are not bound by the framework of conventional Landau theory of phase transitions. The development of photo-induced phase transitions and pump-probe experimental methods that use photoelectron spectroscopy has brought considerable attention to nonequilibrium phenomena. We are working to identify the basic scientific principles for phenomena in these kinds of systems that are far removed from equilibrium.

How are large-scale numerical calculations being used in research on this topic?

What we really want to know is the behavior in the thermodynamic limit where systems are made up of many particles on the level of Avogadro's number. Since it is not possible to arrive there by means of actual calculation, we have to perform calculations for as large a number of particles as possible and to confirm convergence to the thermodynamic limit in order to ensure the reliability of the calculations. Also, as we are dealing with quantum systems, another major issue is the degree to which low temperatures can be handled. For nonequilibrium problems, how long calculations can be performed is another important issue. In addition, in simulations of the complexity of an actual material, the computational cost is increased even further. When you're trying to conduct calculations in as realistic a manner as possible, for a large size, at a low temperature, and for a long period of time, each one of these four items requires computational power that is almost equal to the entire resources of the K computer. It's crucial that you are able to devise a way to do all of these things as you pursue your research.

Currently, in terms of the number of atoms, it's now possible to handle from several hundred to several hundred thousand atoms. In terms of time, we can calculate up to about the picosecond. It's only been during the past ten years or so that techniques have been established for making quantitative estimates of the condensed matter properties of actual materials with strong electron correlation. In the sense that we're now able to make predictions based on materials that actually exist, we're approaching a very important time in history.

To use superconductors as an example, through large-scale calculations such as those possible on the K computer, we're now able to debate the stability of superconductors made of actual materials for the first time. The research that we've done recently is to use first-principles approach to calculate the magnetic properties of a group of iron-based superconductors that were discovered about four years ago. This enabled us to demonstrate that, in some materials, the strength of electron correlations changes systematically, and that it is the primary reason for the diversity of physical properties of the iron-based superconductors.

What will be the impact on society of the achievements of this Priority Research Topic research?

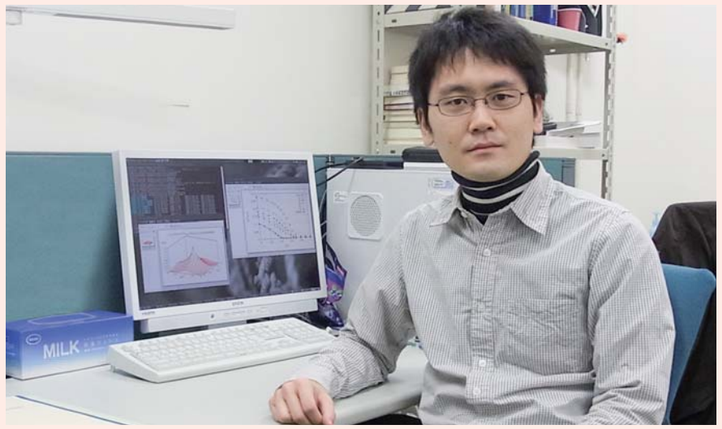
The achievements that we anticipate from research on this topic include quantitative prediction of the transition temperature of high-temperature superconductors, explanation of as-yet undefined superconductor mechanisms, explanation of new quantum-liquid mechanisms, and the establishment of a new theoretical foundation for quantum phase transitions, resulting in the search for and development of new functional materials. We also hope that the study of nonequilibrium dynamics will make it possible to propose design guidelines for new functional devices that use the quantum effect such as switching elements and so on.

It goes without saying that calculating electron states, designing materials and helping to predict physical properties are issues that will have a profound effect on society. Most of the industrial innovations achieved since the 20th century, such as semiconductor elements and devices, would not have been possible without an understanding of the microscopic properties of materials. In the sense of providing theoretical support for producing new industries, the achievements of research on this Priority Research Topic will play a crucial role in superconductor and other energy issues as well as microfabricated devices and other future industries.

Gaining an understanding of novel quantum states and new phenomena will also reveal natural structures and laws unknown heretofore. Looking back at history, we can see the profound impact of new concepts in condensed matter physics on particle physics, biology, chemistry and other fields. It is thought to be very likely that large-scale calculations using supercomputers will give us a clearer understanding of such new concepts in the future. Moreover, this research will not only make a contribution to directly relevant fields of academic study. In the sense of their cultural value as assets of humanity, the new conceptual discoveries and explanations achieved through this research will also make a major contribution to society.

Approach of Priority Area Researcher

Development of variational Monte Carlo method and study of quantum spin liquid

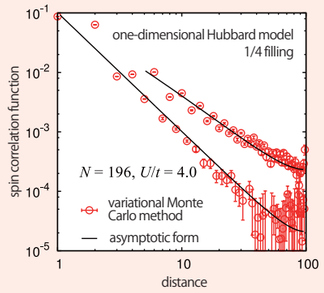


Satoshi Morita
Graduate School of Engineering, The University of Tokyo

Strongly correlated electron systems show many interesting phenomena such as superconductivity and quantum spin liquid (QSL), and attract increasing attention not only as research subjects for fundamental physics but as next-generation devices. In order to simulate strongly correlated electron systems, we have developed the variational Monte Carlo method, which can treat large-size system with high accuracy.

As a CMSI researcher, I have optimized the many-variable variational Monte Carlo method on the K computer and applied this method to study QSL. I finally achieve about 60 times speed-up and more than 90% parallelization efficiency in about 20,000 nodes. Such a speedup and high parallelization are making it possible to simulate a more complicated system in a realistic computational time. We also confirm that this method produces highly accurate results consistent with the exact theory in the one-dimensional Hubbard model.

Quantum spin liquid is a state in which spins fluctuate like a liquid. Competing interactions (geometrical frustration) and quantum fluctuations destroy magnetic order even at zero temperature. Since a QSL state is controllable with small external force, it has potential of application as a new magnetic device. The J_1-J_2 Heisenberg model on square lattice is one of the typical systems which are expected to realize QSL. We reveal that the generalized variational wave-function with the quantum number projection in the many-variable variational Monte Carlo method can represent a QSL state with triplet spin gap. A future challenge is to elucidate physics of QSL in ab initio effective models.



Spin correlation function of the one-dimensional Hubbard model. The numerical data are in excellent agreement with theoretical curves for Tomonaga-Luttinger liquid, which has large quantum fluctuations specific to one-dimensional systems.

Interview with Priority Research Topic Leader

Electron states and dynamics : new developments in molecular theory and integration of heat fluctuations

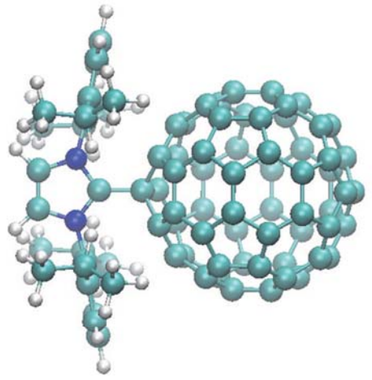
Interviewee :
Seiichiro Ten-no
Professor, Graduate School of System Informatics, Kobe University

Interviewer :
Takehiro Yonehara
CMSI Molecular Science Division Researcher
Graduate School of Arts and Sciences, The University of Tokyo

Overview of the Research Topic

Yonehara The aim of theoretical molecular science is to predict, understand and eventually control real-world chemical phenomena. In this field, two things are extremely important: (1) determining whether theories can be applied to molecular systems and material systems of a realistic size, and (2) developing calculation methods that are easy to use and capable of making highly accurate predictions. The theoretical side has universal significance in the sense that it provides reliable reference data for experimentation.
In the theoretical materials science, which is based primarily on electron states, electron correlation—which defines the many-body correlations among electrons—holds the key to quantitative predictions. First, could you tell us a little about this Priority Research Topic?

Ten-no The objective of this Priority Research Topic is to challenge problems that can only be solved using the K computer, and to achieve major research achievements that have significance for society as well. The code for electron state calculations for molecules that use Gaussian basis functions is extraordinarily complex, and even for someone well-versed in the use of the K computer, a variety of techniques are required. Currently F12 theory massively parallel modules have been provided, and production runs for nanocarbon materials and so on are being conducted. Throughout the latter half of the mission, it will be essential to make it possible to conduct material design that includes excited states in organic electroluminescence (EL) and artificial photosynthesis, and to search for materials that can substitute for rare earths, and thereby to produce a flow of scientific knowledge to other research groups.



F12 calculation of IDipp·C_{60}. Collaboration with Prof. Shigeru Nagase at Fukui Institute for Fundamental Chemistry.

Yonehara How did this topic come to be established for the Priority Research Topic?

Ten-no Up to now, the main method that has been used in materials design and other application fields is the density-functional approach. However, there are many drawbacks in this approach from the theoretical point of view. Our motivation was that, by making it possible to run the perturbation theory and coupled cluster theory that have been developed in the molecular science field on the K computer, we might achieve a material science that is fundamentally different from the one that we have known up to now.

Research outcome and future prospects

Yonehara Could you tell us about some specific recent achievements?

Ten-no The molecular quadrature method used in the F12 method is well suited to massively parallel computing, and up to now we have pursued hybrid parallelization. This has made it possible to achieve extremely high execution efficiency even with several hundred thousand CPU cores. In addition, the execution efficiency of the integration that is needed for molecular orbital calculation was a bottleneck, but here as well, we converted the code that used the quadrature method to SIMD and thereby managed to develop it into a useful calculation method.

Yonehara In addition to accurate knowledge of molecular structures including electron states, chemistry often requires microscopic information on reaction dynamics. Could you talk about the possibility of applying your own research techniques to reaction dynamics, and the issues that might arise in such cases and how you imagine they might be resolved?

Ten-no With regard to low-lying excited states, careful calculation of the matrix elements for nonadiabatic coupling with the potential surface generally makes it possible to determine what is happening. You need reaction dynamics in order to quantify things to the point where it's almost as if you've seen what happened with your own eyes. But in general the interesting phenomenon is the multiple degree of freedom dynamics, so I don't think this can be separated from the electron state calculations. I hope that one day techniques for dynamics will develop to the point where they can be incorporated into electron state theory.

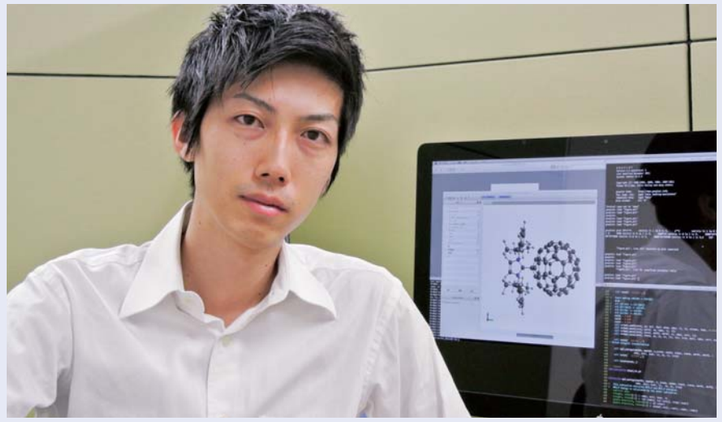
Appeal of computational materials science

Yonehara Finally, could you speak directly to the younger generation (university students and graduate students) about the appeal of molecular science and computational materials science, and about the usefulness of computers in scientific research?

Ten-no I think the fascinating aspect of this area of research is that theoretical calculations are able to predict real-world materials science, and that a bottom-up approach is used to achieve this. For many years, I've felt that developing basic theory offers a better chance of producing major breakthroughs than the use of large computers. Nevertheless, considering the scale of the massively parallel computing environments in recent years, I think that supercomputers are getting to the point where they provide a major advantage for conducting scientific and engineering calculations. I think combining the K computer with the highly precise quantum chemistry theory that has been developed in the field of molecular science will, in the future, reveal essential truths about materials science that we have not been able to see up to now.

Approach of Priority Area Researcher

Determination of crystal structures and interaction energies of organic conductors by massively parallel quantum chemical calculation

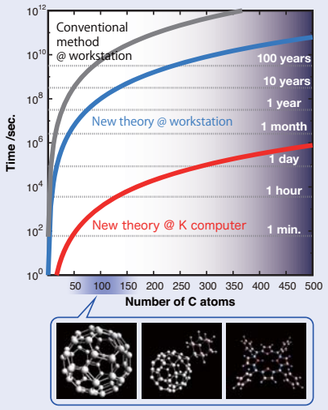


Yu-ya Ohnishi
Graduate School of System Informatics, Kobe University

I am currently developing a new explicitly correlated theory incorporating higher order perturbation terms to achieve more accurate calculations at the same time as studying the microscopic structure and its determinant of molecular crystals consisting of fullerene and porphyrin derivatives, which are expected to be future organic conductors, by using the MP2-F12 method implemented in GELLAN. Although the experiments have elucidated that a certain crystal structure improves the efficiency of the devices as well as the character of molecular does, it is considerably difficult to measure the strength of intermolecular interaction energy, which is closely related with the crystal structure. In order to help to design a better device, we are trying to show this property by performing the highly accurate calculation with massively parallelized GELLAN program.

Computational chemistry aiming to the theoretical understanding of chemical phenomena of atoms and molecules has been developed toward higher accuracy and larger system. It is nowadays possible to obtain highly accurate result, which is comparable to the sophisticated experiments, as far as the system consists of a few atoms. However, the highly accurate calculation of the system including more than ten atoms is still difficult because the computational cost increases by more than fifth power of the basis set size. There are two ways to tackle this problem: one is developing a new theory that enables us the highly accurate calculation with smaller number of basis sets, and another way is to implement the program for massively parallel environment so that the calculation of large system is feasible. The explicitly correlated second-order many-body perturbation (MP2-F12) theory implemented in GELLAN program by us has achieved both approaches. As shown in the figure, we can calculate the large system such as fullerene with high accuracy owing to this new theory and implementation.

Relation between the size of molecule and the computational cost for the highly accurate calculation



New theory and massively parallel implementation enable us highly accurate calculation of organic conductors.

Interview with Priority Research Topic Leader

Prediction of electron functions in nanostructures using the density functional approach

Interviewee :
Atsushi Oshiyama
Professor, Graduate School of Engineering, The University of Tokyo

Interviewer :
Kanako Yoshizawa
CMSI Condensed Matter Physics Division Researcher
Institute for Solid State Physics, The University of Tokyo

Overview of topic and objectives

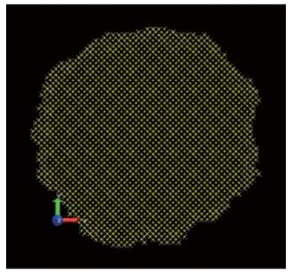
The objective of this Priority Research Topic is to establish a high-speed calculation technique that makes it possible to use state-of-the-art supercomputers to perform first-principles calculations (using density functional theory) for nanostructures ranging in size from several tens of thousands to several hundreds of thousands of atoms. This will make it possible to determine the atomic and electron structure and device properties of these nanostructures and the mechanism by which the nanostructures are formed. This group is working closely with CMSI Research Group 1, which is studying more basic questions. Within CMSI Research Group 2, the role of this Priority Research Topic is the application of basic scientific knowledge to real-world technology. Achievements in the research for this topic will make it possible to use first-principles calculations in quantum simulations, device simulations and other types of technology computer-aided design (TCAD).

In terms of actual calculations, two main methods are used for research and development: the Real-Space Density Functional Theory (RSDFT) and CONQUEST, an order-N first-principles application program. RSDFT introduces a grid into real space and calculates electron orbitals, electron density and potential and other quantities on grid points, and solves the Kohn-Sham equation. Unlike the density functional method that uses plane wave basis sets, this method does not require fast Fourier transformation (FFT), which uses communication between all CPUs. This method also makes it possible to set arbitrary boundary conditions for the wave function, such as nonperiodic system, periodic system and so on.

Rather than determining the eigenfunctions of the Kohn-Sham equation, CONQUEST determines a one-body density matrix. With the conventional algorithms, the computational complexity required for N atoms is proportional to N^3, while it is merely proportional to N by the order-N method. The order-N method thus enables first-principles calculations for ultra-large scale systems that are made up of tens or hundreds of thousands of atoms or more.

Current state

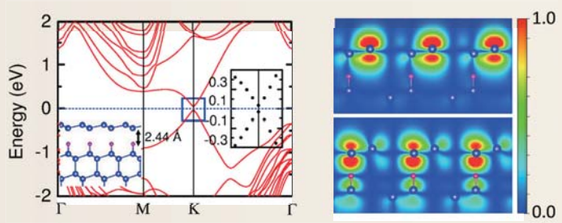
RSDFT was optimized for a massively parallel multicore architecture and achieved an effective performance of 3.08 petaflops (execution efficiency 43.6%) in calculations for a 100,000 atom silicon nanowire conducted using 70% of the overall resources on the K computer. This achievement was awarded the ACM Gordon Bell Prize (Sustained Performance Prize) at SC11, the international conference on high-performance computing. However, it would be difficult to perform simulations for several hundred thousand atoms without occupying 70% of the total resources of the K computer, and so at present RSDFT is only suitable for calculating several tens of thousands of atoms. RSDFT's ability to perform highly efficient parallel calculations also enables it to handle with comparative ease systems consisting of several thousand atoms, something that would require an enormous amount of time to calculate using other methods. RSDFT has successfully determined the charge injection energy in silicon nanodots consisting of several tens to several hundreds of thousands of atoms, the electron state of silicon nanowires, the interaction between carbon nanotubes and silicon interfaces, the structure of silicene (silicon analogue of graphene on thin film) and so on. We have also improved functionals and remedied the bandgap problem by introducing the hybrid exchange correlation energy.



Cross-section of a 10 nm diameter silicon (Si) nanowire, revealing modeling of the atomic-scale irregularities in the lateral surface produced during the wire formation process. In all, electron state calculations were conducted for 14,336 atoms.

Future anticipated benefits

We are approaching the limit of miniaturization of semiconductor devices, and research is being pursued into nanoscale devices that use the quantum effect. Accelerating first-principles calculation methods to the greatest degree possible in order to enable simulations of the quantum effect that controls nano-level phenomena will result in new device designs and guidelines. Specific benefits that are anticipated include predicting the structural stability and electronic functions of nanodots and nanowires (which are expected to become the initiating agents for next-generation devices), establishment of quantum theory and identification of device characteristics for the transport of electrons, heat and atoms for next-generation devices and nano-junctions, establishment of device simulator as basic technologies for the post-scaling era, and so on.



Band structure of a silicon monolayer (silicene) with a honeycomb structure and density distribution of orbits near the Fermi level. The RSDFT calculations indicated that hydrotreating of the Si (111) surface resulted in the formation of a stable silicene film, and Dirac cones were produced near the Fermi level.

Impact and contribution to society

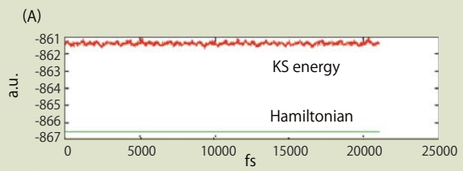
To stimulate the semiconductor industry in Japan, it will be essential to use first-principles calculations in semiconductor simulations, and to expand this effort to include prediction of device material functions, development of new functional materials, and the search for new nanostructures. Achieving increased speed for RSDFT and CONQUEST on supercomputers will also lead to the development of software designed for use on supercomputers. However, it will not be possible to achieve high-performance calculations by hardware evolution alone; software that can make effective use of this evolution will also be needed. For this reason, software will have to evolve along with supercomputers. This Priority Research Topic will make a contribution to Japan's progress and tradition of supercomputer technology.

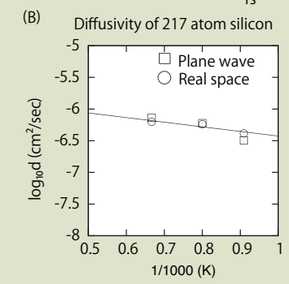
Approach of Priority Area Researcher

Development of Car-Parrinello molecular dynamics based on real-space density functional theory

Kenichi Koizumi
Graduate School of Engineering, The University of Tokyo

Car-Parrinello molecular-dynamics (CPMD) method was developed by R. Car and M. Parrinello in 1985 and its effectiveness is now covering almost all fields of science such as physics, chemistry, and biology. CPMD is based on quantum theory and it can simulate the breaking and reformation of chemical bonds, which are impossible to be described by classical molecular dynamics. However, its effectiveness is still underestimated being hindered by huge computational costs. To simulate chemical reactions in device-scale system including more than thousands of atoms, usage of the massive parallel computation is inevitable. Therefore, we are developing CPMD based on real-space density functional theory (RS-CPMD) that is a suitable method to extract the powers of the massively parallel computations. Now, we have developed a stable code enabling over 500,000 step simulations using 217 Si atoms and those results nicely reproduce those of a plane-wave code. However, there remain some rooms for improving the efficience because the optimization to the K computer is still insufficient. Now, we are trying to tune the code and will realize device-scale CPMD simulations that are difficult to perform by the standard plane-wave codes.





(A) Kohn-Sham energy and Hamiltonian of the total 50ps simulation (500,000 steps) at 1250K. Heating is 10ps, equilibration is 20ps, and production run is 20ps. Note that our Hamiltonian is totally constant.

(B) Diffusivities of crystalline silicon including an interstitial defect. The temperatures are 1100K, 1250K, and 1500K. The results of RS-CPMD reproduce those of a plane-wave code at high temperature.

Interview with Priority Research Topic Leader

Development of the molecular science of viruses through all-atom simulations

Interviewee :
Susumu Okazaki
Professor, Graduate School of Engineering, Nagoya University

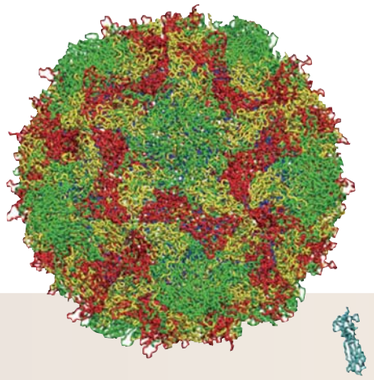
Interviewer :
Yoshitake Sakae
CMSI Molecular Science Division Researcher
Graduate School of Science, Nagoya University

What is the reason for using the K computer to conduct virus simulations?

Protein simulations have often been conducted in the field of molecular science. Up to now, however, they've mostly been single proteins or proteins with ligands added. At most, they've been simulations of protein complexes consisting of several proteins. We wanted to try simulating enormous systems, in which many more proteins come together and, for the first time, have functions as life activities. From among the components of these enormous systems, we chose to study virus capsids. The virus capsid is the basic structural unit of a virus. In an all-atom model that includes water molecules, it consists of some ten million atoms. In order to simulate a ten million atom system, a supercomputer such as the K computer that has high computing capacity is indispensable.

What special measures did you have to devise in order to use the K computer for this purpose?

In protein simulations, it's particularly important to accurately determine the long-range force. The Ewald method is one of the main methods used for accurate calculation of long-range force, but this method requires fast Fourier transformation (FFT). So the number of parallel nodes that can be used is limited to 200 to around 500, and this limits the applicable range of the system to several hundred thousand atoms.



The poliovirus and the D1 and D2 domains of the CD155 receptor. The water molecules used as a solvent have been removed from the image. (1 atmospheric pressure, 37°C)

To get around this problem, we did two things. The first was to introduce an algorithm called the fast multipole method (FMM) that is suited to parallel computing. It enables efficient parallelization even on a computer of the same class as the K computer with more than 80,000 nodes.

The other thing we did was to tune the program to match the K computer hardware. In particular, we simplified the data for large-scale parallelization, optimized communication for the 3-dimensional torus, took steps to reduce data transfer to and from memory (cache optimization), enhanced SIMD execution and so on. This type of tuning was only possible through close communication with experienced computer science personnel at RIKEN and Fujitsu. As a result, even though our program (Modylas) is a general purpose utility, we achieved 41.1% of the theoretical peak performance and 5 milliseconds in actual time for each MD calculation step. We're currently continuing with the tuning process and working to provide the enhanced features needed to estimate free energy and other types of thermodynamic quantities.

What type of ripple effect do you anticipate that the achievements of research into this Priority Research Topic will have in the fields of molecular simulation and virology, and in society at large?

Viewed from the field of virology, our research is expected to lead to the discovery of antivirals and other drugs. Through simulations, we analyze the affinity between the virus and the receptors inside the cell membrane, and by showing the principle through which this is manifested, we will be able to propose new molecules that function as inhibitors and so on. We're also considering various other research topics, such as the affinity between viruses and antibodies, artificial vaccines and so on. We think that these research topics are important from the standpoint of society at large, since they relate directly to people's health.

In the field of molecular simulations, it will eventually become commonplace to perform large-scale simulations for systems with more than a million atoms. I think there will also be further progress in the methods used to handle the enormous quantities of data that will be obtained as a result, as well as analysis methods for thermodynamic quantities and so on. Large-scale systems are an area in which there are many possible research topics, not only in life science but in the fields of chemistry and materials as well. One example is the study of polymers, an area in which new material development is anticipated. In the future, you'll see studies of various polymers that could not be targeted up to now in the field of computational chemistry.

Finally, could you talk about the future prospects for this research?

One is the dissemination of our program. We're currently making preparations to provide the program to people who want to conduct simulations of large-scale systems. Another is a more careful study of the molecular theory of large-scale systems. We plan to conduct simulations of not only viruses but also other large-scale systems in the fields of life science, chemistry, materials and so on. Our goal is to be able to more rigorously explain the principles that control the materials involved in these phenomena.

Approach of Priority Area Researcher

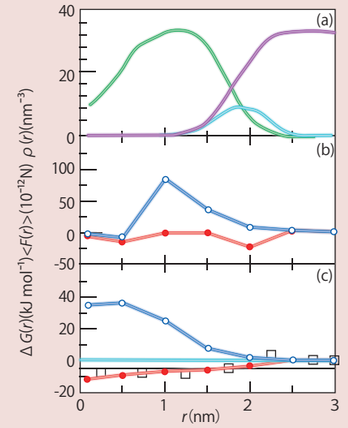
Free energy calculation combined with molecular dynamics simulation

Kazushi Fujimoto
Graduate of School of Engineering, Nagoya University

Solubilization, membrane penetration, binding between virus capsid and receptor are caused by intermolecular interaction between these molecules. Free energy analysis is effective tool in order to clarify physic chemically the penetration or binding.

We develop molecular dynamics (MD) software, which can calculate the free energy, in order to obtain free energy profile between the virus capsid and receptor. The free energy profile of a methane and water molecule penetrating into a sodium dodecyl sulfate (SDS) micelle was calculated by our MD software. Figure shows the calculated mean force and free energy profile. In Fig. (b), the mean force of the methane molecule at r = 2 nm is attractive to a large degree. It is found that the methane is taken into the SDS micelle by this attracting force. On the other hand, the mean force of the water molecule within a range of 0.5 to 2 nm was repulsive force. Therefore, the water molecule dose not penetrates into the SDS micelle core. In Fig. (c), the methane molecule can penetrate into the SDS micelle without free energy barrier, and move about there. The water molecule cannot penetrate into the SDS micelle because of highly unstable.

The position and strength of connection can be clarified by using the free energy profile. The free energy of profile between the virus capsid and the receptor will be calculated.



(a) Number density of the hydrophobic (—) and hydrophilic (—) of the SDS micelle and the water molecules (—). (b) Mean force and (c) free energy profile of the methane (●) and water (○) molecules. — and □ represent our previous work and calculation data of Matubayasi et al., respectively.

Interview with Priority Research Topic Leader

Large-scale calculations for basic processes in fuel-cell related materials

Interviewee :
Osamu Sugino
Associate Professor, Institute for Solid State Physics, The University of Tokyo

Interviewer :
Ryota Jono
CMSI Molecular Science Division Researcher
Graduate School of Engineering, The University of Tokyo

Present status and problems in the area of fuel cells

Jono The K computer is a massively parallel supercomputer made up of some 83,000 nodes, enabling it to handle more realistic environments than less powerful computers. Conversely, this may create new problems that have not been seen in model calculations up to now. What kind of problems do we face in terms of methodology in the area of fuel cells?

Sugino Now that we are able to directly calculate large-scale systems, it is possible to reveal and explore electrode interfaces. What is important here is that, unlike ordinary reactions that take place in a solution, voltage is applied when chemical reactions at the electrode interface are simulated, so the effect of the electrical field must be taken into consideration. Up to now, however, not much attention has been paid to creating realistic environments around molecules. Techniques for conducting simulations at a fixed voltage at electrode interfaces in particular must also explain the phenomena that occur at the actual device interface. Our group developed a method called the Effective Screening Method (ESM) for conducting simulations with the voltage held to a constant level, and we have incorporated it into many simulation packages. Combining this method with other techniques for the calculation of statistics makes it possible to calculate various kinds of physical quantities at electrode interfaces under the applied voltage.

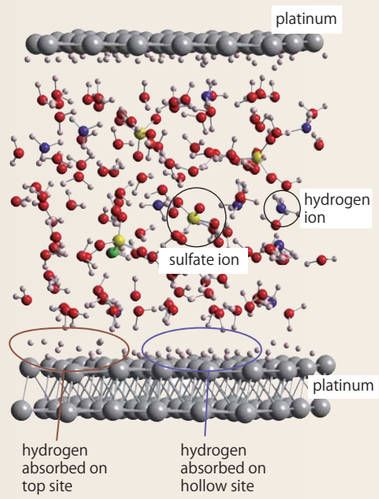
Jono The ESM method makes it possible to accurately depict electrode interfaces for the first time. What problems currently need to be resolved with regard to the electrode interfaces used in fuel cells?

Sugino In a nutshell, I'd say it's the "element strategy" for platinum substitutes. However, this will not be easy to achieve. First, the phenomena that are actually occurring must be reproduced by means of calculations, and the reaction mechanism will have to be understood. Only then can substitute metals be proposed. Electrochemical experiments are being performed to investigate in detail the reaction at the platinum electrode surface at which hydrogen is decomposed. This is ideal for verifying the accuracy of our calculations. Based on preliminary calculations, we have confirmed that, by placing water molecules up to approximately one nanometer from the platinum surface, it is possible to reproduce the properties of both the bulk water and the water near the surface, and that by conducting the simulation for 100 picoseconds or more, the recombination of the hydrogen bonds can be observed. From calculations performed on the K computer based on these findings, we think it will be possible to calculate various physical quantities at electrode interfaces using the methodologies developed up to now, and we plan to show that these can be accurately reproduced.

Collaboration with experimental scientists

Jono The question of what physical quantities can be calculated through the use of the K computer is an important one for many fields, not only fuel cells. Now that experimental scientists themselves have begun to perform calculations, I think the creation of a system by which, in five or ten years when many researchers are given easier access to the K computer, researchers will not have to begin by developing new methodologies but will instead be able to start right in on scientific and technological research, is an important task in terms of improving the environment. The search for platinum substitutes is one of the most important research topics in the Element Strategies Initiative. Could you talk a little about the collaboration system for this effort at CMSI?

Sugino In order to show that calculations can be used to accurately reproduce experimental phenomena, communication with experimental scientists will be essential. Also, rather than just considering ideas for platinum substitutes within CMSI, it would be more efficient to conduct the design based on a variety of opinions. We plan to hold exchanges of views through regular interchange with company researchers and collaboration with the Element Strategies Initiative.



Snapshot of a hydrogen decomposition reaction simulation at a platinum-electrode interface. The ESM method realized the simulation in an environment in which voltage was applied, making it possible for the first time to reproduce the hydrogen decomposition reaction in a real matter.

Jono Finally, could you talk about the future prospects for this research?

Sugino From now on, large-scale experiments using synchrotron radiation, lasers, neutrons and so on will be conducted for interface systems. Measurements that take a close look at interfaces will be conducted repeatedly, and static atomic structures and dynamic processes will be made clear. As a result, I think fields such as microscopic electrochemistry will be developed, and these will produce new fusion domains of science and will lead to applications that we cannot even begin to foresee yet. The theory, too, will have to delve into areas such as excitation, nonequilibrium, ultra-high precision and so on if it is to be able to explain the experiments that are being performed. And I think computational theory, the evolution of computers and the development of algorithms will become even more important.

Approach of Priority Area Researcher

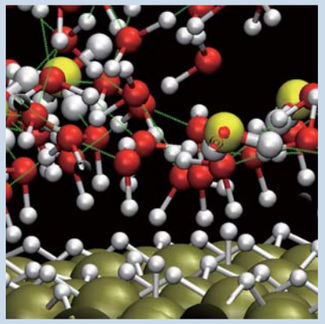
Elucidation of interface reactions between water and electrode metal by large-scale simulation

Hidetoshi Kizaki
Graduate School of Engineering,
Osaka University

First-principles simulations based on quantum mechanics, which make progress dramatically, have played a huge role in figuring out various phenomena in the field of materials science. Recently, first-principles simulations for mechanisms of electric chemical reactions have also made progress dramatically. Since we could not observe elementary steps of reactions directly in traditional experiments of electric chemical reactions, so far reactions mechanisms have been discussed by considering reaction kinetics between reactants and products. However, the dramatic progresses of first-principles simulations enable us to investigate elementary steps of reactions under atomic-scale criteria, traces of those on electrode interface and its dependence on electrode potentials and electrode metals.

For example, it is important to study the interface reactions between water and the electrode metal in the field of fuel cell. Therefore reaction simulations that take an influence of complicated water structures and electrode interfaces into account have been performed. As a result, the adsorption mechanism of H atom on a Pt surface in transferring electronic charge from hydronium ion, H_3O^+, to Pt-electrode, which is Volmer mechanism as a first step of hydrogen generation reaction, has been reproduced. This enables us to obtain a significant key of solving the hydrogen generation reaction mechanism by investigating an interaction between H_3O^+ and a metal surface and investigating H-adsorption dependence on behavior of water and electric potential.

However, due to the limitation of computational resources, the dependence on super cell size of periodic boundary conditions remains in the traditional simulations of electrode interface. Moreover, in order to take statistically adequate sampling of infinite geometry of metastable water and investigate the reaction path of H-adsorption dependence on the electric potential and the electrode metal, a large amount of calculation is required. To solve the problem, large-scale fast parallel computations are indispensable. By using the K computer and more realistic models, we aim to solve the whole electrode reactions of fuel cell.



Electrode interface model of H_2O/Pt (111). Pt (111) – 3 x 2√3 unit cell includes 32 H_2O molecules. A proton is hydrated.

Interview with Priority Research Topic Leader

Mechanism of hydrogen and methane hydrate formation and dissolution and thermodynamic stability

Interviewee :
Hideki Tanaka
Professor, Graduate School of Natural Science and Technology, Okayama University

Interviewer :
Tsutomu Kawatsu
CMSI Molecular Science Division Researcher
Graduate School of Natural Science & Technology, Kanazawa University

What are hydrogen hydrate and methane hydrate?

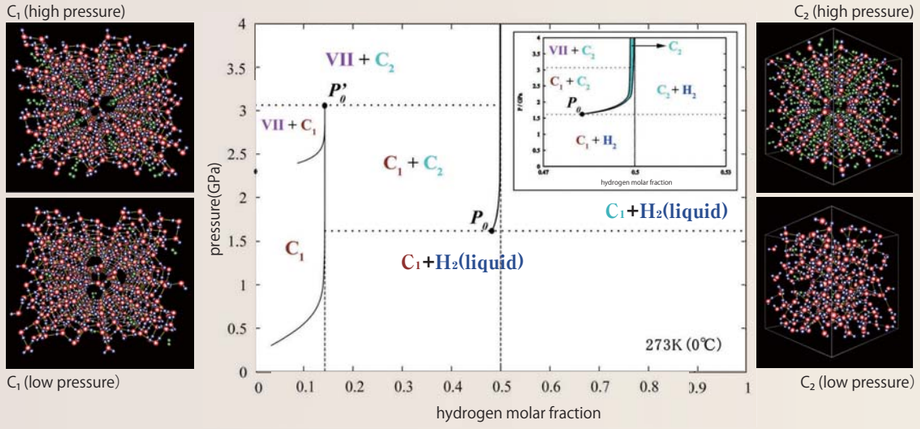
Hydrates are crystalline solids consisting of water molecules and other gaseous molecules formed in high-pressure environments. In hydrogen hydrates, hydrogen molecules are encapsulated in water lattice. Depending on the temperature and pressure, hydrogen hydrate may form a cage-like clathrate hydrate structure, or the hydrogen may be contained inside the interstitials in ordinary ice. The occupancy of hydrogen in the ice will also vary depending on the conditions. The term "methane hydrate" is often heard on TV these days. This is a methane clathrate hydrate, with a structure in which methane is contained inside a cage made of water molecules . In the real world, the cage-like structure is not formed in the absence of methane.

How much progress has there been in research in this area?

We have studied hydrates for around 20 years, so some knowledge has been accumulated in this area. Even a less computationally demanding method enables to obtain a phase diagram (figure below) of the structure obtained, which is in considerable agreement with the experimental results. If pressure is applied to hydrogen hydrate, it is possible to trap hydrogen in ice up to a mass of about one-ninth of water. However, this requires a pressure of 20,000 atmospheres, making it absolutely impossible to load the substance on a vehicle and transport it. However, other substances can be added to reduce the pressure, so this process is expected to find applications.
Currently, large-scale simulations for dissociation of methane hydrate are being conducted on the K computer using the molecular dynamics software program Modylas. The simulations show that when methane hydrate is heated, it melts from the surface inward, but it takes a long time when it is surrounded by water. When methane is placed in liquid water, this results in oversaturation due to its low solubility and any further dissolution of methane is prevented. At higher concentrations, however, bubbles are formed, and the methane escapes into these bubbles, so the hydrate once again begins to melt. Simulations are enabling us to begin to understand processes like these.

Why is research being conducted into how methane hydrate melts?

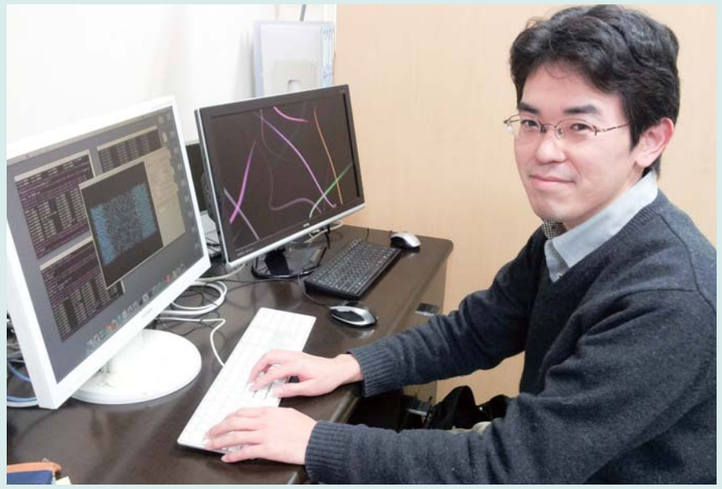
It is known that there is twice the reserve of methane hydrate as other fossil fuels, and it is expected in industrial usage. However, methane hydrate is found on the ocean floor, and at least 87% of its mass is composed of water, so excavating it in solid form would not be cost-effective. We need to find a way of melting it prior to excavation and gathering together just the gaseous methane. In thermodynamic terms, it is possible to melt the methane by burning it with the quantity of heat required to burn about 10-20% of the total quantity of methane, but various conditions are needed for it. Simulations are being performed to study these conditions.



Phase diagram of hydrogen hydrate derived from simulations: This figure shows the types of hydrogen hydrates that are produced at 0 °C with various pressures and hydrogen compositions . C_1 and C_2 are types of hydrogen hydrate. C_1 has hydrogen encaged in a diamond-like cubic crystal ice known as Ice I_c, while C_2 has hydrogen encaged in an orthorhombic crystal ice known as Ice II. VII is cubic crystal ice with a different structure. H_2 indicates a state in which the hydrogen is not encaged in ice but exists outside in liquid form. Regions denoted by two labels stand for coexistence of the corresponding two phases. The images on the left and right show the structures of C_1 and C_2, respectively. In the images, green hydrogen molecules are encaged in the lattice of red and blue water molecules. Under high pressure, there are large numbers of hydrogen molecules encapsulated in each cage , but under low pressure there are only a few. In the case of C_2, the ice crystal structure breaks down at low pressure.

Approach of Priority Area Researcher

Microscopic mechanism of dissociation process of methane hydrate

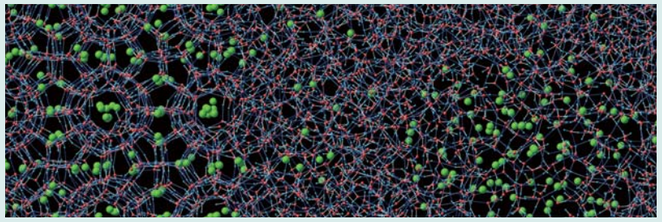


Takuma Yagasaki
Graduate School of Natural Science and Technology, Okayama University

Methane hydrate is a solid comprising hydrogen-bonded water cages, which trap methane molecules. Nowadays, many efforts have been made to obtain natural gas from methane hydrates in marine sediments by dissociating them undersea. The dissociation of undersea methane hydrate is also important in atmospheric sciences because it is related to global warming. The mechanism of the hydrate dissociation is still unclear at the molecular level, although it is an important process in many fields of science. I'm now trying to clarify this issue.
One of the most exciting things in research is observing unexpected phenomena. I got this fortune in this study. In general, the melting temperature of a solid is determined by the bond strength between particles, and does not depend on the surrounding environment. However, our molecular dynamics simulations revealed that the melting temperature of methane hydrate in liquid water is significantly higher than that in methane gas at the same pressure.
When the hydrate dissociation occurs in liquid water, released methane molecules immediately become solvated in water. However, this process is highly suppressed because of the very low solubility of methane. This is the reason for the higher melting temperature in water. This mechanism is unique to gas hydrates and cannot occur in usual one-component solids. It was expected from the mechanism that bubble formation causes an increase in the dissociation rate. We have confirmed this in the following calculations.
Our mechanism suggests inhomogeneous melting of methane hydrate due to bubbles. However, it is difficult to examine this phenomenon by small-system simulations. Effects of heat transport, gradient of methane concentration, and translation of bubbles are important for the hydrate dissociation, but analyses of them also require large-system simulations. We will address these issues by using the K computer.

What are your plans for future research in this area?

For hydrogen hydrate, we are working to develop models and theories in order to improve accuracy in predicting its thermodynamic stability. For methane hydrate, we plan to conduct even larger-scale simulations in order to examine dissociation kinetics by performing simulations in the presence and absence of methane bubbles. Current simulations do not allow us to track formation and growth of bubbles in water.
We are also making plans to use simulations to determine whether it is possible to melt the hydrate by applying external field.



A snapshot in the course of the methane hydrate dissociation in water. Released methane molecules form a bubble. This bubble enhances further dissociation.

Interview with Priority Research Topic Leader

Development of multiscale structural design and assessment techniques to improve the performance of metallic structural materials

Interviewee :
Masanori Kohyama
Prime Senior Researcher, Research Institute for Ubiquitous Energy Devices, National Institute of Advanced Industrial Science and Technology (AIST)

Interviewer :
Kazuhito Shida
CMSI Materials Science Division Researcher
Institute for Materials Research, Tohoku University

Objectives of research for this Priority Research Topic

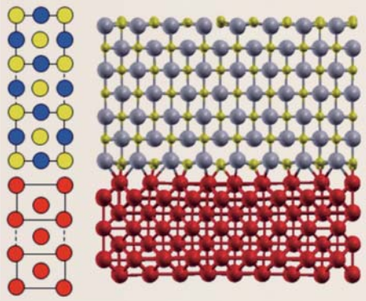
The objective of research in this area is to gain an understanding of the mechanical properties of iron and steel and other metallic structural materials from the atomic and electron level on up. The strength of a metal is determined by its ease of mobility of dislocations (linear defects). For this reason, metallic materials are not monocrystalline but polycrystalline (aggregates of crystal grains), forming a microstructure in which compounds have been deposited. Microstructures achieve high strength by preventing dislocation mobility by means of their grain boundary (interface between crystal grains), deposits, solute atoms, defect clusters and so on.
First-principles calculations are possible for simple defects and interfaces of such metals. Due to lattice misfit, however, the non-coherent (partially coherent) interfaces between deposits and metals require extremely large supercells consisting of several thousand to several tens of thousands of atoms, making it difficult to perform first-principles calculations. In this Priority Research Topic, the K computer and a cutting-edge calculation method are being used to achieve large-scale first-principles calculations for the interfaces between different phases, grain boundaries, dislocations and so on. The aim is to gain an understanding of the detailed interatomic bonds and energy in microstructures, as well as the dynamic behavior and the effect of alloy content and additive elements.

Calculation method

OpenMX, a large-scale first-principles calculation code, is being used in this area. OpenMX calculates electron structures using localized atomic orbital basis sets based on density functional theory. A density matrix is determined for clusters within a set range for each atom, and self-consistent calculations are performed to determine electron structure, total energy and the force acting on the atom. The electron structure is determined in a localized manner, making it possible to use order-*N* calculations, in which the total calculation time is directly proportional to the number of atoms. Use of the K computer is expected to enable large-scale parallelization, and optimization is underway.
QMAS, a plane wave basis set PAW method code, will also be used. Although it cannot handle large systems, QMAS can be used to calculate local stress and local energy, and it is capable of determining the stress and energy distribution at interfaces and grain boundaries and in the area of dislocations with a high degree of accuracy.

First-principles calculations for interfaces between different phases

We have begun with calculations for the titanium carbide (TiC) / iron interface. In iron and steel, TiC, niobium carbide (NbC), vanadium carbide (VC) and other substances are deposited to improve mechanical properties. Solidified transition metal atoms and carbon (C) atoms are deposited as a compound phase, so initially a "coherent interface" in which the iron atoms and carbon atoms meet in a coherent fashion is formed between iron (Fe) (100) // TiC (100) and Fe[100] // TiC[110]. Due to lattice misfit, a coherent interface at which the soft iron stretches slightly in the direction parallel to the interface is formed. The coherent interface itself is stable. As the deposits grow, however, the strain energy on the iron side increases, until overall it outweighs the benefit of the coherent interface formation. At this point, it is predicted to change to a "partially coherent interface" that has less strain even though coherence is sacrificed in the process (see Figure).



Model of compound / iron coherent interface (left) and partially coherent interface (right). Example of NbC (100) / Fe(100) interface. (Prepared by Hideaki Sawada of Nippon Steel & Sumitomo Metal Corporation)

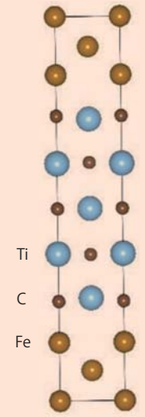
It is necessary to be able to handle both coherent and partially coherent interfaces with first-principles calculations, and to properly estimate the strain energy in the area around deposits. As the number of atoms in the cell is large (several thousand to several tens of thousands), first-principles calculations for partially coherent interfaces can only be executed using the combination of the K computer and OpenMX. At present, we are making good progress in obtaining calculated results for stable atomic arrangements and energy in partially coherent interfaces. With regard to the stress near the interface, QMAS calculations have resulted in the discovery of a new type of stress resulting from the electron structure of the Fe atoms at the interface, and this will no doubt attract considerable attention in academic circles.
In iron and steel, solidified hydrogen tends to invite brittle fracture. Capturing the hydrogen at the interface between the deposits and the iron is expected to make it possible to prevent this brittle fracture. We plan to pursue a detailed study of hydrogen capture by determining the structure of coherent and partially coherent interfaces. We also hope to conduct large-scale calculations for dislocations and grain boundaries using OpenMX. In the case of dislocations, attention has focused on the need to understand the interaction between dislocations and the solidified additive elements.

Benefits for society

The development of structural materials with outstanding strength, toughness and thermal resistance will enable highly efficient energy conversion in various types of generators and internal combustion engines, as well as reduced energy consumption through the construction of lightweight transport vehicles. This technology will also be indispensable for building highly reliable large structures and other elements of a safe and secure social infrastructure. Scarce elements are often used in the additive elements and alloy content of structural materials, and the understanding on a microscopic level that will be provided by research achievements in this area will make a major contribution to the technical development of substitutes for scarce elements.

Approach of Priority Area Researcher

First-principles calculations of iron-MX interfaces (M=transition-metal; X= C, N): the perspective of local energy and local stress



Fe(100)/TiC(100) coherent interface model (5-layer/5-layer supercell)

Vikas Sharma
Research Institute for Ubiquitous Energy Devices, National Institute of Advanced Industrial Science and Technology (AIST)

Development of high-performance metallic materials for structural and thermal applications is crucial to attain more efficient use of energy in the society. In order to improve the mechanical performance, strength and toughness, of iron or steel, precipitates such as transition-metal carbides or nitrides are generated inside it by thermal processes. The size of precipitates, the structure and nature of iron/precipitate interfaces and the stress around the interfaces are crucial to control the mechanical performance. The presence of lattice misfit between the precipitate and iron is an essential issue, which induces the misfit stress at the interface, affecting the size of precipitates and the bulk mechanical properties. In our project, large-scale first-principles calculations of semi-coherent iron/carbide (nitride) interfaces without misfit strains are performed by order-*N* scheme. On the other hand, it is important to make basic analysis of local stress and local energy at the coherent iron/carbide (nitride) interfaces based on the behavior of electrons. I basically deal with this subject. We use the projector augmented wave (PAW) method with plane-wave basis based on the density-functional theory with the help of the QMAS (Quantum MAterials Simulator) code developed in AIST. By this code, we can obtain local energy and local stress in each local region inside the supercell of iron/precipitate interfaces, via the energy-density and stress-density calculations combined with proper integration techniques to settle the gauge-dependent problem. We have started with a Fe(001)/TiC(001) coherent interface, where we have found the interface stresses caused by the lattice origin and the electronic origin.

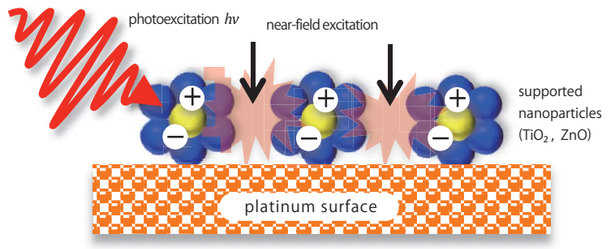
Photo-induced electron dynamics in nanostructures and development of quantum devices with optical and electronic functionality

Interviewee :
Katsuyuki Nobusada
Associate Professor, Institute for Molecular Science, National Institutes of Natural Sciences

Interviewer :
Masashi Noda
CMSI Molecular Science Division Researcher
Institute for Molecular Science, National Institutes of Natural Sciences

What type of research are you conducting for this Special Support Topic?

Electronic devices use the movement of electrons, but we can develop new devices by utilizing light functions in addition to such electronic functions. Our objective is the theoretical design, from a basic physical standpoint, of quantum devices with optical and electronic functionality that are smaller and faster, consume less energy, and have a greater ability to withstand external influences. Our highest priority is to propose design guidelines, from a computational science perspective, that can aid in the development of next-generation devices for the propagation of electromagnetic field energy (waveguides), as well as quantum data transfer devices, solar cells and photocatalysts efficiently converting photovoltaic energy into electricity, chemical energy and so on.



Theoretical design for a light energy conversion nanodevice with broadband, high-efficiency visible light response characteristics. Clear couplings of electrons and electromagnetic fields are produced through near-field light interaction occurring in orderly rows of nanoparticles placed on the platinum (Pt) surface.

Why do you need to use the K computer to conduct theoretical design?

The functionality of the optical and electronic next-generation quantum devices considered in our research is governed by the complex interactions and motion of electrons and light occurring in extremely tiny domains on the order of a few to a dozen or more nanometers. To complement the experimentation and development research whose goal is device design, we will also conduct device design on the basis of theoretical calculations, and we plan to make extensive use of the findings in actual device design. It will be extremely important to pursue device development from the standpoint of both theory and experiment.

The behavior of light and electrons occurring in nanometer-size devices can be expressed in equations based on quantum mechanics. Solving these equations in a manner that envisions an actual device will require calculations on an extremely large scale. Using approximately 200,000 cores, or about one-third of the total resources of the K computer, our group has completed a program efficiently describing the behavior of light and electrons.

Can you tell us about the future prospects for research in this area?

Research areas for the development of next-generation devices vary widely, from basic research to application development, and for this reason it is vitally important to clearly identify the issues to be resolved. We plan to use the K computer to its maximum potential to gain an understanding of the mechanisms of device operation from a basic academic standpoint and formulate theoretical predictions for the discovery of new functions and so on, in order to establish a nano-optical response theory that can serve as a guiding principle for device design.

Fundamental study for development of high-performance Li-ion battery

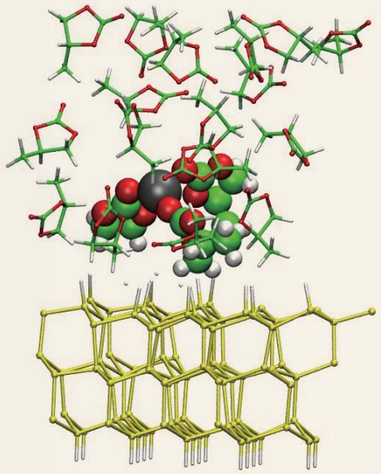
Interviewee :
Minoru Otani
Researcher, Nanosystem Research Institute,
National Institute of Advanced Industrial Science and Technology (AIST)

Interviewer :
Nicéphore Bonnet
CMSI Priority Area Researcher
Institute for Solid State Physics, The University of Tokyo

The challenge of finding our way to sustainable energies is putting an increasing demand on computational studies. In our group, we are using the K computer with the objective to shed light on a key mechanism that takes place in lithium-ion batteries.

The emergence of a sustainable, non CO_2-emitting, energy economy depends heavily on the development of autonomous power systems for application in smart-grid energy storage and transportation. In this regard, Li-ion batteries are a leading technology whose performance–measured in terms of energy density, power density, recharging time, durability, cost, and safety–depends critically on the structure and composition of the electrodes and electrolyte. In particular, the properties of the solid-electrolyte interface (SEI)–the specific phase that results from the chemical decomposition of the organic solvent on the surface of the anode–are known to be very sensitive to the insertion of small quantities of chemical additives into the electrolyte. Because, in addition, the SEI is known to simultaneously control the electrode resistance against corrosion and the Li-ion insertion-extraction rate, a detailed knowledge of the SEI structure is essential in trying to reduce the degradation of the battery discharge capacity upon successive charge-discharge cycles.

In practice however, the SEI is hard to characterize experimentally, implying a strong interest in directly simulating the SEI formation mechanism in the computer. Recently, we have used the first-principles code OpenMX+ESM on the K computer to run 500-atom simulations in which the anode is represented by a slab made of silicon–that has higher Li insertion capacity than carbon–and the electrolyte is composed of one molecule of $LiPF_6$ salt dissolved in propylene carbonate. When putting the system under bias, we have been able to directly observe the progressive migration, desolvation, and adsorption of the Li ion on the surface of the electrode. Following these promising results, we are now conducting simulations containing up to 4000 atoms, which will allow us to assess the critical effect of ppm concentrations of chemical additives and/or traces of water on the Li-ion insertion process and SEI formation mechanism.



Snapshot from MD simulation of the electrode/electrolyte interface of a lithium-ion battery: desolvation of the lithium ion (in black) from propylene carbonate in the vicinity of the electrode.

Report: 3rd CMSI Workshop

New Computational Materials Science Made Possible by Massively Parallel Computing

The 3rd CMSI Workshop was held December 3-5, 2012 at the Okazaki Conference Center in the National Institutes of Natural Sciences (NINS), with more than 100 researchers in attendance.

As in previous years, representatives from each area of research presented reports on achievements attained during the year. This year, the workshop also included some of the presentations submitted by researchers not currently affiliated with CMSI. This was an effort to move CMSI activities a step forward in terms of locating and training new researchers. In the administration of the workshop as well, there was an active effort to elevate young researchers, and 16 Division Researchers served as chair during the course of the three-day workshop.

In the presentations by invited speakers, Mr. Akiyoshi Kuroda of the RIKEN Advanced Institute for Computational Science (AICS) spoke on the topic of "Can the FFT Run Fast on Massively Parallel Computers." He presented that multi-axial parallelization in the plane wave basis set density-functional approach had been successful in achieving more than 20% of peak performance for the entire K computer system, and that even greater performance improvements are anticipated through the use of a three-dimensionally partitioned FFT library.

Professor Isao Tanaka of Kyoto University gave a presentation entitled "Materials Informatics based on First-principles Computing," in which he stressed that materials informatics is increasing in importance as a gateway to the development of new materials, but that the number of researchers in this area is extremely low as compared with other countries. For this reason, he made an impassioned appeal for development in terms of both research and personnel, as a task requiring urgent action.

There was also a panel discussion on the future of supercomputers jointly sponsored with the High Performance Computing Infrastructure (HPCI) Consortium. The panelists were Professor Hiroshi Nakajima of Kyoto University, Mr. Kazuo Minami of RIKEN AICS, Professor Naoki Kawashima of the Institute for Solid State Physics, Professor Isao Tanaka of Kyoto University, Associate Professor Katsuyuki Nobusada of the Institute for Molecular Science, and Project Professor Synge Todo of the Institute for Solid State Physics. Despite being held after the main program had finished on the first day, the panel discussion prompted a spirited discussion between the panelists and attendees.

In the poster session, the Poster Award, presented for outstanding research by young researchers (35 years of age or under), is a regular feature of the workshop. The young researchers exercised a great deal of ingenuity in their presentations, and wherever one looked young researchers could be seen engaged in serious discussions in front of their posters.

In this year's workshop, the awards were given not only to posters but to presentations as well, and two new categories were established: the "Young Researcher Award" and the "Visualization Award."

The Poster Award winners and their research subjects are presented on Page 20.

CMSI Calendar

For more information, see the CMSI website
http://cms-initiative.jp

●1st TUT-CMSI Science Visualization Symposium 2013
(sponsored jointly with Toyohashi University of Technology)
Date: March 5, 2013
Venue: UDX NEXT-3 and UDX Theater (Akihabara)

●2nd CMSI Kobe Hands-on: ALPS Tutorial
Date: March 6, 2013
Venue: CMSI Kobe Branch (RIKEN Advanced Institute for Computational Science (AICS) R501)

●CMSI Industry-Government-Academia Cooperation Symposium
Date: March 12, 2013
Venue: Akihabara Dai Bld. Conference Center

● K Computer Users Interim Report Seminar
Date: March 14 - 15, 2013
Venue: RIKEN Advanced Institute for Computational Science (AICS)

●The Chemical Society of Japan 93rd Spring Annual Meeting
Symposium "Chemistry in the Age of Supercomputing"
Date: March 25, 2013
Venue: Ritsumeikan University Biwako Kusatsu Campus

●The Physical Society of Japan 68th Annual Meeting
Symposium "Computational Physics Advances Toward the Exascale Age"
Date: March 27, 2013 (afternoon)
Venue: Hiroshima University

●23rd Computational Materials Design (CMD®) Workshop
Date: September 2 - 5, 2013
Venue: Institute for NanoScience Design, Osaka University

●CMSI International Workshop
Date: October 17 - 19, 2013
Venue: The University of Tokyo (Hongo Campus), Nagoya University, RIKEN Advanced Institute for Computational Science (AICS)

●CMSI International Symposium
Date: October 21 - 22, 2013
Venue: Ito International Research Center, The University of Tokyo

The 3rd CMSI Poster Award

We introduce the 3rd CMSI Poster Award winners and their research subjects.

CMSI Poster Award

Ryui Kaneko

Graduate School of Engineering, The University of Tokyo

Analysis of J_1-J_2 Heisenberg model by the many-variable variational Monte Carlo method

By using the many-variable variational Monte Carlo method, we calculate the ground state of the J_1-J_2 antiferromagnetic Heisenberg model, and find a spin-gapped quantum spin liquid phase, sandwiched by the Néel and striped antiferromagnetic phases.

CMSI Young Researcher Award

Satoshi Morita

Graduate School of Engineering, The University of Tokyo

Optimization of many-variable variational Monte Carlo method

I have optimized and massively parallelized the many-variable variational Monte Carlo code. I have achieved 60 times speed up of the performance and more than 90% parallelization efficiency with the help of a number of refinements such as a generalization of the fast update algorithm for Pfaffian and redesign of data structures. (See p.5 for more details.)

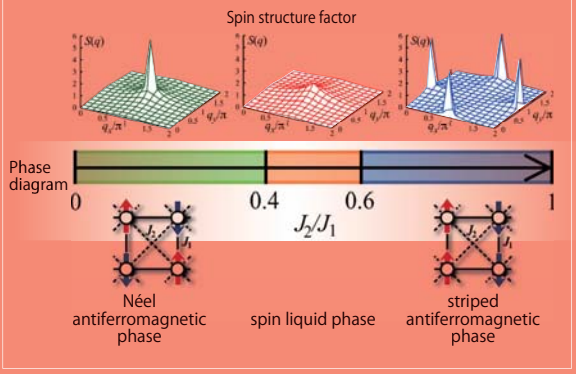
CMSI Visualization Award

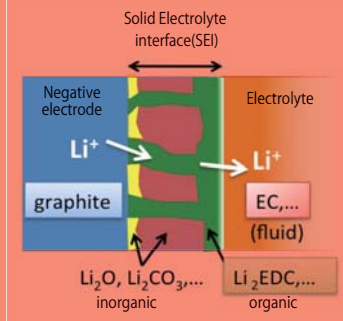
Nobuko Ohba

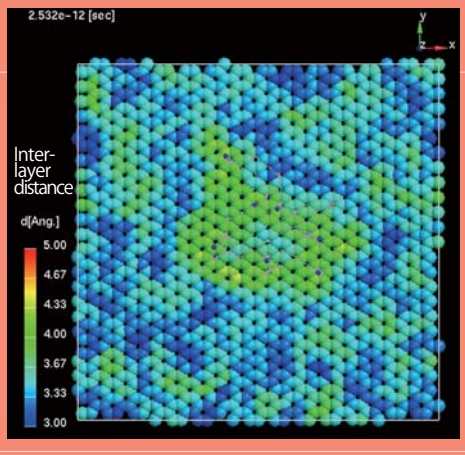
Toyota Central R&D Labs., Inc

Divide-and-conquer-type real-space-grid DFT and its application to hybrid QM-CL simulation

Numerical analysis of the Li diffusion in graphite (negative electrode) in Li-ion battery by using the divide-and-conquer-type real-space-grid density functional theory (DC-RGDFT). It is found that the moving area of Li's is limited. The visualization of simulation results was made by using "viewer" developed by T. Kouno (CMSI).







Torrent No.7 Feb. 2013

2 **Special：Research Topics in CMSI**
New paradigm introduced by the K computer
Tatsuya Sakashita

4 Interview with Priority Research Topic Leaders and Special Support Topic Leaders
Search for new quantum phases in strongly-correlated quantum systems and explanation of dynamics
Masatoshi Imada×Tsuyoshi Okubo

6 **Electron states and dynamics: new developments in molecular theory and integration of heat fluctuations**
Seiichiro Ten-no×Takehiro Yonehara

8 **Prediction of electron functions in nanostructures using the density functional approach**
Atsushi Oshiyama×Kanako Yoshizawa

10 **Development of the molecular science of viruses through all-atom simulations**
Susumu Okazaki×Yoshitake Sakae

12 **Large-scale calculations for basic processes in fuel-cell related materials**
Osamu Sugino×Ryota Jono

14 **Mechanism of hydrogen and methane hydrate formation and dissolution and thermodynamic stability**
Hideki Tanaka×Tsutomu Kawatsu

16 **Development of multiscale structural design and assessment techniques to improve the performance of metallic structural materials**
Masanori Kohyama×Kazuhito Shida

18 **Photo-induced electron dynamics in nanostructures and development of quantum devices with optical and electronic functionality**
Katsuyuki Nobusada×Masashi Noda

18 **Fundamental study for development of high-performance Li-ion battery**
Minoru Otani×Nicéphore Bonnet

Approach of Priority Area Researchers
5 Satoshi Morita
7 Yu-ya Ohnishi
9 Kenichi Koizumi
11 Kazushi Fujimoto
13 Hidetoshi Kizaki
15 Takuma Yagasaki
17 Vikas Shrama

19 **Report: 3rd CMSI Workshop ／ CMSI Calendar**

20 **The 3rd CMSI Poster Award**

Cover：Colorful pencils are spreading out; they overlap and create new colors like a broad range of researches in CMSI.

Torrent : The Newsletter of the Computational Materials Science Initiative (CMSI) No.7, Feb 2013

CMSI is a research network promoting Field 2 "New Materials and Energy Creation" within HPCI Strategy Program (SPIRE) of the MEXT, Japan.

Published by
Computational Materials Science Initiative

Edited by CMSI Publicity Committee
Office Institute for Solid State Physics, The University of Tokyo
5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan
TEL: (+81) 4-7136-3279 FAX: (+81) 4-7136-3441 http://cms-initiative.jp ISSN 2185-8845

Production Assistance : Sci-Tech Communications Incorporated Design : Takada Office Inc.

cmsi Computational Materials Science Initiative