MANA NEWS LETTER

CONVERGENCE

No.24 | 2016 | October

International Center for Materials Nanoarchitectonics (MANA)

Nano Revolution for the Future

Leader's Voice

Pioneering New Fields with Unwavering Research Concepts

Takuzo Aida

Asking the Researcher

Takao Mori

Solving the Energy Problem by the Power of Nanotechnology

– Aiming at Control of Phonons –

MANA Principal Investigator,
Nano-Power Field

Group Leader,
Thermal Energy Materials Group

Takao Mori

PROFILE

Dr. Takao Mori completed his Ph.D. in the Department of Physics, Graduate School of Science, The University of Tokyo in 1996 and became a JSPS Research Fellow (PD) in the Department of Applied Physics, School of Engineering, The University of Tokyo the same year. He joined the National Institute for Research in Inorganic Materials (NIRIM; a predecessor of NIMS) of Japan's Science and Technology Agency in 1998, and joined the National Institute for Materials Science (NIMS) in 2001.

He is Laboratory Director of the Materials for Thermal Energy Conversion Open Laboratory in the NIMS Open Innovation Center, External Collaboration (EC) Division, and Visiting Professor at Hiroshima University. He is also Chief Researcher of the Thermal Management and Thermoelectric Materials Group, "Materials Research by Information Integration" Initiative, NIMS.

Asking the Researcher

Solving the Energy Problem by the Power of Nanotechnology

— Aiming at Control of Phonons —

The coming era of limited energy will be very difficult for everyone on Earth, and there have been high expectations for thermoelectric materials, which convert waste heat directly to useful electricity. We interviewed Dr. Takao Mori, who has been engaged in research to elucidate the mechanisms for high performance in the materials with Nanoarchitectonics, asking how we can overcome the issue with science.

Interviewer: Akio Etori, Science Journalist

The energy problem and thermoelectric materials

In the flow of energy supply, the energy loss in the use of primary energy such as petroleum, coal and natural gas is extremely large. Effectively utilized energy accounts for no more than about one-third of the original energy. Virtually all of the remaining two-thirds is discarded as waste heat.

For this reason, large expectations have been placed on thermoelectric materials in recent years. Thermoelectric materials are solid materials which have the property of mutually converting thermal energy and electric energy. The phenomenon of direct conversion of a temperature difference in an object to electric voltage was discovered in 1821 by the physicist Thomas Seebeck and is called the Seebeck effect. However, even today, in the 21^{st} century, technologies for direct conversion of waste heat to electricity utilizing the Seebeck effect have still not reached practical application. The main reason for this is the fact that no thermoelectric material with adequate performance has yet been developed. To solve this problem, Dr. Takao Mori of MANA is engaged in research aimed at achieving high performance in thermoelectric materials from the standpoint of nanoarchitectonics. "We've taken on the challenge of solving a global-scale problem, namely, the energy problem, by studying materials from a truly small, 'nano' viewpoint."

To begin with, Dr. Mori explains the two large hurdles to high performance in thermoelectric materials. First, the index that represents the performance of thermoelectric materials is expressed by $Z = S^2 \sigma/\kappa$, where Z is the figure of merit, S is the Seebeck coefficient, σ is electrical conductivity and κ is thermal conductivity. In order to increase the figure of merit Z, it is necessary to increase the Seebeck coefficient S and electrical conductivity σ simultaneously. However, this is not easy because a tradeoff relationship generally exists between S and σ. "In semiconductors, σ increases if the carrier density is increased, but S becomes smaller. In insulators, S is extremely large, but σ is small, which means current does not flow."

As the second hurdle, a material with good electrical and poor thermal conductivity is required. Since the voltage generated in a thermoelectric material corresponds to the temperature difference, transmission of heat in the material should be prevented as much as possible. In other words, in order to generate good voltage, the temperature difference needs to be maintained. This is also no simple matter because "conduction of electricity" and "non-transfer of heat" are generally mutually-contradictory properties.

As an additional problem, the thermoelectric materials that were considered promising in the past used elements such as bismuth (Bi), tellurium (Te) or lead (Pb) which are scarce and expensive and/or toxic. To realize wide practical application of thermoelectric materials in society in the future, Dr. Mori believes that it is important to develop thermoelectric materials using raw materials which are abundant in nature and can be obtained at low cost. "Considering global conditions, we should avoid a situation where we must inevitably depend on rare metals, particularly in resource-poor countries like Japan."

Creation of new thermoelectric materials by nanoarchitectonics techniques

In his current research, Dr. Mori is developing thermoelectric materials mainly from two directions. The first involves precise control of the nanostructure in thermoelectric materials by utilizing nanoarchitectonics. "The length of the mean free paths of the phonons and electrons that carry thermal energy are generally different. The approach of creating a nanostructure that can scatter phonons more selectively by utilizing these different mean free paths is widely used around the world. That is, heat is effectively scattered in the material, but due to the short mean free path of electrons, the electrons are hardly affected and can pass through the material. The key point is what kind of nanostructure we should use."

Conventionally, mechanical methods, for example, using a ball mill, were frequently used to introduce a nanostructure into the material. However, Dr. Mori and coworkers have succeeded in fabricating a new nanosheet of a thermoelectric material (Fig. 1). "Nanosheets of a copper tellurium compound (CuTe) are delaminated by a wet bottom-up process using a three-stage chemical reaction. In a sample using this nanosheet, heat could be scattered with comparatively little loss of electricity, and the thermoelectric effect was improved by 30% in comparison with conventional materials. This in itself is a significant improvement in performance. Actually, however, this material still does not have the ideal structure from the viewpoint of nanoarchitectonics. Thus, a dramatic improvement in performance is expected if these can be arranged more skillfully to produce a bulk material with a high-order layered structure."

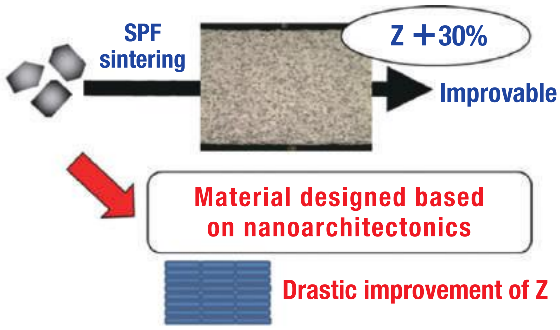


Figure 1a: Possibility of nanosheet of thermoelectric material: The performance of the nanosheet thermoelectric material produced by the wet bottom-up process created by Dr. Mori and coworkers can be improved by 30%, even in samples not optimized by spark plasma sintering (SPS) at all. However, in the future, dramatic improvement of performance is expected if it is possible to arrange the sheets in a high-order structure designed by nanoarchitectonics.

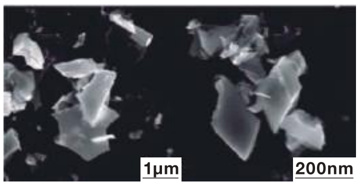


Figure 1b: Electron microscope image of delaminated nanosheet of copper tellurium compound (CuTe)

The champion thermoelectric material in the mid- to high-temperature range, realized with a rare earth-free composition design

As potential champion thermoelectric materials in the mid- to high-temperature range, many researchers around the world are studying materials with caged crystal structures. High performance can be achieved in this type of thermoelectric material because phonons are effectively scattered by utilizing the phenomenon called "rattling", in which atoms doped in the cage structure are vibrating ("rattling") inside the cage. However, practical application is difficult because rare earth elements, etc. are frequently used as the dopant, which incurs supply risks on the material side, and oxidation resistance is also poor.

To avoid these problems, Dr. Mori's group discovered a method in which high performance is obtained from the caged crystal structure without depending on rattling of rare earth atoms. They developed a thermoelectric material with the world's highest performance, comparable to the best materials using rare earths, by forming an appropriate porous structure in the material as a new nanostructure (Fig. 2). "In spite of the rare earth-free composition design, conversion efficiency is equivalent to 15% or more. I think this is an important advance toward the long-desired goal of practical application."

This research achievement received the nano tech Grand Award 2016: Research Project Award (Green Nanotechnology Division).

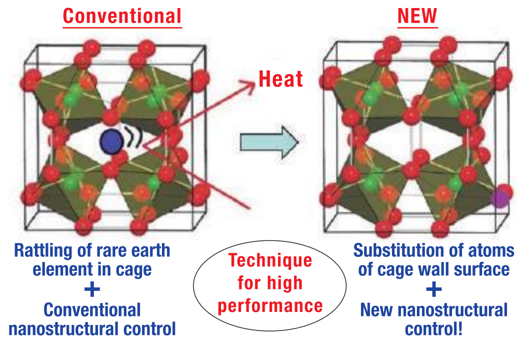


Figure 2a: (Left) Conventionally, high performance was achieved in thermoelectric materials with a caged crystal structure by utilizing rattling by doping rare earth elements. (Right) The new thermoelectric material discovered by Dr. Mori's group is rare earth-free.

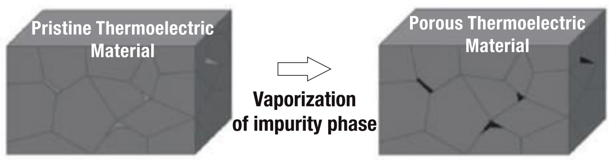


Figure 2b: Synthesis of new high performance thermoelectric material. Atoms in the cage wall structure are substituted, and pores are formed as a new nanostructure in the material by vaporization of an impurity phase which is intentionally created based on the phase diagram of the material (diagram showing the relationship between the phases of a substance and its thermodynamic state). Due to the existence of appropriate pores, the material conducts electricity but heat is easily shielded.

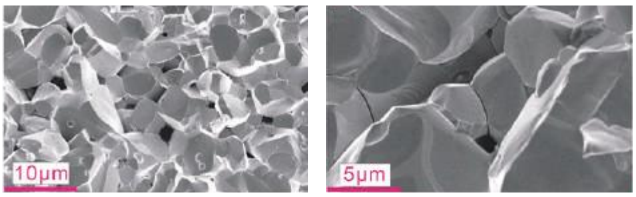


Figure 2c: Electron microscope images of new high performance thermoelectric material. The existence of pores can be confirmed.

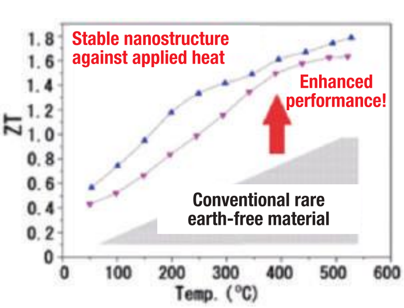


Figure 2d: Graph showing performance of new high performance thermoelectric material using pores. Dramatically higher performance is realized in comparison with the conventional rare earth-free material.

Keen interest from industry

In 2015, the research topic "Development of novel magnetic semiconductor thermoelectric materials and thermoelectric generation devices," under the leadership of Dr. Mori, was selected as a CREST Project of the Japan Science and Technology Agency (JST), and a team type research project was launched with the cooperation of NIMS and Tsukuba University, which are research organizations in the Tsukuba area. The ultimate goal is to create power generation devices which will contribute to practical application by theoretically elucidating and developing the mechanism of high thermoelectric performance by magnetism. This approach also includes the use of advanced nanostructural control.

Thermoelectric materials have attracted keen interest also from industry. Dr. Mori says that the NIMS Open Innovation Center, in which he himself is involved, is functioning extremely well in this regard. "We are enjoying active participation by companies, and we now have the best conceivable environment for research and development. Although there is still not a large market for thermoelectric power generation, our researchers are taking on issues that are close to basic research together with companies. Thanks to this interest from the corporate side, we've learned a lot about the issues and needs from the viewpoint of application."

How to overcome the cost issue is also a problem. "For example, solar power wasn't profitable at first, and subsidies from the government were necessary for popularization of that technology. However, solar power is now an extremely large industry. It's necessary to have a spirit of challenge, which doesn't give up because the hurdles are high, but asks how we can overcome those hurdles. Both researchers and companies have to have that spirit."

Control of phonons – a dream of human science

When we asked Dr. Mori who has had the greatest influence on him in his life to date, he replied, "It's still my father." He went on to say, "Because my father was a particle physicist, I was always interested in science since childhood. My father was a particle physicist, and I do research in solid-state physics. Although our fields are different, I think he had a really large influence on me, in something that can be communicated, even without words, about the proper stance of a researcher."

Beyond development of thermoelectric materials, Dr. Mori is looking ahead to thermal control as a big research theme. During the 20th century, it became possible to control many of the key elements that make up the physical world, such as electrons, spins, and photons, by the power of science, but precise control of phonons and heat still has not been realized. "In the 21st century, I think that control of heat at a high level will be the greatest challenge for humankind. Thermoelectric materials are also included in this big theme. This is definitely not an impossible goal. Because of the accumulation of our understanding of thermal properties, phonon control and other knowledge to date, I believe that this can be realized. Of course it will be difficult, but I definitely want to follow through and accomplish this." "The nature of phonons is very different from that of electrons. I think this a good chance for today's young researchers because they can take on this important issue based on the accumulation of knowledge to date."

Dr. Mori, who always has a gentle smile, is also the father of one boy who is currently in elementary school. "Without realizing it, children learn by watching their parents. Since I was like that too, as a father, I have to show my son the hard work of being a scientist."

Research Outcome 1

Clarifying the Behavior of Atoms and Electrons in Nanoscale Structures by Theoretical Calculations
― Development of Ultra-Large-Scale First-Principle Simulation Technique ―

Tsuyoshi Miyazaki
MANA Principal Investigator,
First-Principles Simulation Group,
Nano-Theory Field

Problem of first-principle simulations.

Novel materials that display new functions and ultra-high performance are being energetically pursued by controlling the nanoscale structure, which has become possible thanks to progress in nanotechnology. In materials with structure at the nanometer scale, it is essential to understand the behavior of individual atoms. However, large numbers of atoms exist even in regions of this small scale; for example, a cube of crystalline silicon, with each side 30nm long, contains more than 1 million atoms. The forces that act between atoms, and hence the properties of substances, are determined by the behavior of electrons (or the electronic states), and these electronic states are described by quantum mechanics. First-principles simulation method, based on quantum mechanics, is a powerful technique that makes it possible to quantify various phenomena of materials at the atomic and electronic level, and has made important contribution to the development of materials science. A significant challenge that confronts conventional first-principles simulations is the numerical complexity of calculations, and as a result the size of the systems that can be calculated is extremely small, normally being of the order of 1000 atoms.

Order *N* method: Realizing first-principle simulation for million atom systems.

With the conventional first-principle method, it is difficult to calculate large systems because the computational complexity increases rapidly, with the cube of atoms *N*. In a joint project with a group led by Prof Bowler of UCL (University College London) (MANA Satellite Principal Investigator), we are currently developing the first-principles calculation program CONQUEST using a new technique called the Order *N* method, in which computational complexity is proportional to *N*. The efficiency of this program in massively parallel computers is also high, realizing first-principles calculations for ultra-large-scale systems. We have already demonstrated the possibility of first-principles calculations of million (10^6) atom systems with the K Computer. Recently, we also implemented molecular dynamics (MD) simulations with first-principles method, making it possible to achieve higher accuracy and efficiency.

Theoretical and experimental fusion research on core-shell nanowires.

Joint research in close collaboration with experimental groups has become possible by utilizing CONQUEST. In joint research with the Fukata Group at MANA, we investigated core-shell nanowires, consisting of silicon and germanium, as a system for use in next-generation vertical transistors, which enable high density integration. Our aim is to clarify the atomic-scale and electronic structure, impurity states and other features of nanowires of various sizes by performing first-principle calculations with the same size as the nanowires developed by the experimental group, and thereby develop higher performance next-generation device materials.

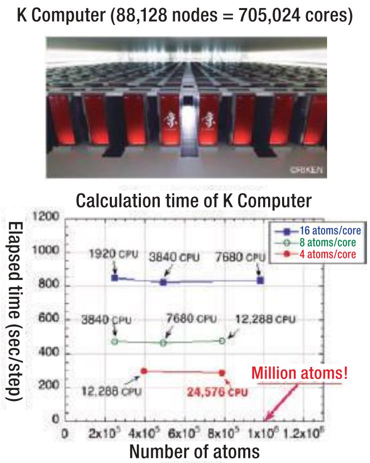


Figure 1: (Left) K Computer, a massively parallel supercomputer, and (right) calculation time on the K Computer when using the Order *N* method first-principle calculation program CONQUEST (*x*-axis shows number of atoms). Because the Order *N* method is used and parallelization efficiency is ideal, even the number of atoms is doubled computation time stays the same when double numbers of CPUs are used. It shows first-principle calculation of million atom systems is also possible.

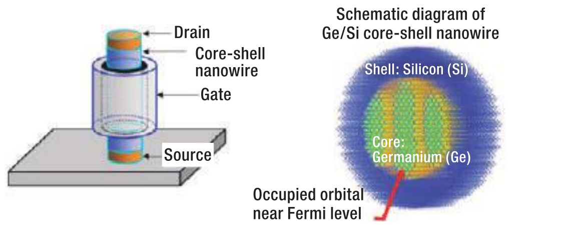


Figure 2: (Left) Schematic diagram of vertical transistor using core-shell nanowire, and (right) optimized structure calculated by first-principle calculation and one orbital occupied by 1 electron near the Fermi level (this orbital contributes to conduction in case of the p-type). It can be understood that this orbital is localized in the core region formed from germanium.

References

1) M. Arita, D. R. Bowler and T. Miyazaki, "Stable and Efficient Linear Scaling First-Principles Molecular Dynamics for 10000+ Atoms", J. Chem. Theory Comput. 10, 5419 (2014).

2) A. Nakata, D. R. Bowler and T. Miyazaki, "Optimized multi-site local orbitals in the large-scale DFT program CONQUEST", Phys. Chem. Chem. Phys. 17, 31427 (2015).

PROFILE

Deputy Director, Center for Emergent Matter Science, RIKEN. Professor, Department of Chemistry and Biotechnology, School of Engineering, The University of Tokyo. Graduated from the Division of Applied Chemistry, College of Engineering, Yokohama National University in 1979. Prof. Aida completed his Doctor of Engineering degree in the Department of Applied Chemistry, School of Engineering, The University of Tokyo in 1984, and served as an Assistant in that department from 1984. He was later appointed Associate Professor of the same department, and was named Professor of the Department of Chemistry and Biotechnology, School of Engineering, The University of Tokyo in 1996. He has held his present position at RIKEN since 2013. He serves on the Review Board of the journal Science and on the Advisory Board of the Journal of the American Chemical Society. He has also received numerous awards, including the Award of the American Chemical Society in Polymer Chemistry and Award of the Chemical Society of Japan in 2009, the Fujiwara Award in 2011 and the Leo Esaki Award in 2015.

Leader's Voice

A Conversation with Prof. Takuzo Aida

Interviewer: Akio Etori, Science Journalist

Pioneering New Fields with Unwavering Research Concepts

Ideas built into molecules

— I understand that you're involved in a diverse range of research, from aqua materials to chemistry of energy conversion, supramolecular polymers and soft materials.

Actually, I'm interested in the correlation between structure and properties. Nanoscience has steadily progressed to the point where we can relatively easily realize our expected designs and functions at around the nanoscale when assembling a structure from molecules. But upward to the mesoscale, and the macroscale that is visible to the naked eye, we face many difficulties in controlling the structure, as the molecular assembly processeses don't converge on a single structure. I'm currently seeking strategies to bridge the gap, this "missing link" between the nano world and the ordinary world.

— It's difficult to build up structures from nano to macro size while keeping the expected structures, right?

That's right, because there are various kinetic traps in molecular assembly at the meso and macro levels. Different multiple structures are created due to multiple kinetic traps and mixed without constituting a single entity. This means we can't fully realize our ideas with molecules. On the other hand, human beings are made up of hierarchical and anisotropic structures that are the accumulation of molecules to the macroscale. This is enabled with certain physical perturbations of a living body. It is possible to make nanosized structures in a flask without pertubations, but quite difficult to avoid kinetic traps, the obstacle for expanding to the mesoscale and macroscale.

One successful example is the aqua material that we reported on in 2010, which is 98% water, but is free-standing and moldable. We previously adopted clay nanosheets as a component, but are now using titanium oxide nanosheets from Dr. Takayoshi Sasaki of MANA in our latest research. These titanium oxide nanosheets differ from other nanosheets in that they orientate perpendicularly to a magnetic field. This means each nanosheet can be aligned parallel to each other. Since these nanosheets have a negative charge, strong repulsion is generated between the nanosheets aligned parallel. By gelating these parallel-aligned nanosheets, we can develop a hydrogel that has anisotropic electrostatic repulsion.

We then found that this hydrogel expresses an unusual mechanical property we had never seen. If we arrange the nanosheets of the hydrogel oriented in the horizontal direction and try to compress the hydrogel orthogonally, it is highly resistive against compressive force, as the component nanosheets repel each other. This means that the gel can function as a rigid material. On the other hand, if we compress the hydrogel in the horizontal direction, it easily deforms, as the inner friction in the same direction of the nanosheets get extremely weak because of the large repulsion between the component nanosheets. This special mechanical property does not appear without an anisotropic structure carried through to the macroscale.

The importance of guiding research concepts

— What materials were you interested in originally?

I studied physical chemistry during college, but I moved to synthetic polymer chemistry in graduate school. I gained a lot of experience through work creating polymers by using catalysts. I became independent at age 37, and considered working on control of radical polymerizations as an extension of that. However, about half a year later, a research group in the U.S. published a paper about the functions of vitamin B12 in the body with exactly the same idea as mine. I took it as a sign that I should abandon continuing research based on the previous work in my field. I discussed the issue with my students and dropped it the same day. It was a turning point for me –I decided to more freely do exactly what I want to do.

My teacher, Prof. Shohei Inoue, said that the life cycle of a research project is about five years, meaning that spending too much time on a project and going into minute details isn't particularly meaningful. I'll work at something as long as it excites me, but I try not to cling to it.

— What were the differences between your polymer research until then and synthetic chemistry?

The biggest difference was the fact that the process of creating something wasn't important; the most important aspect was the properties and functions of the product. Synthetic chemistry attaches importance to the beauty of creation and the efficiency of the process. In materials research however, it's important to create new properties and functions.

When I started an ERATO project sponsored by the JST (Japan Science and Technology Agency), we couldn't do any interesting research for the first two years. I had a group meeting with project members, and they said that as the director of the project I hadn't presented a direction that they should follow. I've valued research concepts ever since. Deciding what molecule you should create, and deciding to do it, is the result of pursuing a research concept, which is a top-down approach.

This doesn't mean that the concept itself gives you concrete guidelines. Physicists are concept-oriented. For example, they begin from a concept like, "Why does an apple fall from a tree?" On the other hand, chemists focus on things. While being able to make things is good, ideas tend to move in the direction of, "What shall we do with

Leader's Voice

A Conversation with Prof. Takuzo Aida

these things?" Likewise, in materials science, research to implement the known properties and functions possible with one material using a different material is uninteresting.

What's most important is a guiding concept which provides the focal point for research. Still, I'm a chemist, so we want to design materials by ourselves as much as possible. I feel I am keeping this balance in my work.

Nanoarchitectonics has taken firm root around the world

── As a member of the MANA Evaluation Committee, what are your thoughts on MANA after its first ten years?

What research institutes need are distinctive, globally-competitive strengths, rather than a broad but shallow approach that dabbles in everything. When you look at conditions in Japan today, that's a question that answers itself. In that sense, I think that MANA has established a distinctive "brand" that is really different from other research organizations.

MANA also brings together diverse human resources along the axis of materials. That structure is important. MANA is one of the world's preeminent organizations, where outstanding researchers in different fields of specialization collaborate and work together in friendly competition as "next-door neighbors". That kind of environment is necessary in research.

Ten years ago the word "nanoarchitectonics" had a big impact in promoting new research, but the word is now acknowledged and widely known. I have high expectations for how this base will be used moving on to the next phase in the coming years.

── MANA is engaged with basic research for the development of new materials that will support the coming age.

The most important thing for scientists involved in basic research is breaking new ground. It might be a harsh thing to say, but doing basic research in an existing field is nothing but play. I think that hints for creating a truly new research field can be often found via ideas for practical applications. If you find that a practical application of something is impossible, that's an opportunity. Why is it impossible? Because the basis to make it possible hasn't appeared yet. This means you have found an unseen basic research field. If you think it's worth doing, then have the courage to do that basic research. I also work as a corporate consultant because companies often times produce seeds for important basic research. Strong, outstanding applied research can also have as remarkably high value as basic research. However, we should avoid applied research aiming at profit for business, which means that introducing "the concept of cost" to science by thinking about the economy, provision of materials, and the price of oil, among other things.

── So new research concepts can also be the product of applied research?

It's very difficult to come up with new concepts. They might come from a conversation with a student or a consultation at a company. It's important that you have an open mind toward things that come from outside yourself. Don't try to fit yourself into some predetermined frame, and don't be bound by one's sense of values. On the other hand, if you lack persistence in your interests, you won't be able to overcome adversities. We have to consider how and what values to adhere to and what values we should disregard. How we resolve this kind of contradiction within ourselves is a perpetual problem as a scientist.

From the left, Prof. Atsushi Maruyama,Tokyo Institute of Technology, Prof. Aida in his mid thirties, and Prof. Yukio Nagasaki, University of Tsukuba.

Research Outcome 2

Using Molecules to Control Electron Tunneling

— Development of Molecular Device Aiming at Ultra-Low Power Consumption Devices —

Yutaka Wakayama
Group Leader, Quantum Device Engineering Group, Nano-System Field

Importance of low power consumption nano devices.

Our everyday environment is virtually overflowing with IT devices. Although miniaturization and high density integration of the transistors that are the heart of those devices have finally approached their limits, there is also another challenge which must not be forgotten, and that is the problem of electric power consumption. According to one estimate, if their current level of power efficiency remains unchanged, IT devices will account for 20% of all power consumption around the year 2025. For this reason, development of devices for lower power consumption is becoming an urgent issue. To solve this problem, we are grappling with the development of novel electronic devices that are driven by very small amounts of electric current.

Potential of molecules.

Tunneling transistors, which employ the tunneling phenomenon of electrons, attracted attention as possible low power consumption devices from an early date. However, this technology still has not reached practical application because it is necessary to fabricate quantum dots precisely, which are the key constituent element in tunneling transistors, at a size of 10 nm or less. Even today, in spite of progress in micro-fabrication techniques, this is still a difficult challenge. Our research is an attempt to solve this problem by using molecules as quantum dots. Because the size and structure of molecules can be controlled freely, precise design of electronic states is also possible. Other superior features of molecules include the fact that different molecules can be incorporated simultaneously in one transistor, and it is possible to use photoisomerization molecules, which react to light. Thus, molecular quantum dots are expected to realize completely new functions that do not exist in the conventional type.

Development of new molecular tunneling device.

One challenge in the development of tunneling transistors using molecules is how to fabricate a realistic transistor structure from nanoscale component substances. For this, nanomaterials assembly technology, in other words, material nanoarchitectonics, is truly necessary.

As shown in Fig. 1, we constructed a double tunnel junction by stacking various molecules, insulation layers and metallic electrode on a silicon (Si) substrate by our original precision film-forming method. When the principle of electrical conduction in this junction was first analyzed using fullerene molecules, it was found that conduction was realized by resonant tunneling via molecular orbits. Fig. 2 shows the electric current characteristics at this time and the energy band diagram showing the principle. Since electrons tunnel one by one through molecules, this shows the possibility of operating a transistor with an extremely small current. By further extension of this principle, we also demonstrated characteristic operations of molecules, for example, multistage tunneling control by simultaneously incorporating heterogeneous species of molecules, and electron tunneling type optical switches using photoisomerization molecules, etc. As an additional advantage, because this device is constructed on a Si substrate, integration of devices by using existing micro-fabrication technology is also possible.

As a result of this work, we succeeded for the first time in the world in operating a vertical tunneling transistor device using molecules. Based on this, we aim to realize devices that simultaneously achieve all of the goals of miniaturization, high density integration and low power consumption in the future.

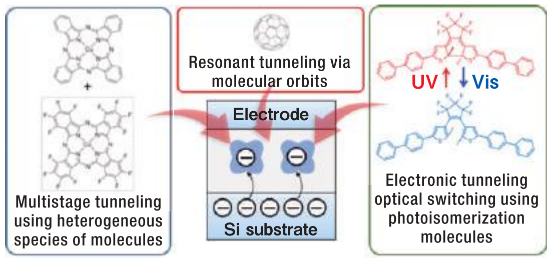


Fig. 1: Schematic diagram of double tunnel junction using various molecules as quantum dots. Multistage tunneling by mixing heterogeneous species of molecules, and optical switches using photoisomerization molecules are also possible.

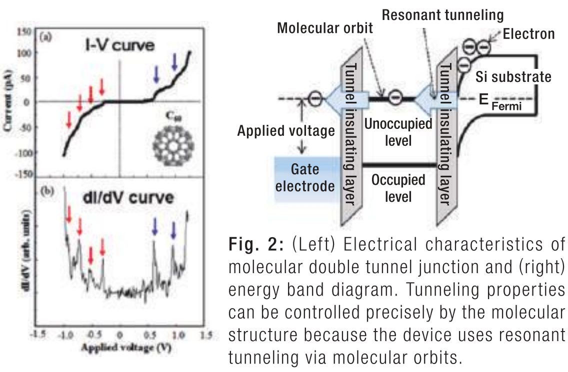


Fig. 2: (Left) Electrical characteristics of molecular double tunnel junction and (right) energy band diagram. Tunneling properties can be controlled precisely by the molecular structure because the device uses resonant tunneling via molecular orbits.

References

1) R. Hayakawa, N. Hiroshiba, T. Chikyow, Y. Wakayama, Single-electron tunneling through molecular quantum dots in metal-insulator-semiconductor structure, *Adv. Func. Mater.* 21, 2933-2937 (2011).

2) H.-S. Seo, R. Hayakawa, T. Chikyow, Y. Wakayama, Multilevel operation of single-electron tunneling with binary molecules in a metal-insulator-semiconductor configuration, *J. Phys. Chem. C* 118, 6467-6472 (2014).

Mentor Program

Guided by Voices, We Push the Limit

For young researchers, it is encouraging to know that there is someone to give them good advice. Young researchers can receive direct advice from famous scientists via the mentor program at MANA. We asked one of the mentors, Toshiaki Enoki, Professor Emeritus of the Tokyo Institute of Technology, about the advantages and importance of the mentor program.

The Important thing is thinking of and launching research yourself

Through MANA's mentor program, I have sent a lot of advice to young scientists and found that young researchers' way of thinking tends to narrow. For example, researchers who engage in systematic routine research over a long period of time as a member of a big lab are more likely to lose the initiative to launch their own original challenging research. Although they could get the latest information or knowledge at a symposium, there are few chances to get new ideas or viewpoints about their research theme through discussion with researchers from outside of their laboratory. In that sense, we can see the importance of having a mentor program which offers exchanges of opinions between young and experienced scientists.

Actually, some young researchers have their original independent research themes. They have a lot of ideas, and you can feel their positive attitude toward research through the discussion. On the other hand, there are also many young scientists who, for a variety of reasons, have difficulty with such independence. For such researchers, the mentor program exists to open their eyes to their own research target. Of course it is very important to do good work as part of a laboratory, but to be a leading scientist, the attitude toward creating and investigating new research by themselves is essential. I believe the role of mentors is to encourage them to think and launch their own research through discussion with us.

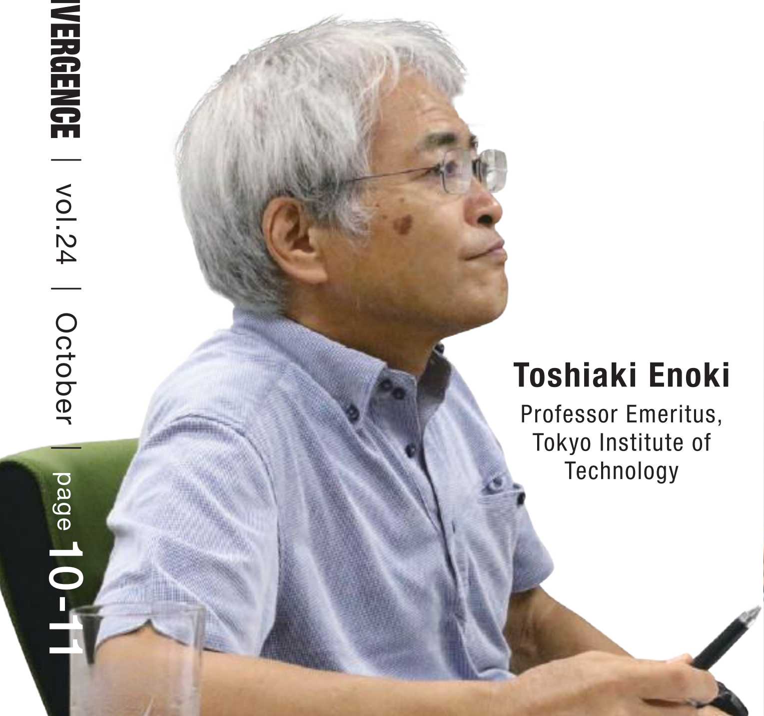
Voices from young researchers

Cuiling Li

“Mentors give my research another point of view. Experienced researchers offer advice that provides a different angle, and makes my research more interesting.”

Ovidu Cretu

“We have more discussion-based communication with mentors than supervisors. Interesting advice about my initial research plan and its future brought diversity to my research.”



Toshiaki Enoki
Professor Emeritus,
Tokyo Institute of
Technology

NEWS & TOPICS

EVENT REPORTS

2nd International Symposium on Nanoarchitectonics for Mechanobiology

The 2nd International Symposium on Nanoarchitectonics for Mechanobiology was held on July 27 and 28th. The symposium featured 5 plenary lectures, 7 invited talks, 8 MANA research presentations, and 45 poster presentations.

Through active discussions by material scientists, computational scientists, mechanical engineers, and molecular biologists enhanced their international network of researchers involved with mechanobiology. 138 people, including participants from industrial company attended the symposium.

10th Nanotechnology Students' Summer School

The event was held from 13 to 19, June at Flinders University, Australia. This year's project theme was "Go to Mars". 24 PhD students from Flinders University, UCLA, University of Auckland, University of Otago, Victoria University of Wellington, and NIIMS were selected to attend this event, and allocated to one of four groups to combine a mix of scientific expertise and cultural backgrounds. Each group was tasked to make; discussions, reports, and final presentation about how latest technologies can contribute to human being to survive on the Mars. During the summer school, students learned how to deal with international collaborative research through group discussions, thought experiments, journal researches and so on.

EVENT NOTICE

MANA International Symposium 2017

The MANA International Symposium 2017 will be held from February 28th to March 3rd at the Tsukuba International Congress Center. Special lectures, invited talks by distinguished international scientists, and the latest MANA research presentations and poster presentations will also be held.

http://www.nims.go.jp/mana/2017/index.html

Tsukuba Biomedical Engineering Collaboration Forum 2017

The Tsukuba Biomedical Engineering Collaboration Forum 2017 will be held on January 20th. Under the theme of "Life Innovation Driven by Nanotechnology", this forum will enhance the cooperation of nanotechnology research and biomedical engineering to lead medical/health life innovations. Presentations not only by researchers but also by industrial companies will be held.

http://www.nims.go.jp/mana/ikourenkei2017/index.html

AWARDS

Takeo Minari, Independent Scientist
Liu Xu-Ying, Postdoctoral Researcher
Gold Award of Korea Information Display Society (KIDS)(2016.8)

Katsuhiko Ariga, MANA PI
Selected as an honorary member of Materials Research Society of India(2016.8)

Françoise Winnik, MANA Satellite PI
Selected as a Fellow of the Royal Society of Canada (RSC)(2016.9)

NEW FACES

ICYS-MANA Researcher
Koichiro Uto

MANA Independent Scientist
Jan Labuta

ICYS-MANA Researcher
Curtis James O'kelly

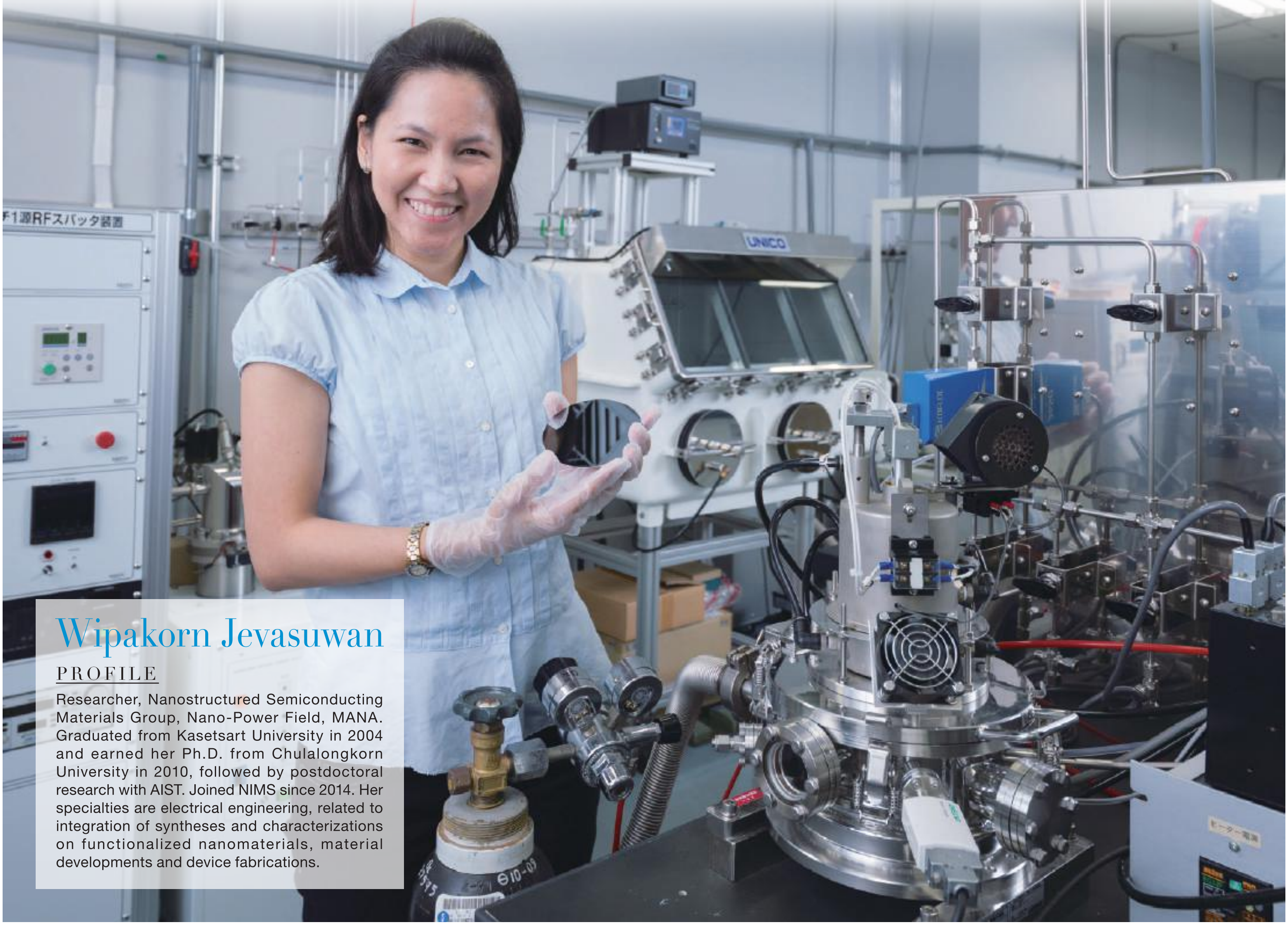
Emerging MANA Researcher

Interviewer and writer: Eri Niyama, University of Tsukuba graduate student D1

Influenced by her father, a chemist who studied water purification, Dr. Wipakorn Jevasuwan from Thailand was attracted to the interest and difficulty of science from a very early age. The weather in Thailand is hot and she thought that the plenty and strong sunlight should be cultivated and useful for something. This led her to go into research on silicon (Si) solar cells. Saying that she would like to contribute to solving the energy problem, she is currently involved in the development of a vertical transistor utilizing Si nanowires, and nanostructural Si solar cells in which pn junctions are formed and integrated with Si nanowires. The structure of nanowires can be fabricated, and their shape can be possibly controlled depending on synthesis methods including chemical (metal-catalyzed electroless) etching, nanoimprinting or CVD (chemical vapor deposition) technique. Moreover, Si nanowires are inexpensive materials with unique physical and geometrical properties; they are also expected to be used in downscaling of personal computers and mobile phones, which is limited with the conventional planar transistor technology.

Dr. Jevasuwan also has great interest in science outreach activities, which means communicating research results to children and members of the general public. Last autumn, she participated in the Tsukuba Science Festival 2015 as one of the MANA mascot characters called “Smart Polymer Rangers,” and played an active role in visitor response. She smiled as she remembered, and said it was a very pleasant experience.

Before joining MANA, Dr. Jevasuwan was an intern at a Japanese company and worked at Japan’s National Institute of Advanced Industrial Science and Technology (AIST). She has now been in Japan for more than 5 years. In talking about her dreams for the future, she said that she would like to make her utmost like to continuously strengthen the connection between NIMS and Thailand. When we asked her what the most important in doing research was, she looked us straight in the eye and replied, “You must fall in love with what you are doing, do your best and never give up.”



Wipakorn Jevasuwan

PROFILE

Researcher, Nanostructured Semiconducting Materials Group, Nano-Power Field, MANA. Graduated from Kasetsart University in 2004 and earned her Ph.D. from Chulalongkorn University in 2010, followed by postdoctoral research with AIST. Joined NIMS since 2014. Her specialties are electrical engineering, related to integration of syntheses and characterizations on functionalized nanomaterials, material developments and device fabrications.

MANA NEWS LETTER

CONVERGENCE

No.24, Eng. Ed., Issued in October, 2016

Outreach Team
International Center for
Materials Nanoarchitectonics (MANA)
c/o National Institute for Materials Science (NIMS)
1-1 Namiki, Tsukuba, Ibaraki, 305-0044 JAPAN
Phone: +81-29-860-4710
Facsimile: +81-29-860-4706
Email: mana-pr@ml.nims.go.jp
URL: http://www.nims.go.jp/mana/

“CONVERGENCE”
is the keyword used to symbolically describe the entire project of MANA, where outstanding researchers from around the world assemble and converge in the “melting pot” research environment to bring together key technologies into nanoarchitectonics for the creation and innovation of new functional materials.

COVER: MANA Principal Investigator Takao Mori and young researchers

CONTENTS

2 **Asking the Researcher**
Solving the Energy Problem by the Power of Nanotechnology – Aiming at Control of Phonons – / Takao Mori

5 **Research Outcome 1**
Clarifying the Behavior of Atoms and Electrons in Nanoscale Structures by Theoretical Calculations / Tsuyoshi Miyazaki

6 **Leader’s Voice**
Pioneering New Fields with Unwavering Research Concepts / Prof. Takuzo Aida

9 **Research Outcome 2**
Using Molecules to Control Electron Tunneling / Yutaka Wakayama

10 **Progress of MANA**
Mentor Program – Guided by Voices, We Push the Limit –

11 **NEWS & TOPICS**

12 **Emerging MANA Researcher** Wipakorn Jevasuwan