MANA NEWS LETTER

CONVERGENCE

No.28 | March | 2021

Nano Revolution for the Future

International Center for Materials Nanoarchitectonics (WPI-MANA)

Leader's Voice

Yoshinobu Aoyagi

Fusion of Different Fields or Specialties Stimulates New Ideas

FEATURE TOPIC

Computational Science × Material Science

Power of Chemists to Connect the "Image" and "Reality"

Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University
Satoshi Maeda, Director Yuriko Ono, Specially Appointed Assistant Professor
International Center for Materials Nanoarchitectonics (WPI-MANA), NIMS
Takashi Nakanishi, Group Leader Ayako Nakata, Senior Researcher

FEATURE TOPIC

Computational Science × Material Science

Power of Chemists to Connect the "Image" and "Reality"

Institute for Chemical Reaction Design and Discovery (WPI-ICReDD) Hokkaido University
Satoshi Maeda, Director
Yuriko Ono, Specially Appointed Assistant Professor

International Center for Materials Nanoarchitectonics (WPI-MANA) National Institute for Materials Science (NIMS)
Takashi Nakanishi, Group Leader
Ayako Nakata, Senior Researcher

What image of "chemistry" awaits in the future when everyone is asked to live in the "space where the virtual and the real are fused" because of COVID-19? Originally, chemistry was the study of leading an image (virtual) envisioned by researchers manifested into reality (real) by way of experiments. Nowadays, the fusion of computational and experimental sciences has made it possible to conceptualize images more clearly. The researchers of ICReDD and MANA explained what they do between image and reality and what fusion world exists between calculation and experiment from the perspectives of three computational chemists and an experimental chemist.

Texts : Osamu Shimizu (Academic Groove)

Image-led material development through chemistry

— In material development, I imagine a researcher first envisions an "image" of a new material, and then transforms it into a real material after repeating experiments and calculations. Can you explain from the perspective of your field of expertise how this is done in your research environment?

Nakanishi: Three researchers here are computational chemists and I am the only experimental chemist today. Hence, I will share how I, as a "material scientist (chemist) who creates things by experiment," create the "real." There are two approaches. One is a problem-solving style in response to society's demands, to develop materials for required functions. The other is a new material exploration style where scientific curiosity drives the investigation and development of materials. For example, when a new substance like graphene is invented, I am curious to determine its origin. It is that kind of curiosity-led research to which I refer. MANA advocates the concept of "Nanoarchitectonics (nanoarchitecture)." Inventing a function to solve problems by combining atoms, molecules, and other nanomaterials is a nanoarchitecture itself. Sometimes, the image predicted by the support of computational science is developed into reality.

Maeda: My approach in research is to "invent a calculation technique based on theoretical chemistry." Quoting Dr. Nakanishi, much of my research these days involves problem-solving. However, I used to work on basic research in the past. With "the exploration of chemical reaction route" as my theme, I focused on a precise theory that covers every possibility. After formulating such a theory to a degree, I began developing it into experiments. This phase involves assembling a model appropriate for the test object and calculation. In this process, a few approximations are incorporated. I would repeatedly perform a trial-and-error method, often asking questions such as "would it be okay if I add this or that approximation?" until the image becomes a reproduction of reality.

Nakata: My field is also computational science. Computational science is sometimes called "the third science". The first is experimental science, which is the embodiment of "reality" itself. The second is theoretical science, like the equation of motion. This deals with the image. The third science, namely, computational science, is "simulation" by calculation. This also deals with the image. When problems in reality are complicated, and cannot be solved by writing equations on paper, we run a simulation with the help of machines, such as supercomputers. If the problem cannot be solved in a strict sense, we incorporate several approximations, as Dr. Maeda mentioned. Several elements and parameters need to be considered, such as the molecular combinations and environments in which chemical reactions occur. How to approximate these elements and incorporate them into the quantum mechanical calculation are the key problems to consider in the development of the image.

Satoshi Maeda
Director
WPI-ICReDD
Hokkaido University

Hokkaido University
Institute for Chemical Reaction Design and Discovery (ICReDD)

In-depth understanding and efficient development of chemical reactions through the interdisciplinary research of computational science, information science, and experimental science.
ICReDD is one of the newest WPI centers, established in October 2018 at Hokkaido University in Hokkaido.

Ono: I did not intend to pursue computational science when I first went to graduate school, and my lab mainly dealt with conducting experiments. One day, my instructor (Yasuhiko Fujii, Professor Emeritus at the Tokyo Institute of Technology) proposed a question: "Experiments take too long. Can't we predict the experimental results to a degree in advance by calculation?" And that's how we embarked on calculation. We calculated based on historical experimental data, but it was not easy to match the experimental and calculated values. As we pursued this issue on a trial-and-error basis, we learned several other things about the main topic. As far as "how a hypothesis (image) becomes reality (real)" is concerned, how to incorporate approximation and to analyze the vast reaction space are the very things at which computational chemists are skilled. You can almost say that computational science is a study of analyzing reality to improve the accuracy of images.

Encounter with calculation. Latest developments in molecular chemistry

— When you think of chemistry, you used to think of an image where a chemist in a white lab coat repeatedly performs experiments to invent a new material. However, I hear that the support of computational and data sciences is indispensable in today's molecular chemistry.

Nakanishi: The importance of computational science is rapidly increasing in the field of chemical material development. Examining phenomena and functions is seldom sufficient to gain a complete understanding, and comprehensively considering the experimental and simulated results is often required. Furthermore, synthesizing molecules is time consuming and takes an effort. However, we calculate and clarify that "We need a molecule with such a structure to make a material with such a function. We want such interactions of the molecules," before synthesizing these molecules. When we write a paper also, we sometimes create an image diagram that has simulation added to indicate visually the image we are predicting from the experimental results.

Nakata: One of the purposes of theoretical calculation is to "understand (the mechanism)." Therefore, supporting the "meaning of what is happening in the experiment" from the calculation side is my important role. Understanding the mechanism makes the design of new molecules and materials much easier. I would be very happy if I were able to design a material from the theoretical chemistry side through calculation and propose, "How about making something like this?" Computational chemists can shine in techniques through which they incorporate approximations in such calculations. It is fun to perform calculations to improve them.

Maeda: Ten years ago or so, few researchers would have believed if they were told that chemical reactions can be predicted by quantum chemical calculations. Recently though, thanks partially to improvements in calculation techniques and the upscaling of computers, the demand for calculation in research is increasing. If prediction were solely based on calculation, we might attain incorrect answers, or answers that do not reflect reality. Hence, validation by experiment is critical. I am currently working on finding a new chemical conversion in calculation and then validating it by collaborating with experimental chemists. To clarify any misunderstandings, our computational science is different from data science. My understanding of data science is that it is the study of finding new combinations from the vast accumulation of experimental or computational data. In quantum chemical calculations, chemical reactions are predicted without any prior information, in the first principle manner. As the popularity of data science grows, it is easily confused with computational science.

Yuriko Ono
Specially Appointed Assistant Professor
WPI-ICReDD
Hokkaido University

Nakanishi: I agree. Data science is not good at studying new things, as it is based on historical data. Data science is said to be good at interpolative prediction but not at extrapolative prediction.

Nakata: The data to which you are referring, I believe, are experimental data. There are attempts to handle calculation results as data and use them in data science or machine learning. The advantages of generating data from calculation are that constant accuracy can be guaranteed at all times, and high-quality data can be prepared. Calculation can also provide data regarding materials that are not yet invented.

Serendipity and teamwork

— Often the spark of a new idea to conduct original research comes to researchers through serendipity. Does serendipity happen differently in experimental chemistry and computational chemistry?

Maeda: This is precisely one of the missions of ICReDD, which is "Can we derive a spark of an idea from calculation?" After two years at my current post, I feel that "(highly accurate) calculation is slower than experiment." In other words, it is often faster to run an experiment on an idea someone else has proposed rather than validating it by calculation. Furthermore, when experimental chemists and computational chemists collaborate to optimize conditions for reactions and catalysts, wisdom attained through the experience of experimental chemists becomes important in extracting ideas from the calculation results. Hence, I want to be able to apply calculation to help find ideas that humans cannot come up with, even if they spend their entire lives thinking about them.

Nakanishi: My spark of idea and serendipity often comes in the form of "realizing as I experiment." It often occurs in the process of trying as hard as I can to understand a phenomenon appearing in the experimental results that I do not understand. Sometimes I realize "Oh, that was serendipity" after I have gained the understanding. I feel that the difference between computational chemists and experimental chemists is increasingly diminishing. Hence, a spark may flash in such a close collaborative environment.

— Sparks flash differently even in computational chemistry and experimental chemistry. Perhaps there are substantial differences in the respective cultures and ways of thinking. How would a collaborative research between these fields progress?

Ono: I feel that various processes proceed through the shortest possible path in collaborative research between computational chemists and experimental chemists. At ICReDD, experimental chemists set a challenging goal. We make a prediction in the initial calculation to attempt to achieve this goal. We then have several discussions, and if a good system is found, we proceed with the process of experimentation to realize the goal. In examining the initial calculation results, it is quite difficult to screen the results with only the knowledge of calculation. Hence, we obtain inputs from experimental chemists to screen the results. We mobilize all the knowledge of computational chemists and experimental chemists and endeavor to achieve the goal through the shortest possible path. I think there are two types of experimental chemists in general: the type who has high expectations from calculation and the type who focuses on experimental results over calculation. My instructor, by whom I was influenced, was the former. I moved to calculation from experiment. However, calculation is not always the correct answer. In interdisciplinary research, I believe it is important to show the information that cannot be seen via experiments alone using calculation.

Nakata: In the old days, theoretical and experimental research used to be conducted separately. Now, these two are increasingly fused. I feel the result of calculation is like an ideal, or an image, and it becomes real once you speak with experimental chemists. As Dr. Ono said, realistic information from experimental chemists is very important.

Nakanishi: I believe the type of person we need in the current research environment is someone who understands computational science, data science, and experiments and can coordinate with the respective professionals. Projects will go smoothly if you have this type of person.

Takashi Nakanishi
Group Leader
WPI-MANA
NIMS

Does the future of chemistry lie with robots conducting experiments?

— The Japanese government is advocating "Society 5.0" with a vision of a "future society where the virtual and real are ideally fused." How do you think chemistry will change in such an era?

Ono: I cannot be certain of things very far in the future, but I can imagine a future in which we calculate a highly accurate prediction in advance and then propose to the experimental chemist what is promising and will become real; in other words, the overall speed of development will be accelerated. For this to happen, close cooperation between experiment and calculation will be necessary.

Nakata: Data science proposes several choices. However, the reason why they are promising is still not completely understood in many cases in today's data science. The advantage of computational science is to understand; therefore, it can help theorize and narrow down that which is promising from the several choices proposed by data science. In other words, I feel that the virtual filtering of the choices proposed by data science will be realized by computational science.

Ayako Nakata
Senior Researcher
WPI-MANA
NIMS

Nakanishi: The current flow of material development by fusing data science and experiments is a cycle of accumulating experimental data, predicting, and then returning to experimentation. Unfortunately, the speed of development inevitably slows down in the experiment phase. As an experimental chemist, I think it is important to master the ability to create things. What I mean is that you need to have the skill to synthesize molecules and create materials regardless of the future advances in computational science and data science.

Maeda: I feel that robots are a possible solution to the problem Dr. Nakanishi just mentioned. A future with robots conducting experiments based on the calculated prediction is possible. In fact, ICReDD has decided to introduce robots for conducting experiments. Of course, there is a concern regarding how well robots can perform complicated acts, as experiments involve several skills. We would like to pursue the possibility in the future.

— Now, here is a simple question. Are there difficult questions that cannot be solved in chemistry, like the abc conjecture and the Riemann hypothesis in mathematics?

Nakata: When there are an enormous number of reaction patterns, how do you examine all of them? This must be one of the difficult questions that cannot be solved.

Ono: I think the theoretical method Dr. Maeda invented fits the bill.

Maeda: That was just something I did a little ahead of time when others were not working on it yet (laugh). Come to think of it, several unsolved problems in chemistry are a matter of degree. In physics and mathematics, we often hear "what was not possible is now possible." However, in chemistry, "we can do it, but not well enough for practical use. We want to make it more efficient or industrially applicable," is equivalent to an unsolved problem.

— So, you are saying that a difficult question to solve is a matter of industrial implementation. In that aspect, the introduction of robots to conduct experiments appears to be a natural choice.

Future prospects. To image-led reality

— We only have a few minutes left. Please share your future prospects.

Nakanishi: I would like to invent at least one raw material or materials that will be a part of a product that is helpful to society. Moreover, I want to leave a legacy to future generations. This might be something that contributes to society, such as discovering a substance and function that will be mentioned in textbooks.

Nakata: I am interested in phenomena in which a conventional material changes significantly (its performance is greatly improved or it can serve a new function) by a small change. I would like to be able to propose something of that sort from a theoretical point, and that can lead to reality.

Maeda: I get a little anxious speaking about the prospect of my organization (ICReDD) (laugh). I want to establish calculation- and information-led chemistry, and understanding- and prediction-driven chemistry. To achieve this, I want to plan a strategy in which calculation and information can contribute at various complication levels.

Ono: When you speak with someone from another discipline, say an organic chemistry researcher, it often takes time to understand each other. Communication is quite difficult. Even though the difference between computational chemistry and experimental chemistry is diminishing, there is still quite a significant difference. I want to continue my efforts toward shrinking that barrier.

The roundtable discussion was held online to comply with countermeasures policy for COVID-19.

Leader's Voice

Fusion of Different Fields or Specialties Stimulates New Ideas

Yoshinobu Aoyagi

Emeritus Prof. Tokyo Institute of Technology,
Emeritus Prof. RIKEN Institute

Basic research is critical in developing the next generation of science and technology

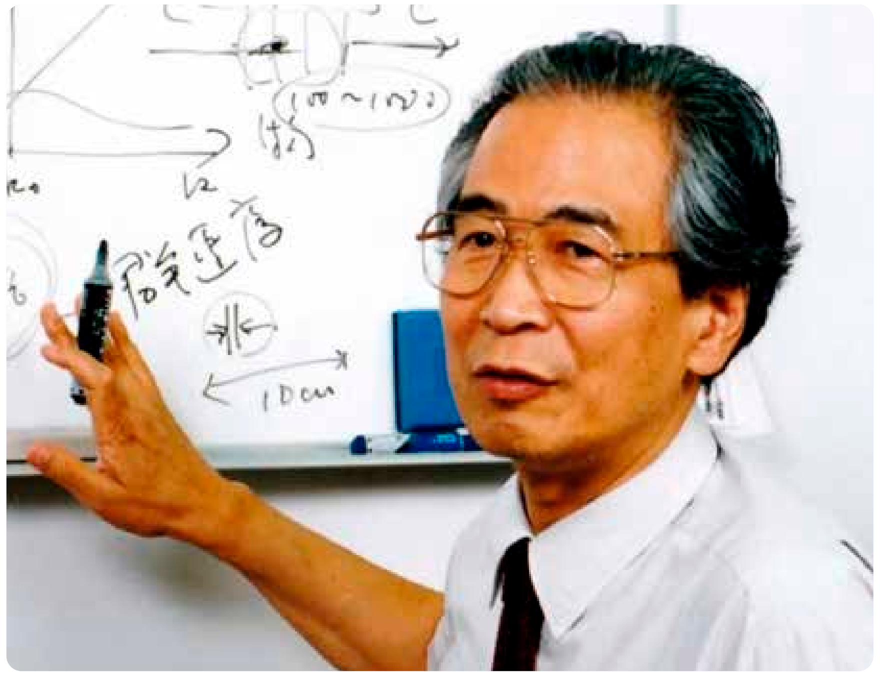
There is no doubt that basic research is the foundation of future science and technology, even in my field of specialty, applied physics.

The fact that Japanese scientists have won several Nobel Prizes in recent years should be regarded as the fruit of basic research over the years. For example, the development of the blue LED, which won Dr. Isamu Akasaki the Nobel Prize for Physics in 2014, is based on the grassroots-style basic research conducted around 1979 on the metal organic chemical vapor deposition on the blue light-emitting material, gallium nitride (GaN).

Even though GaN is durable and emits light well, this study presented several challenges, such as the unavailability of a suitable substrate on which to grow the crystals. Therefore, high-quality crystals could not be grown, and the n-type and p-type GaN necessary for diodes could not be created. In the meantime, zinc selenide (ZnSe) was studied as a promising material for a blue light-emitting compound in the 1990s, but it gradually became apparent that its life is too short for practical use. Under such circumstances, Dr. Akasaki persevered and continued his research until its fruition, hoping that developing a blue LED made of GaN with a long life expectancy "would trigger a lighting revolution not seen since the time of Thomas Edison." This grassroots-style basic research is critically important as seed research that may produce great fruit in the future. Without a bud, new fruit will never grow. In curiosity-driven grassroots-style basic research, it is critical to pursue one's strong scientific and technological interests. If you dig deeper, it is possible that an unexpected result will emerge, and a new field of study will be born. It is important in grassroots-style basic research to pause for a moment prior to starting to understand the vision clearly; "What kind of wonderful world will be uncovered if this research works, and what are its challenges?" One's research may often reveal unexpected phenomena or results. After analyzing these phenomena and results, one will need the ability and deep insight to determine accurately whether they are worthless, or if you are on to something. A clear vision is necessary in order to do so.

The scientific and technological nation Japan should strive to be

Japan has few natural resources and can only survive through science and technology. Some people say, "There are no more big and new things to work on in science and technology," but this is not true. There are mountains of grand opportunities that Japan can excel in and should tackle in the fields of materials, electronics, informatics, energy, biological, medical, and chemical sciences. Nature does not come divided into fields. Now that these individual scientific fields have matured to a certain degree, it is only natural that the seeds of ambitious and new interdisciplinary research should sprout.



Not interesting if the research is not ambitious

It is important that ambitious research themes be interesting. Now, what does "ambitious" mean? A few phrases come to mind, but when I submit or examine a new research proposal, I always ask, "What is new about this? What solution does it propose to what problem? How will the world change if this research goes well? What kind of wonderful world will it reveal?" I ask this to myself as well as to my students. The most important thing, I believe, is that the results of the research will contribute to humanity and society, and ultimately help someone locally or worldwide. Contribution to humanity and society does not only mean in terms of productivity per se, but also includes discovery of new laws of nature and recognition of phenomena, i.e., contribution to human wisdom. Several ambitious research projects will fail, but researchers must pursue results that could change the world with a stubborn will and flexible mind.

It is also important to have a broad view and to discuss in depth with professionals from various fields in order to find an interesting topic of research. I have several "strategic" researcher friends in various disciplines around the world, and through discussion, I have learned the perspectives of professionals in different disciplines and their worlds.

Together with renowned researchers from around the world
at the banquet of the international symposium in Ringberg, Germany.

Fusion of different fields or specialties to discover fascinating research topics

"Interdisciplinary" is a hot topic of conversation these days. People tend to imagine a completely different discipline from their own. However, if you rethink of it as fields other than your own (other disciplines), "interdisciplinary" research simply means joint research with professionals in other fields, which can dramatically expand the scope of your research, that is, "fusion of different fields or specialties". The ideal would be to conduct a few interdisciplinary studies to evolve your topic. To do this, you need to do good work that is recognized globally (to make your partners think it would be advantageous to work with you), and to build close "strategic" relationships with as many professionals in other disciplines as possible. Become friends with several people who are doing good work, regardless of their workplace, domestically or internationally. If this produces good results, people will naturally come to you.

The advantage of fusion of different fields or specialties is that it is easy to propose novel and interesting research topics. The Atom Switch device, an example of success at the International Center for Materials Nanoarchitectonics (MANA), is a wonderful fruit of interdisciplinary collaboration among professionals in the basic research of STM and electronics. When you look for a new "fusion" research topic jointly with researchers in other disciplines, ambitious and interesting research will be born. When a young researcher joins a new lab, he/she can formulate a fascinating research topic for him/herself as well as for the lab if the varied expertise of the researcher and the lab can be fused. Learn the equipment, people, and research topics of the new lab, and then propose an interdisciplinary theme in collaboration with your own research.

Dinner with Professor M. Stuke of Max Planck Institute, Germany.

Mindset of facing obstacles

Fusion of different fields or specialties may be the weakness of Japanese researchers. Perhaps several of them are afraid of being different from others or of failure. Recently, an American graduate of Stanford University said, "Even if I fail and lose everything, I am confident I will get more than what I have now in my life in a completely different field." Focusing on success rather than failure, what bold words these are! Interdisciplinary collaboration, that is, fusion of different fields or specialties, requires such strong confidence and a supportive environment. If success gives you recognition, you can challenge all you want, don't you think?

It is also essential to have someone who encourages you and gives you advice in finding yourself in a new field. There is a saying to "make use of whoever is useful, including your parents." What matters is the result. I believe that the experienced professionals who have helped build this science-and-technology-orientated nation with their wisdom and technology can assume the role of the parents.

At the International Nanotechnology Conference in Pontresina, Switzerland.
Professor Yoshinobu Aoyagi (second from left) and
former MANA Director Professor Masakazu Aono (second from right).

PROFILE

Prof./Dr. Yoshinobu Aoyagi

**Emeritus Prof. Tokyo Institute of Technology,
Emeritus Prof. RIKEN Institute,
Senior Researcher of Ritsumeikan Univ.**

Awards: Ohkohchi Memorial Prize, Ichimura Science Special Prize, National Invention Award, Jpn. Applied Physics Prize, Prize of Agency of Science and Technology, MNC Most Impressive Presentation Award, Best paper award of Jpn J. Appl. Phys., Fellow of Jpn. Society of Appl. Phys., Micro and Nano Processes International Conference Award.

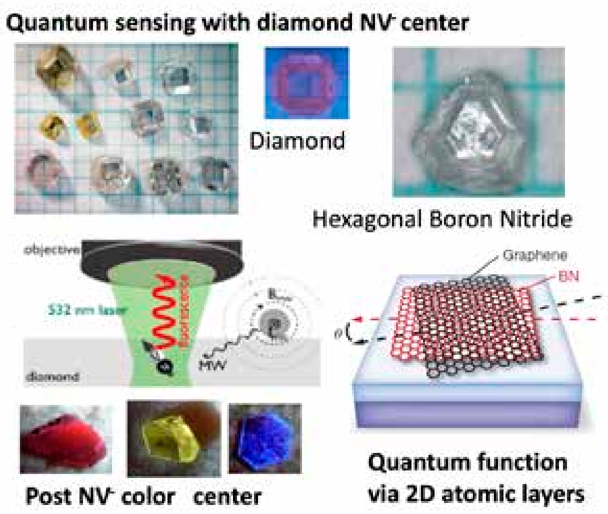
MANA RESEARCH TOPICS

Introducing MANA's latest nanotechnology research and projects

01 Quantum Material Project

The quantum technology innovation strategy aimed at the use of quantum science has been taken up as a national policy. In this strategy, it is important to develop quantum materials that are the basis of quantum computing, sensing, communication, and other technologies. NIMS has been conducting research on quantum technology development, material synthesis, physical property observation, etc. for a long period. From the last year, MANA has started 'Quantum Material Project' with the aim of contributing to the strategy policy. We aim to develop a material for realizing Q-bit and to develop a new quantum photonics.

Takashi Taniguchi
NIMS Fellow
Project Leader of Quantum Material Project

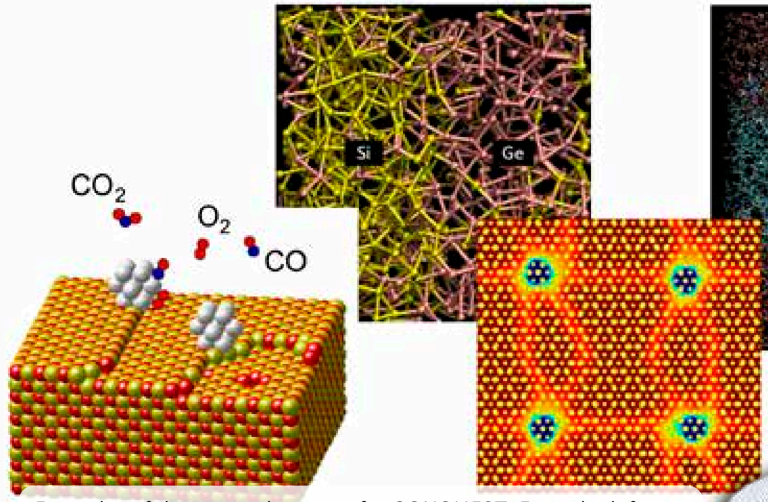


Quantum sensing with diamond single crystal & Exploration of quantum function with 2D materials

03 CONQUEST

Development and release of first-principles calculation program that can handle 1 million atoms

First-principles electronic structure calculations are powerful methods that allow us to explore the atomic-scale structure and properties of materials. However, due to the high computational cost of the calculations, it is not possible to calculate complex structures containing many atoms, such as interfaces, nanostructured substances, and biological systems. We have developed a paradigm-breaking program that enables first-principles calculations even for very large-scale systems containing millions of atoms, by making use of new approaches such as the localised orbital method and the order N method. We have released the program as an open source, freely available code, so any researcher can use this new approach.

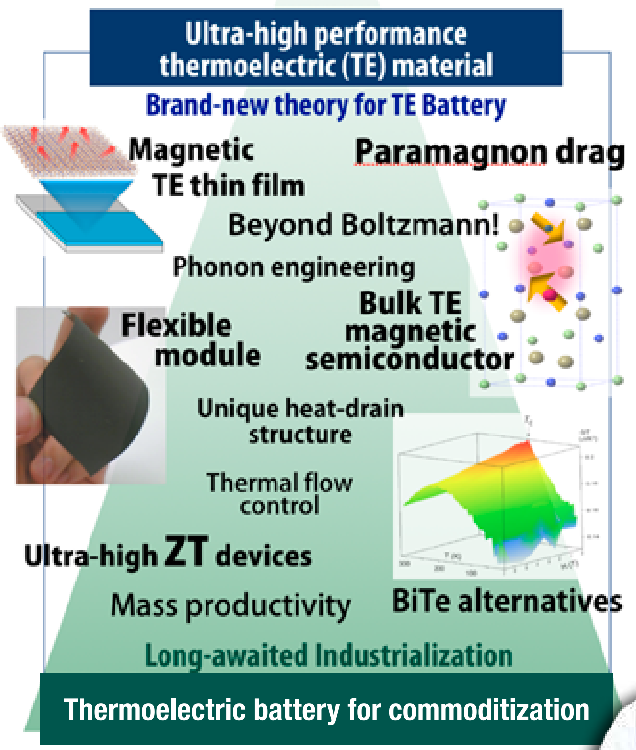


Examples of the research targets for CONQUEST. From the left, atomic structures of catalyst of metallic nanoparticle, Si/Ge interface, vortex structure in ferroelectric oxide, and ion channels.

Tsuyoshi Miyazaki
MANA Principal Investigator
Group Leader of First-Principles Simulation Group

02 Development of innovative thermoelectric materials and devices utilizing magnetism and nanostructures

JST-Mirai Program



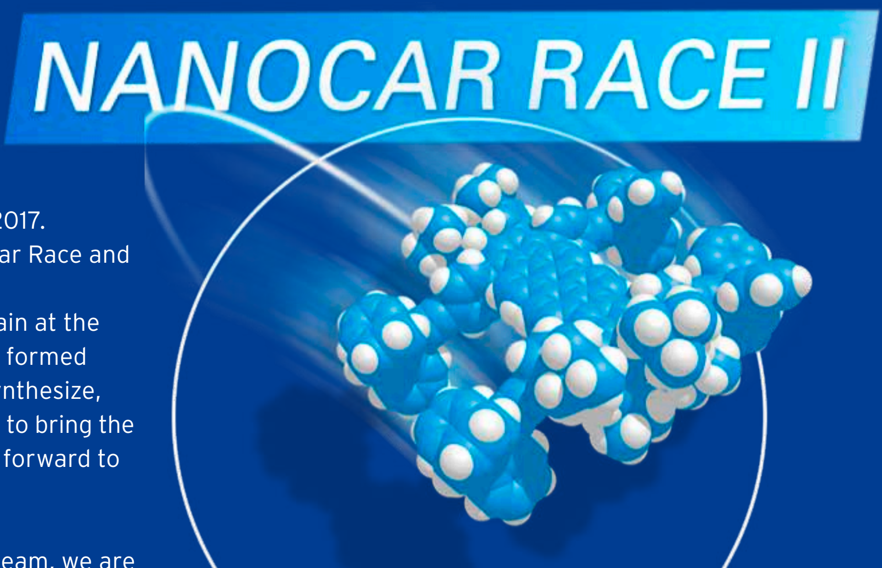
Our group is taking on the challenges of the 200 years long dream of commercializing thermoelectric power generation by discovering new principles for enhancing thermoelectric performance. We have discovered the enhancement of the thermoelectric effect, by controlling nanostructures and utilizing magnetism, which enable surpassing of the conventional trade-off between electronic and thermal properties, and we have pioneered the new field of high-performance magnetic semiconductor thermoelectric materials. Ultra-high performance was also found by thin film growth of related materials through international collaboration. At the same time, we are also developing thermal management technologies and power generation modules using processes compatible to industry.

Takao Mori
MANA Principal Investigator
Group Leader of Thermal Energy Materials Group

MANA Channel

Nanocar Race 2

Nanocar Race is an international scientific competition with the aim of testing the performance of molecular machines and the scientific instruments used to control them.
The race of the molecules takes place on a 100 nanometer track and was held for the first time at the MANA satellite in Toulouse, France, in April 2017.
A NIMS-MANA team participated in the first Nanocar Race and received the "Fair Play Award."
The second Nanocar Race is planned to be held again at the MANA satellite in Toulouse in spring 2022. A newly formed NIMS-MANA team has already started to design, synthesize, and evaluate new molecular machines with the goal to bring the victory of Nanocar Race 2 to NIMS-MANA. We look forward to your continuous support of our NIMS-MANA team.



On the official Twitter account of the NIMS-MANA team, we are sharing the latest information.Please have a look and follow us on MANA's official and unofficial Twitter accounts.

#Nanocar_Race_2 #Molecular_Machines #It's_time_to_win
#Follow_us

Twitter accounts

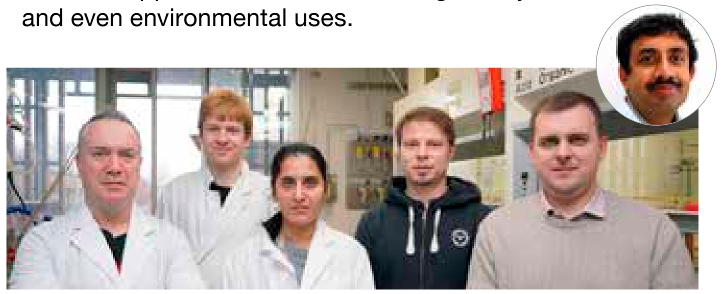
MANA Channel (unofficial) | NIMS-MANA Team | MANA Official

New People & New Groups

Introducing our new researchers and new groups (FY2020)

FUNCTIONAL CHROMOPHORES GROUP Nano-Materials

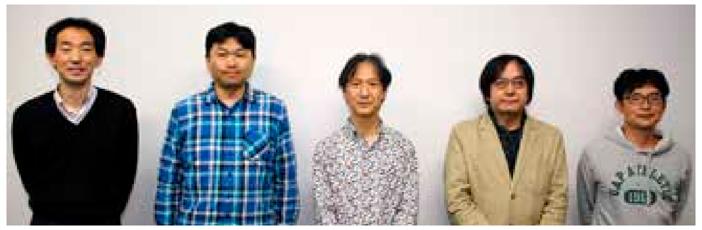
Chromophores are molecules usually considered 'functional' due to color. Functional Chromophores Group investigates nanomolecular materials to uncover functionality based not only on color but also on the detailed molecular structure. Potential applications include, sensing, catalysis, medicinal and even environmental uses.



Jonathan Hill, Group Leader (first from left)
Jan Labuta, Senior Researcher (second from right)
Anirban Bandyopadhyay, Senior Researcher (outside frame)

QUANTUM MATERIAL-PROPERTIES GROUP Nano-Systems

We are a new group joining MANA last April, conducting experimental and theoretical research on superconductivity and topological materials. Superconductivity is a quantum phenomenon that appears on a macroscopic scale. Topological materials, on the other hand, are based on the topological properties of quantum mechanical wavefunctions. Our group name may seem ambiguous, but the name represents the body.



Taichi Terashima, Group Leader (third from left) Masanori Kohno, Chief Researcher (second from left) Hiroyuki Yamase, Principal Researcher (first from left) Minoru Tachiki, Principal Researcher (second from right) Shuuichi Ooi, Senior Researcher (first from right)

QUANTUM SOLID STATE MATERIALS GROUP Nano-Materials

We are mainly engaged in research focusing on oxides with the aim of developing new materials that contribute to advanced quantum technology. We are also collaborating with researchers inside and outside MANA to conduct research that contributes to topological quantum information processing by realizing new junctions between high-temperature superconductors and topological materials.

Kazunari Yamaura, Group Leader (fourth from right)
Alexei Belik, Principal Researcher (third from right)
Yoshihiro Tsujimoto, Senior Researcher (second from left)

NANOPARTICLE GROUP Nano-Materials

We are researching to create "breakthrough energy conversion materials" that contribute to the realization and succession of a safe and healthy society. The core material is nanocrystals. We are working on the control, utilization, and application of "quantum characteristics" that manifests in nanostructures, and are expanding our research into photonics, medical thermal phononics, and optoelectronics.

Naoto Shirahata
Group Leader

Sun Hong-Tao
Principal Researcher

INDEPENDENT SCIENTIST

Takayuki Harada

Takuya Iwasaki

ICYS-WPI-MANA

Adrian Diaz-Alvarez

NIMS FELLOW • NIMS DISTINGUISHED FELLOW • NIMS SPECIAL RESEARCHER

Takashi Taniguchi
NIMS Fellow

Hideo Hosono
NIMS Distinguished Fellow
Electro-Active Materials Team

Hiroshi Mizoguchi
NIMS Special Researcher
Electro-Active Materials Team

MANA RESEARCHER

Masahiro Goto
Chief Researcher

Makoto Tachibana
Senior Researcher

Kensei Terashima
Senior Researcher

Deng Xiao
Researcher

Nano Revolution for the Future

News & Events

Information from MANA about international conferences, events and the latest news

C MANA INTERNATIONAL SYMPOSIUM 2021 jointly with ICYS

2-3 March 2021, ONLINE

The "MANA International Symposium 2021 jointly with ICYS" has been held online on March 2-3, 2021. MANA International Symposium is held each year to present research achievements of MANA to the international scientific community. The event has been the 14th in the series. Further information is available on the official website.

C The 3rd ICYS & MANA Reunion Workshop

4-5 March 2021, ONLINE

"The 3rd ICYS & MANA Reunion Workshop" organized by ICYS and MANA alumni has been held on March 4-5, 2021, after the MANA International Symposium 2021.

N Nine researchers from MANA selected as Clarivate Analytics "Highly Cited Researchers 2020"

24 November 2020

Clarivate Analytics releases its annual list of Highly Cited Researchers. Highly Cited Researchers have produced multiple papers ranked in the top 1% by citations over the course of the last decade. In 2020, nine researchers from MANA have been selected as "Highly Cited Researchers 2020."

N New MANA brochure for companies

25 November 2020

For NIMS Week 2020 (online), MANA has issued a new brochure for companies "Nano Revolution for the Future." The brochure introduces examples where basic research from MANA has led to applications and proposes promising nanotechnology research from MANA for the Carbon Neutral Society and Society 5.0.

E Online Joint Seminar for Teachers "Todoke! WPI's Latest Research"

5 December 2020

On December 5, 2020, the online seminar "Todoke! WPI's latest research" for junior and senior high school teachers has been held jointly by four WPI centers. From MANA, principal researcher Naoyuki Kawamoto introduced his research activities and exchanged opinions with participants.

N Obituary: Professor Françoise Winnik

18 February 2021

Prof. Françoise Winnik, MANA Satellite Principal Investigator, Professor of University of Helsinki, passed away on February 13th, 2021. She has interacted with many MANA researchers, postdocs, and students, providing guidance and encouragement based on her outstanding knowledge and experience in nanoscience. We never forget her great contribution to MANA and express our deepest condolences.

Editor's Note

"Online Roundtable"

Due to the unexpected global outbreak of the new COVID-19 virus, the year 2020 definitely became a prosperous new era of online services. With the "stay-at-home" requests, the opportunity to use various online services has increased dramatically. Among them, the online video conferencing software must be a super utility player, like MVP players in the world of professional sports. Thanks to this software, we were able to successfully hold and record this issue's feature topic, the roundtable discussion, despite the going out restrictions. In public, they say that the online video conferencing software is not only used for conferences and events, like MANA activities, but also for private gatherings such as online drinking parties and alumni associations. It seems that the software became a tool that is inseparable from the remote environment. What we used for necessity, became a tool that we love to use. In an environment where we can't meet, new unexpected encounters are born thanks to the freedom and joy to participate in an event that we are interested in, from anywhere. Even after overcoming the COVID-19 disaster, MANA would like to continue to connect with you through the online conference system that people around the world can enjoy. (KT)

Who's who in MANA

Being part of the multicultural working environment at WPI-MANA

Andreas Doenni
Team Leader, Planning and Outreach Team, MANA

Q1: Can you explain your research activity?

During my Ph.D. in Physics at ETH Zürich in Switzerland, I worked at a large-scale facility and performed neutron scattering experiments on materials provided by external users. Later as a postdoc in Japan, I became an external user by myself. I started to prepare and characterize new materials in order to measure them at large-scale facilities. Especially NIMS has excellent facilities to prepare new high-quality materials, for example under high pressure. Over the years, I have published more than 100 research papers, many of them internationally co-authored.

Q2: When did you join NIMS?

I joined NIMS in 2006 as a researcher. One year later, the WPI-MANA project started at NIMS and I received the chance to work there in the middle management as a Team Leader. My presence in this function is like a *bridge* between different cultures and like a *glue* between foreign and Japanese researchers.

My presence is like a *glue* between foreign and Japanese researchers

Q3: How did the WPI-MANA project change NIMS?

The first NIMS President, Prof. Teruo Kishi, has started to strongly promote the internationalization of NIMS. I think that the two projects ICYS (International Center for Young Scientists, 2003-2008) and WPI-MANA (International Center for Materials Nanoarchitectonics, 2007-2017) have made NIMS the most internationalized research institute in Japan. And I'm absolutely impressed how the WPI-MANA top management under Director Prof. Masakazu Aono has succeeded to make MANA an internationally well-known brand.

At NIMS Open House in April 2017. Swiss Raclette is very popular every year.
Who's the chef? Of course, it's me!

Q4: How do you experience the international working environment at WPI-MANA?

WPI-MANA has a multicultural working environment with about half of the researchers from Japan and about half from abroad. I appreciate it more and more to have the privilege to work in such a stimulating and fruitful environment. For the current MANA (a research center of NIMS and a wpi academy member) under Director Prof. Takayoshi Sasaki I wish that NIMS will continue to profit from the huge achievements for a long time to come. The year 2020 has been full of challenges and difficulties, because of the ongoing COVID-19 pandemic. Let us stay strong and safe and continue on our journey as much as possible.

MANA NEWS LETTER
CONVERGENCE
No.28, March 2021

Planning and Outreach Team
International Center for
Materials Nanoarchitectonics (WPI-MANA)
National Institute for Materials Science (NIMS)
1-1 Namiki, Tsukuba, Ibaraki, 305-0044 JAPAN
Phone: +81-29-860-4710
Fax: +81-29-860-4706
Email: mana-pr@ml.nims.go.jp
Website: https://www.nims.go.jp/mana/

"CONVERGENCE"
is the keyword used to symbolically describe the entire project of WPI-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.

CONTENTS