

# Advanced Institute for Materials Research

# AIMR Magazine / Vol. 10 / July 2020

Advanced Institute for Materials Research (AIMR), Tohoku University 2-1-1 Katahira, Aoba-ku, Sendai, 980-8577 Japan Phone: 022-217-6146 Mail: aimr-outreach@grp.tohoku.ac.jp

https://www.wpi-aimr.tohoku.ac.jp/





# http://www.analysis.org/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/linearity/li

[Special Interview]

# Accelerating Advanced Materials Science ORIMO Shin-ichi

Director, Advanced Institute for Materials Research (AIMR), Tohoku University

[AIMR in the world]

Fraunhofer Project Center at Tohoku University A Platform for Fostering Industry-Academia Collaboration

# Thomas Otto

Director, Fraunhofer Project Center at Tohoku University Director, Fraunhofer Institute for Electronic Nano Systems ENAS

# [Series]

The Resurrected Laboratory TANIGAKI Katsumi Professor Emeritus, Tohoku University

Fresh Eye g-RIPS-Sendai 2019

Math and I

Andreas Dechant Researcher, Graduate School of Science, Kyoto University

# New Staff

OZAWA Tomoki AIMR Junior Principal Investigator

**GAO Xichan** AIMR Assistant Professor



# Accelerating Advanced Materials Science



Director, Advanced Institute for Materials Research (AIMR), Tohoku University

**ORIMO Shin-ichi** 

On October 1, 2019, Professor ORIMO Shin-ichi was inaugurated as the third Director of the Advanced Institute for Materials Research (AIMR), Tohoku University. With coronavirus disease 2019 (COVID-19) crisis occurring six months after assuming the post, Professor Orimo has since spent his days busily supervising efforts to prevent spread as well as leading the "New Normal" as the institute's director. We asked him about AIMR's efforts to overcome this crisis and to embody the goal of "bringing advanced materials science to the world."

# Scientific Principles based on Mathematics-Materials Science Collaboration

AIMR builds its identity on collaboration between mathematics and materials science. This unique concept has been strongly driven by the former director and mathematician KOTANI Motoko since 2011. Up until 2018, such collaborations have been built on three target projects: non-equilibrium materials based on mathematical dynamical systems, topological functional materials, and multi-scale hierarchical materials based on discrete geometric analysis. By applying these newly established mathematical concepts to materials science, AIMR successfully derived "structural characteristics hidden in randomness (irregularity) in materials," which could not have been identified until then, producing outstanding achievements that gained worldwide recognition.

# Launch and Expansion of Advanced Target Projects

To further strengthen collaboration between mathematics and materials science included in these achievements, I launched three new Advanced Target Projects with Professor SUITO Hiroshi, Deputy Director in 2019. The three projects are: 1) control of local structure in topological functional materials, 2) integrated control of bond variation and its time evolution, and 3) improving self-organization technology and controlling biological responses. These ambitious projects aim to evolve conventional static randomness research to "dynamic (kinetic) randomness," or elucidate "reactivity/responsiveness to external fields" of hierarchical structures obtained by the establishment of self-orders. AIMR also endeavors to link micro-scale perspectives (related to atom/molecule control technologies) with meso-macro scale perspectives (related to larger structures and performances) all at once, thereby accelerating materials



Director ORIMO Shin-ichi (left) and Deputy Director SUITO Hiroshi (right)

creation to develop a diverse range of unprecedented physical properties and functionalities.

I specialize in materials science. Aiming to create various materials suited to highly efficient energy conversion, storage, and transportation and to implement them in society, I am working on the discovery of new hydrides with excellent lithium ion conductivity applicable to next-generation all-solid-state batteries. Generally, molecular dynamics calculation is employed to understand ionic conductivity, but at AIMR, research is conducted to explore structural properties hidden in dynamic randomness (i.e. during ionic conduction) through mathematics and materials science collaborations to acquire fundamental understanding of "why ionic retention occurs in materials," "how to reduce this retention," and upon achieving this, "how to increase the ionic conductivity of the whole material." The goal is to create materials with extremely high ionic conductivity. These studies are being conducted as part of 2) integrated control of bond variation and its time evolution.

Furthermore, AIMR proactively encourages the use of the institute's angle-resolved photoemission spectroscope (ARPES), which boasts the world's highest angular resolution, scanning tunneling microscope (STM), and advanced measurement technologies available at the next-generation synchrotron facility currently being built on the Tohoku University campus.



AIMR also aims to build a scientific principle that encompasses diverse advanced materials research projects such as electronics, energy, and biomedical by leveraging advanced measurement technologies as well as collaboration between mathematics and materials science through the three advanced target projects. Needless to say, the scope will not be limited to merely the establishment of a scientific principle, but will also extend beyond that to include the creation of materials that would truly contribute to society. Reinforcing collaborations with industry is thus seen as one of the most important challenges, moving forward. AIMR's identity "collaboration between mathematics and materials science" has attracted enormous interests from industry as well through activities such as g-RIPS. By promoting not only short-term results but also materials creation based on fundamental sciences with a view to the future, AIMR is committed to fulfilling its responsibilities as a research hub for bringing advanced materials science to society.

# **Three Rs Again**

Since joining AIMR in 2013 as the principal investigator (PI) of the Device/System Group, I have experienced at first-hand that AIMR's greatest strength lies in its ability to provide researchers from different fields (i.e. mathematics and materials science) the opportunity to deepen discussions under-one-roof, and share different values among from young researchers to PIs. To further develop this strength, I would like to once again emphasize the importance of the three Rs: Relief, Research, and Recognition.

The first is "Relief." AIMR strives to give priority to the safety of everyone involved at the institute including the Research Division and the Research Support Division, as well as focus on efforts including mental care. In doing so, we hope that everyone at the institute will be able to maximize their skills. The second is "Research." AIMR stands at the frontline, at the very edge of the field of research. But this also means that we are also at the edge of a cliff. I think that it is important to constantly aim to improve ourselves through friendly rivalry, feeling "on-edge" to a certain extent. The third is Recognition. It is vital for our people to continue the awareness of striving to be a research center that is needed now more than ever before, both inside and outside the university, and Japan. To that end, we aim to further strengthen our communicative ability as an academic research center for advanced materials that connects to the world by deepening cooperative ties with the Joint Research Centers at the University of Cambridge in the UK, the University of Chicago in the United States, and Tsinghua University in China, and the Fraunhofer Institute for Electronic Nano Systems ENAS in Germany, which has an agreement for projects, as well as with universities and research institutions in France and Switzerland moving forward.

# Overcoming the current crisis and moving forward on the goal of "bringing advanced materials science to the world"

Since March 2020, we have been forced to limit our research activities in response to the COVID-19 pandemic. This has especially been a hardship to our young scientists and students who were graduating. Amid this situation, Tohoku University has declared that it will encourage research and development based on the "new normal" post-COVID, and promote efforts leading social change.

With the pandemic expected to prolong, AIMR will need to steadily drive its goals of building a new scientific principle and creating new materials through the three advanced target projects promoting collaboration between mathematics and materials science, while taking all possible measures to prevent the spread of COVID-19. For this, we need to remind ourselves of AIMR's strength of being able to provide an under-one-roof venue for researchers from different fields to work with each other. We also need to continue to focus importance on the three Rs for AIMR to fully demonstrate this strength. We often hear researchers saying that they have had more time to think about future research themes and future prospects now that they spend their everyday life and time differently from usual due to the COVID-19 situation. I hope to continue our system of top-down decision-making by the director, which is the basic principle of the WPI Research Centers, while extensively incorporating innovative ideas, opinions and suggestions that lead the way to a new normal.

With support from the many involved at AIMR, I will strive to overcome this difficult situation and embody the goal of "bringing advanced materials science to the world."

#### **ORIMO Shin-ichi**



Born in Hiroshima in 1966. After earning a Doctor of Philosophy from Hiroshima University, served as a teaching assistant at the university from 1995. From 1998 to 1999, joined the Max Planck Institute for Metals Research as a Humboldt Fellow and an overseas researcher from the Ministry of Education, Culture, Sports, Science and Technology. In 2002, was appoint ed assistant professor (later associate professor) at the Institute for Materials Research of Tohoku University and omoted to professor in 2009. Since 2013, served as the PI of the Device/System Group at the Advanced Institute for Materials Science (AIMR). Appointed Deputy Director in 2018. During this time, served as special advisor to the president, membe of the Provost Office, director of the Japan Institute of Metals and Materials, and chairperson of the University-Industry Cooperative Research Committee of the Japan Society for the Promotion of Science, Director of AIMR since October 1, 2019. Visiting Professor of High Energy Accelerator Research Organization. Major awards received include: The Japan Institute of Metals and Materials Meritorious Award (2011), the Minister of Education, Culture, Sports, Science and Technology's Commendation for Science and Technology (Research Category) (2012), and the Science of Hydrogen & Energy Award (2015).

# INDEX

# **01** [Special Interview]

# Accelerating Advanced Materials Science ORIMO Shin-ichi

Director, Advanced Institute for Materials Research (AIMR), Tohoku University

# 05 AIMR in the world

Fraunhofer Project Center at Tohoku University A Platform for Fostering Industry-Academia Collaboration

#### **Thomas Otto**

Director, Fraunhofer Project Center at Tohoku University Director, Fraunhofer Institute for Electronic Nano Systems ENAS

# 07 The Resurrected Laboratory

#### TANIGAKI Katsumi

Professor Emeritus, Tohoku University

# 09 Fresh Eye g-RIPS-Sendai 2019

# 12 Math and I

#### **Andreas Dechant**

Researcher, Graduate School of Science, Kyoto University

# 13 New Staff

# OZAWA Tomoki AIMR Junior Principal Investigator

#### **GAO** Xichan

AIMR Assistant Professor

Editor NISHIYAMA Nobuyuki Design/Printing Hi creative inc. produced by Strategic Public Relations Office, Advanced Institute for Materials Research (AIMR), Tohoku University

# Fraunhofer Project Center at Tohoku University A Platform for Fostering Industry-Academia Collaboration

Director, Fraunhofer Project Center at Tohoku University Director, Fraunhofer Institute for Electronic Nano Systems ENAS

# Thomas Otto

Born in 1957, Germany. He earned a PhD in engineering at Technische Universität KarLMarx-Stadt in 1987. After working as a postdoctoral fellow at Chemnitz University of Technology, he took up the post of development engineer at SENTECH Instruments GmbH in 1997. Then he moved to the Fraunhofer ENAS and assumed the position of deputy head in 2008 and served as director acting since May 2016. He became a director of the Fraunhofer Project Center at Tohoku University in 2018.



Fraunhofer-Gesellschaft is Europe's largest application-oriented research organization with 74 institutes and independent research units in Germany. The organization has made significant contribution to technology transfer in the context of collaboration between universities and industry with the aim of practical application of scientific expertise. As seen in Fraunhofer, there are very well organized and efficient collaboration systems between universities and industry in Germany. We had the opportunity to talk to Professor Thomas Otto, director of the Fraunhofer Project Center at Tohoku University. He explains the present and the future of NEMS/MEMS technology and shares his views on promotion of industry-academia collaboration and further cooperation with AIMR.

# The first Fraunhofer Project Center in Japan

Fraunhofer Institute for Electronic Nano Systems ENAS (Fraunhofer ENAS) and Tohoku University have been cooperating in the field of new materials for NEMS (nano-electro-mechanical-systems) and MEMS (micro-electro-mechanical systems) for many years. To advance our cooperation, Fraunhofer ENAS and Tohoku University's AIMR launched a strategic research initiative by establishing a joint research and development unit at Tohoku University. The Fraunhofer Project Center "NEMS/MEMS Devices and Manufacturing Technologies at Tohoku University" was inaugurated on April 1, 2012. Since its foundation, the center has become a platform for common research development activities of both institutes.

It is the first Fraunhofer Project Center in Japan. At the time of its founding, the deceased Professor Thomas Gessner

who served as former director of the Fraunhofer ENAS and former AIMR principal invesitigator and Professor Masayoshi Esashi who served as former AIMR principal investigator have made immense contributions. The center has been focusing on research and development in the field of smart systems integration by using micro and nano technologies and know-how for state-of-the-art materials.

# Supporting the NEMS/MEMS industry through mathematics-materials science collaboration

New technologies including new materials enter into emerging markets. Basic knowledge for new technologies and materials is developed at universities especially at their centers of excellence like the AIMR. Looking at the NEMS/MEMS industry, we see the development to complete systems. It is especially important to increase function-

ality of systems themselves. The NEMS/MEMS - electromechanical systems play an important role as they are the senses of the systems. There exist a lot of requirements concerning accuracy, stability as well as reliability of the sensors but there is also the need to combine different sensor principles, different types of sensors in one system. Integrating new materials, new working principles, new applications and often less energy consumption are the main achievements. Worldwide you can observe innovative approaches for scalable fabrication of electronics and sensors using novel functional nanomaterials. So for example the outstanding intrinsic properties of single-walled carbon nanotubes (SWCNTs), such as superior mechanical strength and piezoresistivity, facilitate a new class of miniaturized strain sensors standing out by sensitivity and flexibility with respect to substrate material and integration scenario.

Moreover the autonomy of systems increases leading to demands concerning the processing and storage of data, artificial intelligence, the smartness and intelligence of the system as well as the energy supply of the system itself. Especially for smartness of systems mathematical methods are essential. For that reason, the interdisciplinary approach of the AIMR combining materials science not only with physics and chemistry but also with mathematics at an institutional level is very important. This approach at an university level is new and unique worldwide.

Looking at the work of materials science you address beyond CMOS, low-power, multifunctional, high performance devices. Examples are metallic glasses, nanoporous materials, novel atomic layer materials and much more. Combining this with mathematical concepts and analytical methods you create a new material science, which will definitively support the NEMS/MEMS industry in the future.

# The importance of co-innovation center

Our expertise at Fraunhofer is to bring results of fundamental research into application. The Fraunhofer model of applied research is successful worldwide. We know just from the history that also different laboratories at Tohoku University live an open door philosophy. They open their facilities to industrial partners and they work together with them on the commercialisation of new technologies, new functional systems. We know this work especially from Professor Esashi, one of the former directors of the Fraunhofer Project Center at Tohoku University. It is important to have such so-called co-innovation centers. And I believe the AIMR and our project center can be such a place.

# Acting as a bridge to promote industry-academia collaboration

Since 1949, the Fraunhofer-Gesellschaft, Europe's leading

# - AIMR IN THE WORLD

organization for applied research, has been successfully working at and on the interface between science, business and society. Last year we celebrated the 70's anniversary. Let me introduce Fraunhofer's slogans. "With our fascination for research, we are discovering the world of tomorrow. And the day after tomorrow. It is the future that drives the Fraunhofer-Gesellschaft. We ask the right questions and find new answers: Solutions that are of immediate benefit to industry and society." Under these principles, we have been contributing to the promotion of industry-academia collaboration. And moreover, with Fraunhofer's key strategic initiatives, the Fraunhofer-Gesellschaft bundles the competencies of its institutes in order to develop comprehensive system solutions for strategically important topics.

# Personnel exchanges between universities and companies

To commercialize the good achievements of fundamental research conducted at universities, it is definitively necessary to have personnel exchanges between universities and companies. That is mutually beneficial for both sides. This supports not only the exchange of know-how but also the common understanding of the different perspectives. Even the scientists learn what are the needs of the industry and sometimes they get new ideas for their research. Using methods like design thinking sometimes new product ideas arise, but also sometimes new ideas for research. It is a fruitful cooperation for both sides. Of course, therefore a budget is required at both sides. This includes also a budget for use of infrastructure.

There are many different ways how industry and research benefit from common work. A successful cooperation between science and industry often leads to a technology transfer to industry. Additionally, sometimes employees of research institutes start to work in industry, support the introduction of the new technologies.

Other models are based on training of employees from industry. Looking what is ongoing worldwide, sometimes also so-called digital product schools arise, where scientists, students and staff from industry develop new solutions for the companies taking part.

# Next step for the Fraunhofer Project Center at Tohoku University

Up to now we were focusing only on highend smart systems. We will now extend our cooperation to systems with a much shorter lifetime which enter into closed material cycles. In a common project we want to develop compostable electronics which may be used e.g. for toys or for application in agriculture. There we also want to combine the material know-how at Tohoku University with our system know-how.



As a researcher, opportunities for research can come along in unexpected forms. This is an article about research labs, and since I started out in a corporate research lab, I'd like to begin with looking back on my life as a researcher there.

After I graduated from university I joined NEC, which was well-known for computer control, because I wanted to study on intelligent robots in the future. At NEC, I got the chance to research bubble memory cells (memory using magnetic domain walls) which have large capacity for processing huge amounts of data. This research project was part of national policy driven by government, and corporate research institutes belonging to NEC, Hitachi, Toshiba, and NTT joined forces to vie with the global mega-corporation IBM. Unfortunately, the project did not result in commercialization of bubble memory, which was never used beyond limited fields such as space programs, and research on bubble memory came to an end, including work by IBM. The thing that left the greatest impression on me as a young researcher was the attitude of the lead researchers I saw at that time, who devoted their working lives to advancing the research. Subsequently, Japan experienced an unprecedented boom in corporate basic research. NEC established a basic research lab at Tsukuba Science City (on the site of the International Exposition on Science and Technology), and at the same time set up a research lab near Princeton University in the US. The call went out for young researchers wanting to shift to NEC Tsukuba Research Laboratories. In the end, many mid-level researchers working at NEC Central Research Laboratories in Tokyo were hesitant about moving to Tsukuba. I think they felt that leaving the Central Research Laboratories, which were right in the center of the Kanto region, was like heading out into the boondocks. I was still young and had no ties in Tokyo, so I put my hand up for the first group and left for my new post. The result was that those who moved first had the privilege of getting the best spots and equipment in the new lab. This was to prove an asset for my subsequent life as a researcher. I stayed at NEC Tsukuba





Research Laboratories in Tsukuba Science City for 10 years after that. It transformed into a world-renowned research lab with lots of young researchers, many of whom had returned from overseas, and it was a highly stimulating environment. Around this time, I started research on superconductors, which now plays a key role in my current research.

After that I became a research team leader with department manager status at NEC Tsukuba Research Laboratories, and when I wanted stimulation as a researcher, I was given the opportunity to take up the post of professor at the Graduate School of Science, Osaka City University. Professor Yoichiro Nambu, winner of the Nobel Prize in Physics, had taught at Osaka City University, and for me it was a teaching and research institute that roused my curiosity. At that time the university was establishing a material science department integrating physics and chemistry. My six years there were a good opportunity to learn about balancing teaching with research. Interacting with many other professors also provided the chance to take greater interest in physics.

In 2003, I was given the opportunity to take up a new professorship in the Department of Physics at the Graduate School of Science, Tohoku University. Since my son was attending junior high at the time, with the understanding of my family I moved to Sendai alone to take up the post at the age of 49. Although I had a professor's office at Tohoku University, rather than sitting there I decided to work in the lab with the students to maintain my skills as a researcher. No doubt the young students felt some discomfort at having a much older professor sitting in the same room with them, but I think that day-to-day conversation among the students and young staff members played an important role in keeping me up-to-date as a researcher. My main work subsequently shifted to the AIMR, which was set up at Tohoku University in 2007 as part of efforts by the Ministry of Education, Culture, Sports, Science and Technology to promote internationalization of research. In 2011 the Great East Japan Earthquake struck, and I now work in the new AIMR facility in Katahira. In March 2020 I reach retirement age, and will leave my current post in a few months. The time is coming to call a halt on my long journey as a researcher.

Thinking back now over my research career that began at NEC Central Research Laboratories, it feels both long and short. After a career of more than 35 years, I now feel that when I was young I could freely take on challenges without thinking too much about them, but as I got older there was some physical and mental decline, and gradually the spirit of challenge dwindled. Paradoxically, as you go through life it is by no means risky to take risks. Even if you fail, it will open up possibilities for the future. I hope that young people aiming to be researchers will continue to maintain the spirit of challenge for as long as they can.

[February 17, 2020. At the Tanigaki Laboratory in the AIMR Main Building]



# g-RIPS-Sendai 2019

The g-RIPS-Sendai 2019 (Graduate-level Research in Industrial Projects for Students) program was held from June 17 to August 9, 2019 at AIMR, Tohoku University. The event was sponsored by industrial companies including Toyota Motor Corporation, Fujitsu Laboratories Ltd. and NEC Corporation. The program, originally initiated by IPAM (Institute for Pure and Applied Mathematics), UCLA (University of California, Los Angeles) in the United States, has been running since 2001 and was held in Japan for the first time in 2018.

The aim of the project is to bring together the next generation of young research leaders, foster industry-academia collaboration and strengthen cross-cultural exchange.

A total of 8 students from the US and 5 students from Japan with mathematics or mathematics-related backgrounds gathered in Sendai and tackled different research problems which were designed by the sponsors. On the opening day, industrial mentors from the sponsors explained their projects to the students. Each of the four groups presented their results and outcomes at a final meeting. Throughout the event, communication was carried out in English only.

Toyota set up two projects that focus on the design for next-generation mobility services in suburban areas. Taking Tsukuba City as an example, Group 1 developed a comprehensive concept for the improvement of mobility services on the University of Tsukuba's large campus. Group 2 elaborated on an approach toward the optimization of mobility services for patients of Tsukuba Hospital, which is a very important healthcare provider for the region. Although both teams dealt with different problems, they were encouraged to exchange their ideas and views. In the end, both developed their own mathematical approaches and presented individual solutions.

Fujitsu provided computational environments for Group 3 so that they could tackle real-world issues by "Digital Annealer". This new technology helps solve large-scale combinatorial optimization problems, which would be very time consuming on conventional computers; it provides solutions for problems such as the optimization of traffic routes in order to reduce traffic congestion or high-speed clustering for the utilization of big data. The students had to find concrete formulations and efficient algorithms, and find optimal solutions for combinatorial optimization problems.

Group 4 dealt with "Quantum Annealing" under the guidance of NEC. Using computational environments for a D-wave machine provided by NEC, students searched for the proper choices of solvers and the evaluation of solutions on combinatorial optimization problems. Trying to optimize the "bike share rebalancing problem", the students proposed the choices of the annealers and solvers in order to receive most accurate solutions in the shortest possible time. We spoke to Christine Hoffman from University of California, Merced, who participated in this program.

#### —What was your motivation for participating in the g-RIPS-Sendai 2019 program?

I learned about the g-RIPS-Sendai 2019 program while searching for summer opportunities. It seemed like a unique experience to work on industrial focused problems for an international Japanese company. The interdisciplinary and international aspects of the program appealed to me as well. Prior to the program I had never been to Japan, but I think working in Japan and meeting my company sponsors at Fujitsu headquarters allowed me to gain a deep understanding of the company and their mission.

# –Which project were you working on and why did you choose it?

My project was the FUJITSU Laboratories Ltd.: Resolving real-world issues by "Digital Annealer". My graduate research is in gradient-free optimization, but combinatorial optimization problems have always seemed interesting to me. I was excited to learn about advancements in solving computationally expensive combinatorial problems quickly.



Presentation by Christine Hoffman

#### g-RIPS-Sendai 2019



#### -How did the research proceed? Which difficulties or challenges did you deal with?

Fujitsu is real-world problem orientated. I appreciated this strong focus throughout our project. We started brainstorming real-world problems that could be solved using the digital annealer. Then we started solving smaller, simpler problems to understand the software architecture and progressed to adding more complexity and constraints.

### -How was the communication with the Japanese students in your project?

It was a pleasure getting to know the Japanese students from all the g-RIPS projects. Some students gave insight into their project. For example, the groups working on the Toyota university mobility project included students from Tsukuba University who were personally familiar with the transportation issues there. In addition to collaborating with them on the project, they helped us in our daily lives in Japan as well! One of them took me to the grocery store



In a Japanese culture class

and helped me purchase what I needed, despite not being able to read anything.

### -Do you think that this experience has an impact on your future career?

It feels really rewarding working on projects directly aimed at solving current problems. I feel it has opened doors for future career opportunities, in terms of both experience and connection. Fujitsu has an office very close to my home in California and I will be attending a symposium there next month thanks to the connections I made at Fujitsu.

# -Would you recommend other students from your country to participate in the g-RIPS program in the future?

Absolutely! G-RIPS combines so many unique opportunities: industrial project experience, international collaboration exposure, and university project mentor support. I would highly recommend this program.

# -What was your impression of AIMR and **Tohoku University?**

The AIMR has a broad range of research scientists working in many different areas. I was impressed by the diversity in researchers and learned about a variety of research fields that all still have a connection back to materials research.

To see the voices from other participants, please visit the following website "g-RIPS-Sendai: Program report for 2019." https://www.wpi-aimr.tohoku.ac.jp/cmsoi/g-RIPS2019.html

# Math and I

Part 3

# **Dependable Friend**

 $X \longrightarrow Y \longrightarrow Z \Rightarrow I(x, Y) \ge I(x, Z)$ 

# **Andreas Dechant**

Researcher, Graduate School of Science, Kyoto University (Former AIMR Assistant Professor)

# Mathematics as a source of inspiration

As a theoretical physicist, mathematics for me is like an old, a bit extravagant, but dependable friend. Sometimes, spending time together can be rather exhausting. Sometimes, you struggle to understand them or even fight with them. Other times, they provide you with inspiration and new insights. But in the end, you can always depend on them.

Allegories aside, when I started my career in physics, I often viewed mathematics as merely a tool. You have to solve a concrete problem and apply the right kind of math in the right places to make progress. In the process, the rigor of mathematics can sometimes get in the way. In mathematics, everything should be well-defined, proven and airtight. From the point of view of a physicist, this can appear as "extravagancy" : You just want to get the job done and not put up with mathematics nagging about the details. And often, relying on intuition rather than rigor works: You build a rough scaffolding of your theory, and only in the end come back to mathematics to make sure you were actually allowed to do what you just did.

But sometimes, your intuition can fail you in spectacular ways. I vividly remember having this experience a few years ago: My supervisor and I discovered an article proposing a conjecture to which both our intuitions said, "No way! This cannot be correct!" So, we set about trying to prove our intuition. But after a lot of hard work, what we ended up with was a proof of the article's conjecture. And it required a lot more work to have our intuition catch up with mathematical rigor.

The formula which finally allowed us to understand the results has become my favorite mathematical formula: the data processing inequality. In this formula, X, Y and Z are arbitrary sets of data and the arrows indicate operations carried out on their elements. For example,  $X \rightarrow Y$  means that you take objects



In 2010, he received his Diploma in Physics at Augsburg University and completed his doctoral degree program at Freie Universität Berlin in 2014, both in Germany. He became a ISPS postdoctoral fellow at University of Kyoto in 2015 and a postdoctoral researcher in 2017 at the same institution. In 2018, he became an assistant professor at AIMR. Currently he is working as a researcher at Graduate School of Science, Kyoto University

from *X* and transform them in some way to obtain a new set of objects *Y*. The only rule is that you can only use the objects that were contained in X and not add any new ones. The function I(X;Y) is called the mutual information between X and Y: it measures how much information can be gained about X by looking at *Y* and vice versa. The data processing inequality states that this information can only decrease by adding another operation  $Y \rightarrow Z$ .

As its name implies, this inequality has its origins in data processing and information theory. When you have a set of data, you cannot increase the information contained in the data by any operation that only uses the data as input. This also means that once information is lost, you can never get it back. An everyday example is converting a bitmap file X into a JPEG Y on a computer: this operation reduces the information contained in the image and, whatever you do to the JPEG, the information will never increase again and you will not get back the original. In physics, this concept is called irreversibility: during an irreversible process  $X \rightarrow Y$ , information is lost, so we never see it happening in reverse.

Such a seemingly innocent-looking mathematical formula contains so much insight and even philosophy! This realization was what first caused me to view mathematics as a source of inspiration rather than just a set of tools. Rather than being opposites, rigor and intuition must work in tandem to make progress.

This view of mathematics has only deepened since coming to AIMR. As a theoretical physicist, I have always been on the more "mathematical" side of science. However, here I learned that mathematics can also inspire much more applied disciplines like materials sciences in ways I never imagined.

(September 6, 2019. At the Mathematical Science Group Laboratory in the AIMR Main Building)





# **OZAWA** Tomoki

"I recall that, from my childhood, I had this vague belief that the world should be understandable through the eye of science. A book about Einstein that I read when I was at junior high had a big impact on me, and I decided that I wanted to be a physicist." Associate Professor Ozawa studied in Japan up to university level, but physics is international. He thought that he didn't have to continue studying in Japan, and went to the United States for graduate school. He then worked as a post-doctoral researcher in Italy and Belgium, spending 12 years overseas.

He specializes in theoretical research on condensed-matter physics. When lots of things come together, sometimes phenomena appear that can't be predicted at a glance from their individual properties. That's his field of research. Cold atoms (large numbers of atoms cooled to near absolute zero) have been a particular theme of his research since his graduate school days. "When I was doing research in Italy, the researcher in the next room asked me if I knew about topological insulators, and that's how I was lucky enough to get in on the ground floor of research on photonic topological insulators, which are now a hot topic around the world." Since then, he has continued to study various phenomena that occur when

atoms and light come together, with a focus on many-body and topological properties.

In 2018 he came back to Japan and joined the RIKEN Interdisciplinary Theoretical and Mathematical Sciences Program (iTHEMS). AIMR collaborates with iTHEMS, and that's how he started visiting AIMR. "As someone whose research career has mainly been overseas, I feel relaxed in the AIMR environment, where there is a high proportion of foreign researchers." He hopes to run a research lab at AIMR that takes account of diversity.

The most important thing he learned from his overseas research career is that it is natural for scientists to take vacations and enjoy life beyond research. He always keeps in mind that family is at the center of his life. "My wife is also a researcher. We have two children, and we enjoy raising them together."

> OZAWA Tomoki AIMR Junior Principal Investigato

Born in Tokyo in 1983. In 2012 he obtained Ph.D. in physics from the University of Illinois at Urbana-Champaign. After carrying out post-doctoral research in Italy and Belgium and working as a Senior Research Scientist at RIKEN, he joined AIMR in 2020 as an Associate Professor and Junior Principal Investigate

Dr. Gao was always interested in working abroad and broaden her horizon. Her choice to come to Japan was mainly influenced by her passion and curiosity for research and her admiration for the scientific and technological progress in this country: "I was always deeply impressed by the advanced Japanese technologies."

During her PhD program at Liaoning Normal University, Dr. Gao dealt with calculations of interaction energies in DNA. She felt the desire to further expand her knowledge in Computational Molecular Science and apply it to other fields. The position at NIMS is a perfect match for her: "Here I can apply my background to lithium-ion batteries and calculate the reactions. That is very promising research."

At AIMR, she has developed a genetic algorithm based on force field for lithium-ion battery (LIB) applications. The mechanism of lithium ion transport which significantly affects the LIB performance has been explained based on trustworthy classical MD simulations. She hopes that her research will further contribute to lithium-ion battery applications.



A big surprise for Dr. Gao was the international working atmosphere at AIMR: "It is very nice that everyone speaks English!" She emphasized that she has never experienced to work in such an interdisciplinary environment with people from all over the world. Modestly she added: "I know that I have to break the framework of my research background to achieve a deeper understanding of my work. AIMR provides me this chance because I can work together with scientist from other disciplines."

When asked about what she likes about Sendai, she promptly answered with a smiling face: "The shopping mall and the food. I tried Sushi in other countries before. But here in Japan it is extremely tasty due to the freshness of the fish-and affordable. And the Japanese beef tongue (a specialty of Sendai) is extremely delicious. Sendai is also a very convenient city. I find everything I need to enjoy my daily life here."

#### GAO Xichan

AIMR Assistant Professo

Born in 1987 in Liao Province, China. After obtaining her master's degree at Liaoning Normal University in Computational Molecular Science, Dr. Gao finished her doctoral program at the same institution in 2016 and right after, she started working at Tsukuba University, Japan. In 2018, she ioined the National Institute for Materials Science (NIMS) and came to AIMR as a visiting scientist in the same year. Since April 2020, she has been working as assistant professor at AIMR