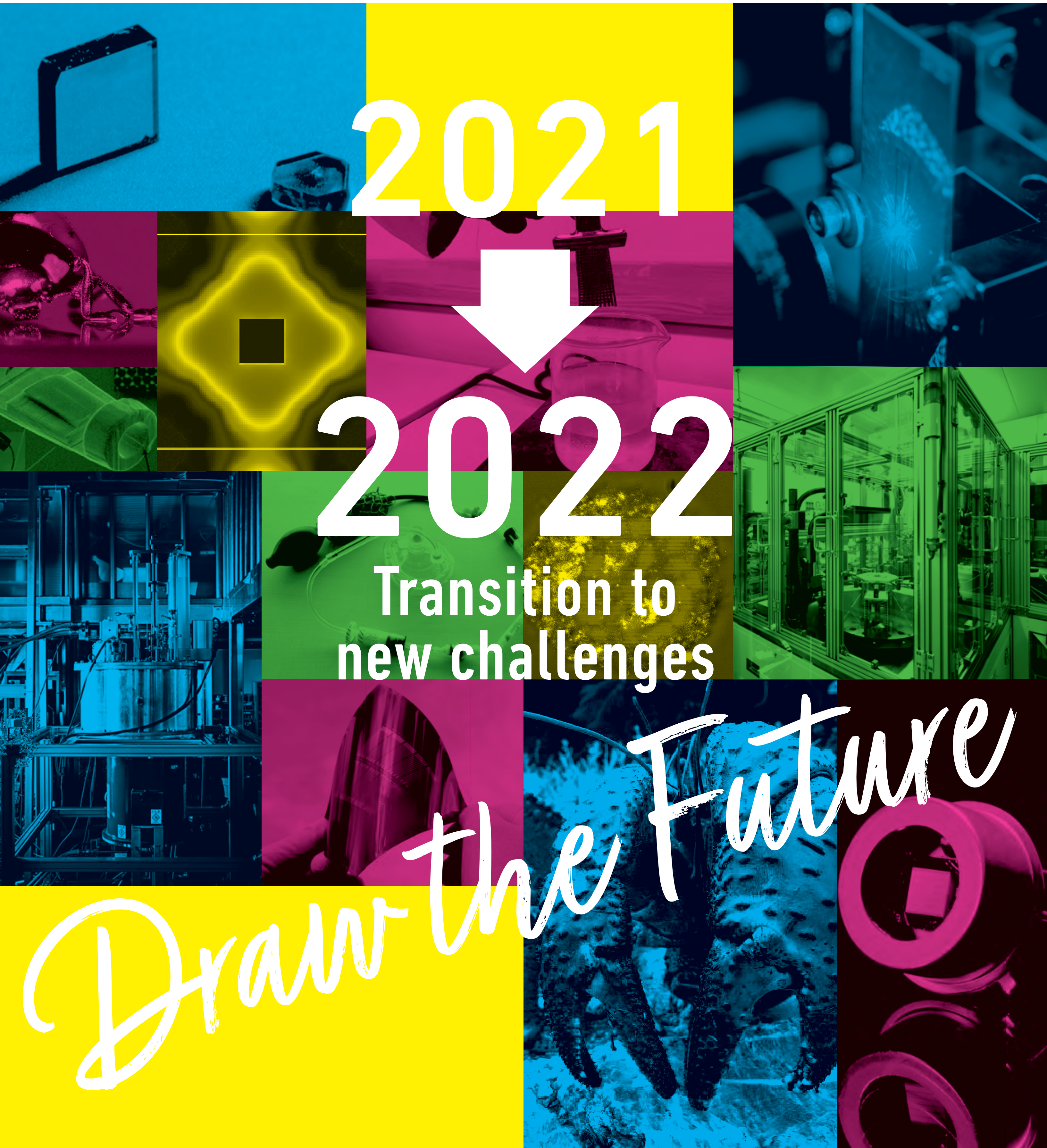
2022

NIMS NOW INTERNATIONAL

NATIONAL INSTITUTE FOR MATERIALS SCIENCE

No. 2



2021 ↓ 2022

Transition to new challenges

Draw the Future

2020

2019

2021

2018

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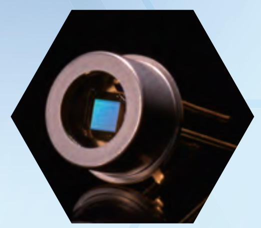
2022

Transition to new challenges



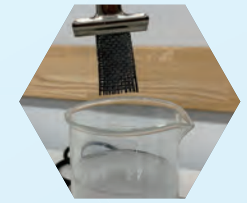
NIMS made significant advances in FY2021—its 20th anniversary year.

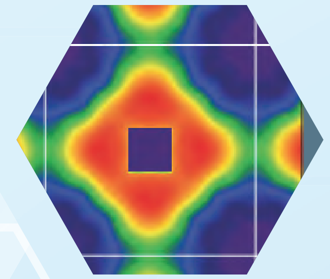
For example, NIMS launched large national projects to develop materials vital to emerging technologies, including next-generation batteries, hydrogen liquefaction and digital transformation (DX) in materials science. NIMS also expanded its Materials Open Platform (MOP) initiative—a framework designed to promote open innovation through collaboration between private companies in the same industries with the goal of strengthening the capabilities of Japan's industrial sector. Japan's major manufacturers of chemicals, all-solid-state batteries and pharmaceutical products have joined industry-specific MOPs at NIMS to conduct joint research and development.

What drives NIMS to undertake these challenges? We are committed to leading Japan's materials research and solving social issues through continuous research efforts. Our recent organizational reforms have boosted its ability to carry out these missions and produce research results.

During FY2022, NIMS will take on new challenges in an effort to make Japan and world more prosperous. This NIMS NOW issue highlights NIMS' accomplishments in FY2021.

Draw the Future





Interview with the President of NIMS

Remembering FY2021 and tackling new challenges in FY2022

**NIMS is committed to solving social problems through research and development.
To enhance NIMS' research capabilities, NIMS President Kazuhito Hashimoto has been pushing forward with organizational and management reform.
FY2021 is the sixth year of NIMS' seven-year medium-to-long-term (MTLT) plan.
According to Hashimoto, his organization's efforts under the plan thus far have borne fruit.
In FY2022, NIMS is expected to play a central role in completing various ongoing projects crucial to Japan's future.
We asked Hashimoto about his vision and ambitions for the coming fiscal year.**

Kazuhito Hashimoto
President of
the National Institute for Materials Science (NIMS)

Supporting both independent and team research

NIMS made significant progress during FY2021 on a number of research projects with potentially significant impacts on the general public. These included energy-related research aimed at achieving carbon neutrality and the introduction of digital transformation (DX) into materials research—a fundamental change in the way materials are developed. In addition, NIMS' collaboration with companies in the industrial sector is beginning to produce tangible results. In this sixth year of the seven-year MTLT plan, I feel that our organizational and management reforms have paid off handsomely.

Since I became President, I've been encouraging all NIMS researchers to spend half of their time researching subjects of personal interest while devoting the other half to team efforts to achieve NIMS' missions. As a national research organization, NIMS must contribute to society through its research. Our R&D is expected to produce solutions to social issues in line with the Japanese government's guidelines. To enhance our research capabilities, we need to boost the research capabilities of our individual researchers. This is why I have encouraged them to pursue their passion projects. My personal experience as a researcher convinces me that this is the best way to improve researchers' abilities.

I would like to explain my vision using a metaphor: an orchestra. A great orchestra is composed of talented soloists who can also fulfill roles specific to each piece of music: some need to stand out by playing leading roles while others need to play softly in supporting roles. This analogy applies to NIMS as a research organization. I encourage individual NIMS researchers to spend half of their time pursuing their own research interests in a manner similar to soloists. At the same time, I ask them to spend the remaining half on team research as if they are members of an orchestra. To thoroughly implement this policy, we have developed an effective research support system and we allocate our budget to ensure that our researchers can perform to the best of their abilities both individually and collectively. In addition, we have designed a performance evaluation system that encourages researchers to divide their efforts between their personal and organizational duties as evenly as possible.

I believe that NIMS researchers have internalized this policy and are diligently carrying it out. This initiative seems to have produced positive, measurable results. The number of research articles published is a common research capability indicator. During 2015, before the implementation of the current MTLT plan, NIMS researchers published 1,222 articles. The number has since increased annually, and in FY2021, we've already published 1,553 articles as of February 15, 2022. Other commonly used research paper indices (i.e., the top 1% and 10% most cited papers) indicate that the quality of our research articles has also improved. NIMS has surpassed Japan's universities and other public research institutions and is now competing with world-top-class research universities overseas in terms of the proportion of papers published that meet these criteria. NIMS' increased research capabilities are also reflected in the increased amount of scientific research funding granted by the Japan Society for the Promotion of Science.

In FY2021, NIMS' proposals on rechargeable batteries and liquid hydrogen research were selected as major national projects (see pp. 10–12). In addition, NIMS' experience in developing its own materials data aggregation systems led to its selection as a main hub for a project to develop platforms to aggregate materials data generated by academics across Japan. This project was launched in FY2021 by the Ministry of Education, Culture, Sports, Science and Technology (MEXT). Furthermore, some of our collaborations with private companies resulted in major successes, including significant results in the Softbank-NIMS joint project to develop air batteries (see p. 13).

Based on these achievements, it's clear that our policy of encouraging our researchers to allocate their efforts evenly between independent and team research is beginning to produce tangible results.

Materials Open Platform (MOP): strengthening Japan's industrial competitiveness

As part of our MTLT plan, we have created MOPs at NIMS to promote open innovation through collaboration with multiple companies in the same industries, rather than one-on-one collaboration. This is a very ambitious initiative to bring together groups of competing companies and encourage them to achieve common basic research goals.

For example, we launched a chemical MOP in 2016 with the participation of Japan's four major chemical companies: Asahi Kasei Corporation, Sumitomo Chemical Company, Mitsui Chemicals and Mitsubishi Chemical Corporation. At the beginning of this collaboration, these long-time rivals were very cautious and dubious of one another, although all understood the significance of working together. To decide on some common goals, NIMS acted as an intermediary, consulting with individual companies on their preferences and intentions to determine workable goals. As a result, the participants reached an agreement to conduct materials informatics research on basic polymeric materials, jointly collect data and perform AI analysis. After five years of collaboration, their research has made significant progress and all seem very satisfied. They have even suggested that we expand this collaboration to include other companies.

Another interesting example is the pharmaceutical MOP launched this fiscal year. Because Japanese pharmaceutical makers are generally smaller than their counterparts overseas, multi-company collaboration is a viable option for them. While it would be impossible for rival companies to jointly develop new drug compounds, they could cooperate on the development of techniques to convert candidate substances into drugs. We proposed this type of collaboration and 11 major pharmaceutical makers in Japan joined the MOP. We're excited to see what kinds of results this collaboration produces (see p. 15). In addition, we recently launched an all-solid-state battery MOP and are planning to start a magnet MOP in FY2022.

Under the MOP framework, private companies are the main players while NIMS researchers play a supporting role. The NIMS researchers who serve as mediators in these collaborative activities may be seen this to be irrelevant to their main duties but I believe that our services will contribute immensely to strengthening Japan's industrial competitiveness.

NIMS as a main hub for the Advanced Research Infrastructure for Materials and Nanotechnology project

Another objective of the current MTLT plan is adopting DX into materials development. Materials informatics—which exploits AI and data science—is becoming an increasingly popular approach to materials development not only in academia but also among private companies. Given that data is the foundation of materials informatics, NIMS must develop effective materials data platforms.

To efficiently aggregate materials data, we're developing a system capable of automatically transferring high-quality data generated by lab equipment to data servers. This system is already connected to 150 lab devices and we're working to link it to more devices. Because lab instruments output data in different formats, it needs to be standardized before it can be aggregated. In addition, metadata (e.g., information on samples and data collection conditions) is vital to effective data utilization. To satisfy these demands, NIMS has also developed a system capable of automatically translating raw data, standardizing its format and transferring it to data servers along with the associated raw data and metadata. These systems also need to be fully protected. Accomplishing all of these goals will be very labor-intensive and expensive. In fact, our previous efforts to develop data platforms required substantial effort and financial investments.

In addition to its data aggregation function, a data platform needs to promote effective data utilization by researchers. For this reason, we launched a new framework in FY2021 to support researchers carrying out data-driven research. Under this framework, experimental researchers are assigned a materials informatics expert with whom they jointly conduct data-driven research. We just had our first meeting with the participating researchers six months after the launch of this project and found that they had already produced results beyond their expectations. This is a strong indication that some data is likely to contain valuable information, as we had long anticipated. Although data-driven research is being rapidly adopted all over the world, I believe that NIMS is currently a frontrunner in this field.

We initially developed data aggregation systems for the benefit of NIMS. However, as a national research institute, we're obliged to spread our initiatives across Japan. Accordingly, we negotiated with MEXT to achieve nationwide adoption of NIMS' data aggregation system. As a result, MEXT launched the Advanced Research Infrastructure for Materials and Nanotechnology project this fiscal year. The aim of this project is to create cloud servers to enable collection and sharing of data from 25 universities and national research organizations across Japan. NIMS will provide all of its techniques and know-how relevant to this project and serve as the main data hub and overall project supervisor.

NIMS' efforts to thoroughly collect data generated by academia and organize it into databases is unprecedented anywhere in the world. As the data aggregation system expands to include a greater number of participants, new issues are expected to arise, such as security and user restrictions. NIMS will play a central role in this project, which is vital to Japan's future.

Rechargeable batteries and liquid hydrogen: keys to achieving a carbon-neutral economy

NIMS is also engaged in major research and development efforts related to carbon-neutral technologies, and has been particularly focused on the development of rechargeable batteries for the last several years. In this fiscal year, MEXT designated NIMS the Center for Advanced Battery Collaboration and tasked it with leading Japan's academic community in rechargeable battery R&D. With respect to all-solid-state battery research, we intend to provide nationwide leadership by guiding both the academic and industrial sectors and mediating the MOP collaboration described above.


Prototype magnetic refrigerator capable of liquefying hydrogen

Moreover, NIMS is engaged in liquid hydrogen research as another means of energy storage. Two projects are currently underway: hydrogen liquefaction and safety evaluation of materials in direct contact with liquid hydrogen. In the first project, in FY2021 we succeeded in liquefying hydrogen using magnetic refrigeration for the first time in the world. This technology may potentially be used to liquefy hydrogen much more cheaply than conventional methods and has already attracted the attention of some manufacturers with whom we have begun joint research.

In the safety evaluation project, the long-term stability of materials needs to be assessed under cryogenic conditions sufficient to liquefy hydrogen. NIMS has considerable experience in performing similar safety evaluations, including creep testing (in which materials' long-term reliability is assessed under high-pressure, high-temperature conditions) and material reliability testing under cryogenic conditions as part of JAXA (Japan Aerospace Exploration Agency)'s project to develop a rocket fueled by liquid hydrogen. Japan currently has no public organization capable of evaluating the safety of materials in direct contact with liquid hydrogen and needs to rely on overseas organizations for this task. For Japan to win in the fierce international competition to achieve a hydrogen economy, it should develop its own capabilities to perform fundamental tasks, such as materials evaluation. NIMS therefore submitted a proposal to develop the capability to serve as an authorized material evaluation organization to NEDO (New Energy and Industrial Technology Development Organization), which was accepted in FY2021 (see pp. 10–11).


Research building at NIMS' Sakura site for use by venture companies

Other carbon-neutral technologies being researched at NIMS include thermoelectric power generation and solar cells. As a materials research institute, we are committed to leading research on various carbon-neutral technologies.

Actively supporting venture companies derived from NIMS

In line with Japan's major policy initiative on promoting startups, NIMS has created various systems to support them. The first venture company derived from NIMS, Oxide Corporation, was listed on stock exchanges in FY2021. This was great news for us. NIMS researchers seem increasingly interested in launching startups, perhaps because of Oxide's success. To support these researchers, we have created a system to invest in qualified NIMS-derived venture companies. We created a 100-million-yen fund by allocating a portion of NIMS' revenues, including those from patents. We recently decided to invest in Thermalytica, which specializes in insulation and heat shield materials R&D, after an external evaluation process. This is the first time that this system was exploited.

In addition, we allocated a research building at NIMS' Sakura site for use by startup companies. We plan to provide further support to help grow their businesses.

Recruiting world-class researchers

As a means of enhancing NIMS' research capabilities, we began recruiting outstanding researchers from around the world in FY2021. We announced that we would reward researchers with up to 100 million yen in initial funding. This has drawn a great deal of attention from the Japanese government and the mass media. We have received many applications and are currently negotiating with some of the qualified applicants about employment conditions and other details. We will continue to widely recruit proficient researchers.

Many of the applicants from overseas already have respectable research positions. When we asked one such applicant why he is interested in coming here, he answered that he found NIMS' research environment attractive. Although Japan's research environment is generally considered to be declining in quality relative to global standards, NIMS is an exception. The applicant's remark supports this. We will continue our efforts to further improve our research environment.

We were very productive in achieving our many missions during this fiscal year. Some may wonder what our focus for the next fiscal year will be. My answer is that we will remain fully committed to all of our missions. FY2022 is the final year of our current MTLT plan. We will therefore complete all of our ongoing projects in accordance with the plan and formulate a new MTLT plan to continue producing results.

2021 NIMS Press Release List

As a top runner in materials research, NIMS is creating a new future for materials science that will lead to the next generation. Let's look back on the history of NIMS this year.

Details of all 2021 press releases

1.19 Demonstration of Unconventional Transverse Thermoelectric Generation

2.19 High Efficiency Magnetic Cooling by Using Small Magnetic Field Changes

3.5 Discovery of a Mechanism for Making Superconductors More Resistant to Magnetic Fields

3.10 Highly Fatigue-Resistant FMS Alloy with Enhanced Weldability

NIMS enhanced the weldability of the previously developed fatigue-resistant FMS (iron-manganese-silicon-based) alloy, designed for use in seismic dampers, alloy, designed for use in seismic dampers, without compromising its fatigue durability by modifying its composition.

4.1 New NIMS Structural Materials Data Sheets Released

4.13 Conventional Idea of Electronic State in High-Temperature Superconductors Is Overturned

4.17 Development of a Novel Thermoelectric Material with Conversion Efficiency as High as Bi_2Te_3

4.27 Development of a Portable and Disposable Nitric Oxide (NO) Generator

5.14 NIMS and the Indian Institute of Technology Hyderabad (IITH) launched IITH-NIMS Joint Research Center for Materials Research

5.20 Joint Development of a Toothed Gear Reusability Evaluation Method

Okinawa Churashima Foundation

5.24 Exoskeletal Microstructure of Extremely Hard Coconut Crab Claws

The NIMS Research Center for Structural Materials and the Okinawa Churashima Foundation Research Center jointly ascertained the microstructure and chemical composition of the extremely tough exoskeletons of coconut crab claws, which are capable of generating a stronger pinching force than those of any other crustacean.

5.27 Fabrication of Printed High-Performance Thin-Film Transistors Operable at One Volt

5.27 Development of Ultra-High-Resolution Printed Electronics Using Dual Surface Architectonics

6.3 Tarsal Adhesion Mechanisms of Ladybird Beetles Ascertained

6.4 Special Open Call for Leaders Promoting World-Top-Class Research in Materials Science

6.14 Development of a Viscosity Measurement Technique Applicable to Both Liquids and Gases

6.21 Digitalization and Visualization of Odors Using an Odor Sensor and Machine Learning

NIMS has developed a technique which combines an odor sensor and machine learning that is capable of selecting reference odors out of a dozen samples of different odors.

6.25 Materials Open Platform (MOP) for Pharmaceutical Science Launched
(▸ see p.15)

7.29 Simple Thermoset Plastic Recycling Using a Peptide Solution

Epoxy resin is a type of thermoset resin commonly used in glue, paint and composite materials. NIMS and ISMA have developed a new thermoset plastic recycling system capable of easily decomposing epoxy resins in an aqueous solution of a naturally derived peptide.

8.5 Development of an Antigen Enrichment Technique with Enhanced Sensitivity for Rapid COVID-19 Diagnosis

8.27 NIMS Award 2021 Goes to Prof. Tsuneya Ando, Prof. Allan H. MacDonald and Prof. Pablo Jarillo-Herrero

8.30 Lattice Softness: Key to the Identification of Metals with High Hydrogenation Abilities

9.27 NIMS and Graduate School of Information Science and Technology at Osaka University jointly launch a new collaborative PhD program

10.11 Development of an Artificial Vision Device Capable of Mimicking Human Optical Illusions

10.25 Development of a versatile, accurate AI prediction technique even with a small number of experiments

11.9 Discovery of an Obscure Source of High-Temperature Superconductivity Using an Artificial Neural Network

11.9 Development of a High-Energy-Resolution, LaB_6 Nanowire-Based Field Emission Gun

11.15 Success in Efficient Fabrication of High-Performance Neodymium Magnets Using Machine Learning

NIMS has demonstrated that it is possible to maximize the permanent magnetic property of neodymium magnets, for which demand is rapidly increasing as magnets for traction motors in electric vehicles and other applications, with a minimum number of experiments by applying machine learning to experimental datasets obtained by varying the conditions for their fabrication.

12.15 Development of a Lithium-Air Battery with an Energy Density over 500 Wh/kg
(▸ see p.13)

12.24 Observation of Quantum Transport at Room Temperature in a 2.8-Nanometer CNT Transistor

12.24 NIMS wins the highest award at Japan's PR Award Grand Prix 2021

NIMS won the highest award at the "PR Award Grand Prix 2021" sponsored by the Japan Public Relations Association. Based on the YouTube channel "Material's Eye" with more than 170,000 registered users, we are communicating the appeal of materials science to many people at events such as NIMS Open House and competitions for producing materials. These led a lot of young people to go on to universities with materials science. In this way, our public relations activities which have a great impact on the next generation of young people are highly evaluated.

Liquid hydrogen

Full-scale R&D begins: materials vital to achieving a hydrogen economy

NIMS has launched large-scale projects to develop carbon-neutral technologies, including a magnetic refrigeration technology capable of liquefying hydrogen, systems needed to put this technology into practical use and new materials resistant to liquid hydrogen. We asked Tadashi Shimizu (Director of the Cryogenic Center for Liquid Hydrogen and Materials Science (CLean)) about the current status of liquid hydrogen research at CLean and issues that still need to be overcome.

Tadashi Shimizu
Director, Cryogenic Center for Liquid Hydrogen and Materials Science (CLean)
Director, Nuclear Magnetic Resonance (NMR) Station

Four technological issues related to the development of a hydrogen supply chain

Hydrogen is a key energy source for achieving carbon neutrality. Japan is the first country to have developed a liquefied natural gas (LNG) supply chain in which natural gas is produced and liquefied overseas and transported in tankers to Japan. This means of importing LNG was a necessity for Japan as it is surrounded by the sea and pipelining LNG from abroad is not an option. Japan—the world's largest LNG consumer—is now attempting to develop the world's first hydrogen supply chain. Because pure hydrogen does not exist in nature, it needs to be extracted from hydrogen compounds, such as water. Japan's hydrogen supply chain is expected to operate in a manner similar to the way its LNG supply chain operates: hydrogen will be produced and liquefied in countries where these processes are cheap and then transported in tankers to Japan.

A hydrogen supply chain consists of four industrial steps: hydrogen production, liquefaction, transportation/storage and utilization. All of these steps have major technological issues requiring the development of new materials.

When the current LNG supply chain was created, western countries were ahead of Japan in developing basic technologies, global standards and international rules related to supply chains. As a result, western countries have predominantly profited from major supply chain-related products and the inspection of these products. By comparison, global standards have yet to be set for hydrogen-related technologies, giving Japan a chance to lead the way in developing technologies, standards and rules related to hydrogen supply chains.

I'd like to briefly describe the issues associated with the four hydrogen supply chain processes: hydrogen production, liquefaction, transportation/storage and utilization. First, high-performance catalysts need to be developed to increase the efficiency of hydrogen producing chemical reactions. Because hydrogen can be produced either from water or fossil fuels, catalysts capable of breaking water down into hydrogen and oxygen and of breaking fossil fuels down into hydrogen, carbon and oxygen need to be developed. Second, hydrogen liquefaction is currently a very expensive process, and its cost-efficiency must be dramatically improved. Third, liquid hydrogen transportation and storage equipment needs to be developed using inexpensive materials that are also resistant to embrittlement caused by exposure to hydrogen and cryogenic temperatures. Finally, hydrogen fuel cells compatible with a wide range of systems, in addition to automobiles, should be developed. This will require new fuel cell materials suitable for use in different systems. NIMS has the appropriate materials R&D skills and infrastructure to tackle these issues.

Hydrogen liquefaction technology is vital to achieving widespread use of hydrogen energy. When hydrogen gas is liquefied, its volume can be reduced to approximately one eight hundredth of its original gaseous volume, making hydrogen transportation and storage practical. However, because hydrogen liquefies at the very low temperature of 20 K (-253°C), its liquefaction requires a huge amount of energy.

Vapor compression refrigeration technology is currently used to liquify hydrogen. This technology—also used in air conditioners and refrigerators—cools a refrigerant gas by cyclically compressing and expanding it. This technology was invented more than 200 years ago—about as old as heat engines, such as steam engines—during the Industrial Revolution. It is very unlikely that the performance of this old technology can be substantially improved. In addition, nearly all hydrogen liquefaction systems are conventional products made in western countries. This western world's domination of this market makes it difficult for Japan to create more economical and efficient hydrogen liquefaction technologies.

NIMS leads the development of hydrogen-related technologies

NIMS has focused on magnetic refrigeration, in which the distance between a magnet and a magnetic material is repeatedly changed, causing the material to absorb and release heat. Because this technology only requires changing the intensity of the magnetic fields applied to a magnetic material, it may potentially be much more efficient in liquefying hydrogen than vapor compression refrigeration.

Japan has been a frontrunner in developing magnetic refrigeration technology and NIMS has been researching this technology for many years. Magnetic refrigeration has the potential to be a game-changing technology.

In 2018, NIMS launched a research project entitled, "Development of an advanced hydrogen liquefaction system using magnetic refrigeration technology," funded by the Japan Science and Technology Agency (JST)'s program, "Innovative hydrogen liquefaction technologies desirable in a future society." In FY2021, NIMS succeeded in liquefying hydrogen using a new magnetic refrigeration technology it developed—a major breakthrough.

To put this technology into practical use, we need to develop higher performance magnetic refrigeration systems and magnetic materials.

Computer-based numerical analysis is a new technique that enables researchers to efficiently determine optimum experimental methods. Using this technique, we were able to design a magnetic refrigeration system capable of liquefying hydrogen.

Magnetic materials that perform optimally at 20 K—the temperature at which hydrogen liquefies—need to be developed. No research has previously been conducted to develop such materials. We have adopted machine learning techniques in our effort to discover optimum magnetic materials and this approach has produced promising results. We will continue to improve the performance of our magnetic refrigeration technology, including its hydrogen liquefaction efficiency.

Koji Kamiya(Group Leader of Magnetic Refrigeration System Group) operating a magnetic refrigeration prototype for hydrogen liquefaction

Pick Up

Hideki Katayama
Deputy Director,
Research Center for Structural Materials

Yoshinori Ono
Principal Researcher,
Materials Strength Standard and Technology Group
Research Center for Structural Materials

In this NEDO-funded project, NIMS will evaluate the mechanical properties of materials to be used in liquid hydrogen-related equipment, such as tanks used to store and ship liquid hydrogen. A new evaluation facility, including evaluation equipment and a lab, is being developed at NIMS' Sakura site. Hideki Katayama and Yoshinori Ono, the leaders of this project, share their thoughts on it.

Katayama: To achieve widespread use of hydrogen, the cost of supplying it needs to be reduced by increasing the size of hydrogen supply chain equipment and demand for hydrogen has to be created. With respect to hydrogen supply chain equipment (i.e., equipment needed to produce, transport, store and utilize liquid hydrogen), the reliability of materials used to manufacture it must be properly evaluated by developing effective reliability evaluation technologies.

Ono: In FY2021, NIMS' research proposal entitled, "Development of material evaluation technology vital to liquid hydrogen equipment R&D," was accepted by NEDO under the category, "Construction of a large-scale hydrogen supply chain," supported by the Green Innovation fund. We are preparing cryogenic testing systems to evaluate the mechanical properties of materials to be used in liquid hydrogen-related equipment (e.g., tanks used to store and transport liquid hydrogen). NIMS has experience in evaluating the mechanical properties of materials used in liquid rocket engines at cryogenic temperatures in joint research with JAXA. In addition, NIMS has developed a new method of evaluating materials by exposing them to hydrogen using a test piece with a hollow core. This method eliminated the need to use large equipment. These experiences and techniques are expected to be handy in evaluating the reliability of materials in this project.

Katayama: During the first six months of this project, we have progressed in preparing a new evaluation facility at NIMS' Sakura site by designing evaluation equipment and a lab, among other preparations.

Strengthening NIMS' role as a core battery development center

NIMS has been leading the development of innovative next-generation batteries, including all-solid-state batteries and lithium -air batteries. Its Center for Advanced Battery Collaboration was officially launched this year to research protocols for battery design, development and analysis using AI and other techniques. We asked Kazunori Takada, Director of the Center, about ongoing research projects and future plans.

Kazunori Takada
Director,
Center for Green Research on Energy and Environmental Materials

Development of durable, reliable all-solid-state (ASS) batteries

In 1991, two types of small, high-capacity rechargeable batteries became available: nickel-metal hydride batteries and lithium-ion batteries. This led to the rapid development and popularization of new battery-powered technologies, including mobile phones and laptop computers. Today, development of new batteries superior in performance to lithium-ion batteries is underway to meet the requirements of emerging technologies, such as electric vehicles.

Among the many types of next-generation batteries under development, NIMS has been focused mainly on ASS batteries and lithium–air batteries.

An ASS battery contains a solid electrolyte rather than a conventional liquid one. This battery has the potential to significantly exceed lithium-ion batteries in performance by having a higher capacity, shorter charge time and longer life. Researchers have been working to develop ASS batteries that are sufficiently durable and reliable to withstand more than a decade of use in automobiles and other technologies with long useful lives.

Toyota Motor Corporation has announced that it has developed a prototype automobile powered by ASS batteries and is working to put it into practical use. The sulfide solid electrolytes integrated into these batteries have significantly increased their performance. However, sulfides are highly reactive to moisture in the air, imposing major constraints on battery production processes and making battery production expensive.

Materials Open Platform (MOP) for the development of ASS batteries with oxide solid electrolytes

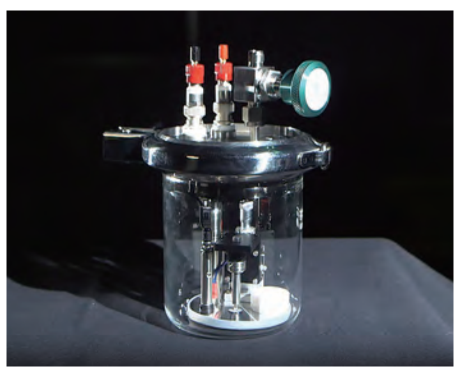
NIMS has been researching and developing battery production processes needed to produce high-performance ASS batteries containing oxide solid (i.e., ceramic) electrolytes. Oxides have the advantage of being stable and easy to handle in the air. To put these batteries into practical use, we launched an ASS battery MOP in 2020 with the aim of facilitating collaboration between automobile, material, battery and other manufacturers.

Some researchers claim that the performance of sulfide ASS batteries has surpassed that of lithium-ion batteries. However, their production processes are complex, making production expensive. For this reason, many manufacturers have chosen to develop oxide ASS batteries as a long-term strategy. However, most of them have somewhat reluctant to fully engage in oxide ASS battery R&D because these batteries still perform poorly and are far from being ready for practical use. To address this issue, NIMS led the effort to launch the ASS battery MOP by inviting relevant private companies. While the COVID-19 pandemic has been disrupting MOP collaboration, we have managed to make progress in preparing tools and fundamental technologies needed to develop oxide ASS batteries.

NIMS has been collaborating with SoftBank Corp. in developing lithium–air batteries, which has produced significant results. In addition, many NIMS researchers are participating in ALCA-SPRING project of JST (Japan Science and Technology Agency) to research and develop magnesium batteries, which contain no rare metals, as well as the above next-generation batteries.

Finally, the Center for Advanced Battery Collaboration established at NIMS officially began operating in FY2021. At this Center, we use AI techniques to create protocols for efficient battery design, development and analysis, eliminating the need for the long process of trial-and-error that characterized battery development in the past.

As described above, NIMS participated in many next-generation battery development projects during this fiscal year with a main focus on ASS and lithium–air batteries. We will continue leading Japan's efforts to develop and achieve practical use of innovative batteries.



Prototype cell for all-solid-state battery

Pick Up

Development of lithium-air battery

Kohei Uosaki
Fellow
Executive Advisor
to the President

Shoichi Matsuda
Senior Researcher
Rechargeable Battery Materials Group
Center for Green Research on Energy and Environmental Materials

The lithium-air battery developed by NIMS in collaboration with Softbank Corp has achieved 500Wh / kg. NIMS has been exploring lightweight batteries, including metal–air batteries with high energy densities with Softbanc Corp. We asked Kohei Uosaki and Shoichi Matsuda, who lead these collaborative R&D efforts, about their future research plans.

Uosaki: NIMS has been conducting basic research on lithium–air batteries with support from the JST/ALCA-SPRING program (ALCA: Advanced Low Carbon Technology Research and Development Program, SPRING: Specially Promoted Research for Innovative Next Generation Batteries) for about 10 years. Lithium–air batteries have the potential to significantly exceed currently most used lithium-ion batteries from the view point of their energy density. In 2018, NIMS and SoftBank established the Advanced Technologies Development Center with the objective of research and development of practical lithium–air batteries suitable for use in mobile phone base stations, HAPS (high altitude platform stations) and other applications. The joint research group recently succeeded in stable operation of rechargeable lithium–air battery with an energy density of 500 Wh/kg at room temperature. This news was publicized in December 2021 in the form of a press release.

High energy density lithium -air battery cell equipped with a porous carbon cathode developed by NIMS

Matsuda: The negative and positive electrodes for current lithium-ion batteries are both composed of heavy materials: graphite and a lithium ion-containing metallic oxide, respectively. By contrast, the negative electrode of a lithium–air battery is composed of light, metallic lithium and its positive electrodes—oxygen in the air—is virtually weightless. Based on the energy density estimation only for weight of electrode materials, the energy density of lithium–air battery can be more than 10 times that of a lithium-ion battery. However, taking other components of actual batteries into account, including electrolytes, separators and packing materials, the energy density of a practical lithium–air battery is estimated to be about two to three times that of a lithium-ion battery.

Uosaki: We have already accomplished the objective of developing a high energy density lithium–air battery in the ALCA-SPRING project. However, our goal is to create a practical rechargeable battery with stable charge/discharge cycles. A battery for use in HAPS should be rechargeable at least 200 times. In general, there is a tradeoff relation between energy density and cycle life, the higher the energy density of a battery, the shorter its lifecycle. We have been seeking ways of simultaneously increasing both battery energy densities and lifecycles through extensive basic research.

Matsuda: We've made two significant technological accomplishments for development of rechargeable lithium–air batteries. First, we established the electrolyte injection technique that can be adaptable for small electrolyte condition. For achieving an energy density over 500 Wh/kg, it is required for reducing the amount of electrolyte—realistic battery conditions.

Although there are several report the have achieved high performance lithium–air battery (e.g., high lifecycle performance), the battery are evaluated under unrealistic conditions, such as batteries containing excessive electrolyte amounts and are evaluated with low capacity limitation conditions. The second technological accomplishment is for developments of self-standing porous carbon membrane for positive electrode. We succeeded in preparing carbon powder based self-standing membrane only using minimum amounts of binder and substrate material without diminishing the mechanical strength of the membrane.

Uosaki: It is very important for batteries to have higher energy densities but many researchers are less concerned about reducing battery weight from the practical view of point, which is directly influenced by the electrolyte amount and the weight of the battery case, separator, current collector and other components. By contrast, NIMS always maintains high standards in meeting all kinds of practical use requirements in its battery R&D.

Matsuda: The success of operation of 500 Wh/kg class lithium-air batteries are based on the results of evaluation of more than 3000 battery cells, which were fabricated manually and these investigation takes over two-year period. To accelerate the R&D, we recently introduced an automated robotic technology that enables us to produce 500 cells a month. In addition, we have adopted machine learning techniques to analyze the battery data by collaborating with MaDIS (Research and Services Division of Materials Data and Integrated System). By the use of machine learning techniques, the suitable experimental plans are recommended. Thus, the research development for searching suitable material combination for realizing long cycle-life lithium-air batteries can be greatly accelerated. We plan to publish these results in the near future.

Uosaki: The long-term goal of the NIMS-SoftBank Advanced Technology Development Center is the development of lightweight batteries, which are not limited to lithium–air batteries. We will therefore explore a wide range of batteries that may potentially have high energy densities, in addition to continuing our research on lithium–air batteries.

Automated robotic technology capable of expediting the production of high energy density lithium -air battery cells

MOP

Materials Open Platform (MOP) for Chemical Industry

Development of an AI technique capable of improving the accuracy of next-generation material property predictions

The MOP for chemical industry is a collaborative framework designed to encourage Japan's chemical manufacturers to jointly conduct fundamental research with common goals. Takashi Nakanishi, a research group leader at NIMS, has been acting as an intermediary between the four chemical manufacturers participating in this MOP. We asked Nakanishi about the current status of MOP collaboration and the results it has produced.

Takashi Nakanishi
Leader of the Frontier Molecules Group
International Center for Materials Nanoarchitectonics

Chemical manufacturers and NIMS construct a sharable database

The MOP for chemical industry was established in 2017 to enable chemical manufacturers to jointly tackle common challenges, thereby boosting their international competitiveness. NIMS was able to convince four chemical companies to join the MOP: Asahi Kasei Corporation, Sumitomo Chemical Company, Mitsui Chemicals and Mitsubishi Chemical Corporation.

In this unprecedented project, our first task was to identify common development goals the participating companies could agree on. Our general direction was to develop polymeric materials using data science—a field in which Japan lagged behind some other countries at the time.

Gathering consistent data about polymer was challenging because many different types of polymers exist with physical properties that vary widely. In addition, we were unsure what types of data to collect to develop techniques of interest. Despite these difficulties and uncertainties, we remained optimistic about the possibility of developing world-class techniques commensurate with the reputation Japanese chemical manufacturers enjoy for being highly skilled. We ultimately decided to develop fundamental materials informatics (MI) techniques applicable to polyolefins, a versatile class of polymers.

In building a polymer database, we initially considered asking all of the participating companies to provide their data or data that is no longer in use. However, we soon dropped this approach due to the companies' stringent rules against data sharing. Consequently, we decided to create a new, sharable database from scratch. NIMS and expert representatives from the member companies led this effort.

We have collected more than 45,000 data points representing 300 types of polymers—a sufficient amount of data to enable effective analysis of polymeric materials with diverse characteristics. We collected this data in accordance with the rules we formulated (e.g., types of lab instruments, measurement methods and data formats). This unique collaboration led to the construction of an exceptionally high-quality database.

Development of an AI technique using the database

This database—a common asset of the four member companies and NIMS—was used to develop new AI techniques. The companies are very satisfied with their accomplishments so far. The MOP for chemical industry has grown from its initial roster of about 20 company researchers to more than 40. This novel collaboration framework allows Japan's top researchers and technicians to openly and enthusiastically work together and exchange information. It is also providing young researchers with valuable opportunities to gain research experience.

On the other hand, because many of the results produced from this collaboration were classified as confidential information, we were unable to publish them. NIMS plans to more widely publicize our activities as part of an effort to strengthen the international competitiveness of Japan's industrial sector. In FY2021, we managed as MOP members to publish a part of our research on the development of an advanced MI technique—an AI technique capable of improving the accuracy of material property predictions after only a small number of experiments—while protecting most of the confidential information. This research article was well received in Japan and overseas due to this technique's applicability to a wide range of materials development in addition to polymeric materials.* It is noted that the MOP is drawing interest from other chemical manufacturers.

FY2022 will mark the chemical MOP's sixth year. We are discussing whether to wrap up some of our ongoing projects and initiate new projects vital to Japan's chemical industry today.

We will continue updating our activities annually by identifying changing needs in the chemical industry with the goal of enhancing the technological capabilities of Japan's industrial sector.

* Link to the NIMS press release:
https://www.nims.go.jp/eng/news/press/2021/10/202110250.html

Materials Open Platform (MOP) for Pharmaceutical Science

Aiming to become a leader in pharmaceutical materials science

The MOP for Pharmaceutical Science was launched in FY2021 with the objective of increasing the global competitiveness of Japan's pharmaceutical industry. Kohsaku Kawakami, a research group leader at NIMS, led the effort to invite pharmaceutical companies to form the MOP. We asked Kawakami about his vision for this project.

Kohsaku Kawakami
Leader of the Medical Soft Matter Group
Research Center for Functional Materials

Filling technical gaps with major pharmaceutical companies overseas

During this fiscal year, NIMS launched the MOP for Pharmaceutical Science with 11 drug firms. This MOP has begun evaluating physicochemical properties of chemical compounds and developing drug formulation techniques mainly focused on antibody and nucleic acid drugs.

While most drug research focuses on potentially active compounds, techniques used to convert compounds into drug products are also very important. For example, a COVID-19 vaccine is composed of fragile messenger RNA (the active ingredient) wrapped in lipid particles. These particles make the vaccine suitable for administration and enable it to work effectively in the body. This illustrates the fact that a drug requires a precise combination of active and inert ingredients.

World-class pharmaceutical companies have their own materials science sections to evaluate the physicochemical properties of drug compounds and develop them into products. By contrast, Japanese pharmaceutical companies have very few materials scientists dedicated to these tasks. I believe that NIMS is in the appropriate position to group these scientists together and support them as they perform these tasks in an effort to close the technical gaps between Japanese pharmaceutical companies and their foreign counterparts.

The importance of materials science is expected to increase in biopharmaceuticals R&D. Conventionally, low-molecular compounds have been used as main drug components. However, biopharmaceuticals composed of biopolymers (e.g., antibodies and nucleic acids) applicable to a wide range of modalities (i.e., therapeutic methods) have become increasingly popular in recent years. Japan's pharmaceutical sector is keenly interested in developing globally competitive biopharmaceutical techniques.

Japanese pharmaceutical companies have traditionally been very capable relative to global standards. However, they are rapidly falling behind in the era of biopharmaceuticals because they are much smaller than their world-class counterparts overseas and have very limited materials science R&D capabilities. We have launched the pharmaceutical MOP to overcome these issues.

Revision of technical procedures and evaluation methods

We have established six joint research groups with different objectives within the MOP: 1) development of analytical methods for antibody drugs, 2) development of techniques to convert antibody drugs into formulations, 3) development of physicochemical property profiling methods for nucleic acid drugs, 4) investigation of mechanisms by which low-molecular drugs are absorbed in the gastrointestinal tract, 5) development of stable amorphous drugs and 6) use of ionic liquids in drug formulation. All member companies are participating in more than one of the joint research groups, and all results produced by group research are shared by all of the companies, including companies not involved in producing the results. Although we have just begun these group activities and have not made any major achievements, we have made satisfactory progress.

For example, group research has made us realize that individual companies perform certain tasks and measurements differently even when using the same techniques. In light of this awareness, we have revised our technical procedures and evaluation methods to improve consistency between the member companies and research efficiency.

R&D procedures differ between Japanese pharmaceutical companies due to their traditional reluctance to share information. However, keeping information secret (e.g., drug development procedures) could adversely affect joint development efforts, delaying commercialization of the final products. Although sharing information may entail some risk, pharmaceutical companies should understand the risks of not sharing information as well.

Techniques used to formulate different drugs for different diseases often have many similarities. It would therefore be more efficient for pharmaceutical companies to develop fundamental formulation techniques together rather than separately. This MOP collaboration is expected to be particularly effective in developing techniques to formulate biopharmaceuticals.

We plan to publicly release the major research findings produced through this MOP collaboration. We will even encourage others to use our techniques if they are helpful. We will also make active efforts to globally publicize our results through presentations at scientific meetings and publication of research articles. We hope to become a frontrunner in pharmaceutical materials R&D so that we can be involved in setting rules for drug development.

Our MOP membership may grow in the future as we have been receiving inquiries from other pharmaceutical companies. We will closely communicate in making decisions on research subjects and new projects.

NIMS NEWS

Special Open Call for Leaders Promoting World-Top-Class Research in Material Science

NIMS has announced an international open call for the recruitment of extremely talented researchers who can promote top world-class research in Materials Science. The successful candidate will be required to lead a new independent research group. In addition, several incentives will be made available, including the special allocation of a generous start-up fund of up to 100 million yen within the first year, to enable the candidate to start research at NIMS. All research fields related to Materials Science, regardless of whether they are basic or applied, are eligible for application.

More detail

English subtitles added to “To the Scientists of the Future” video clips

“To the Scientists of the Future” is a YouTube video clip series created jointly by NIMS and EUPHRATES Ltd. (a group specializing in creative work, including NHK’s educational TV programs). We have added an English subtitle option to these clips.

This scientific video series has been popular in Japan with a cumulative view count exceeding 7 million. These clips demonstrate the various intriguing scientific phenomena and unique materials NIMS has developed using fascinating images that are also entertaining and beutiful.

An English subtitle option makes it accessible to a broader global audience with an interest in science. We hope you enjoy it.

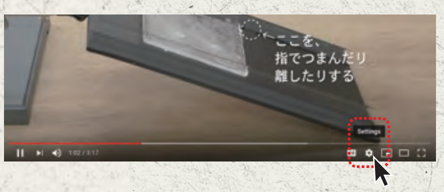
<How to display English subtitles>

1.

On the YouTube website, type “nims euphrates” in the search box and press enter. Select the video clip entitled “NIMS x EUPHRATES 未来の科学者たちへ.”

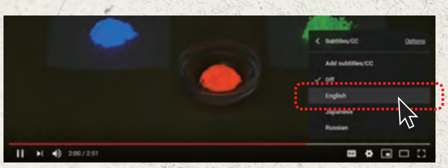
2.

Left-click the “Settings” icon in the lower right corner of the screen and select “Subtitles”.



3.

Finally, select “English” (only Japanese audio is available).



<List of “To the Scientists of the Future” video clips>

▼**Sialon phosphor**

▼**Invisible glass**

▼**Super hydrophobic material**

*Video clips with English subtitles will be released as they become available.

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