The CATALYST

Helping you react with chemical reactions

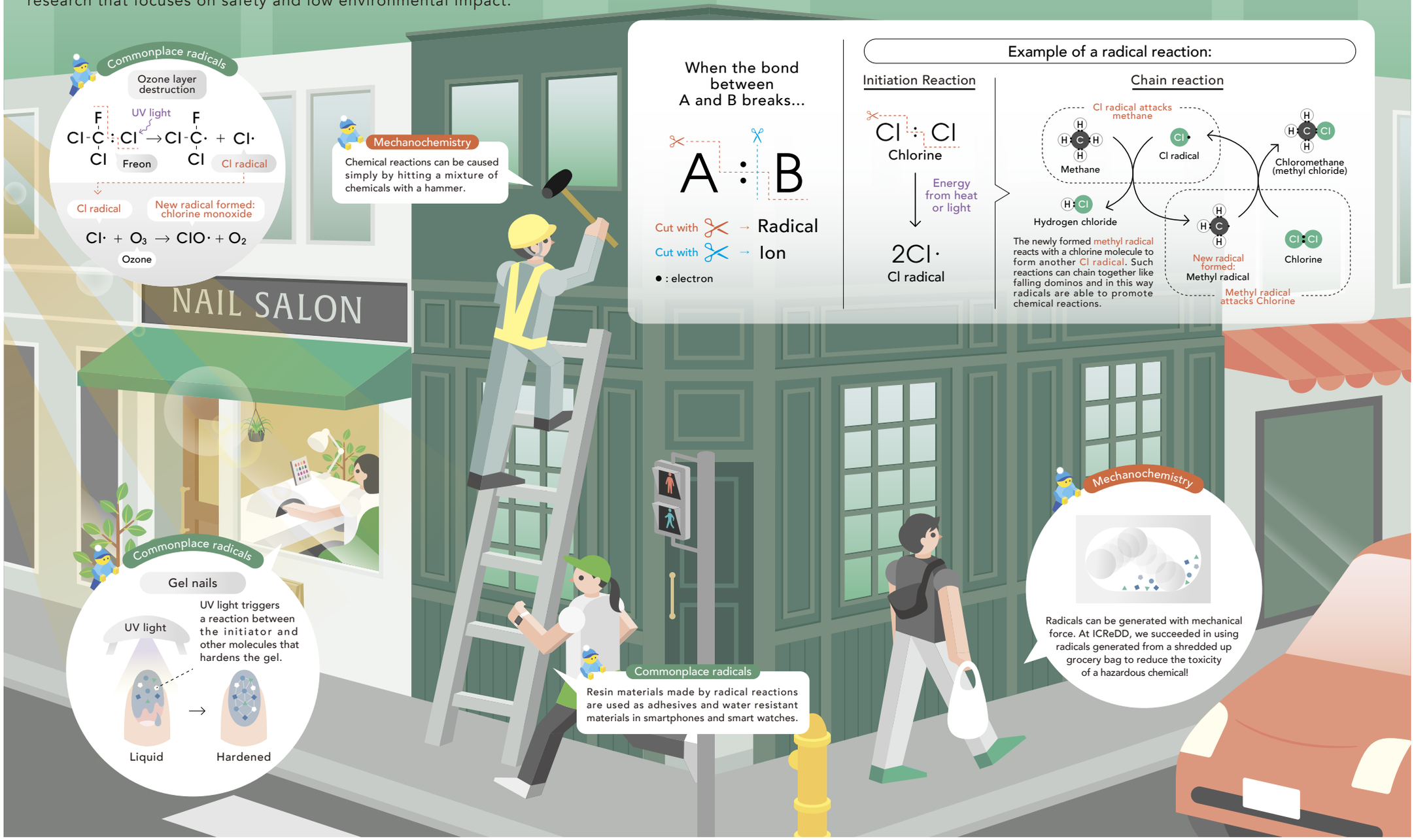
Issue 16
June 2024

Environmentally friendly reaction development:
Force is the key?

ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY

Environmentally friendly reaction development: Force is the key?

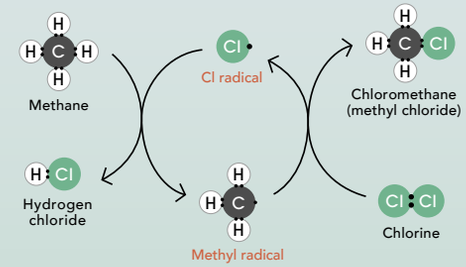
Materials and products that make our lives more convenient also put stress on the environment in the form of hazardous chemicals that result from the treatment of plastic garbage and other waste products. Instead of simply enjoying the convenience brought to our lives, we should think about the future and work to develop new materials and new technologies that are kind to the planet, an endeavor that is also included in the United Nations Sustainable Development Goals. In this issue, we introduce ICReDD research that focuses on safety and low environmental impact.



1. Mechanochemistry

When you imagine a chemical reaction, it is common to think of mixing chemicals together in a liquid and heating the mixture or shining it with a light to cause a reaction. However, in the field of mechanochemistry, solids are hit or smashed together via mechanical force to cause a reaction, hardly using any liquid or any energy from heat or light. Specialized machines called ball mills provide the most effective mixing. A ball, typically made of metal, is placed in a metal jar along with chemical substances. The ball mill rapidly shakes the jar, pulverizing the chemical solids and mixing them together sufficiently to cause a reaction. Alternatively, even a method as simple as hitting chemicals with a hammer can enable a reaction. It may sound like incredibly tough work is being done in these experiments, but as we mentioned in Issue 7 of The Catalyst, methods like this are gaining attention for being safer and more environmentally friendly since they reduce the amount solvent being used and the amount of waste products generated.

2. Radical reactions

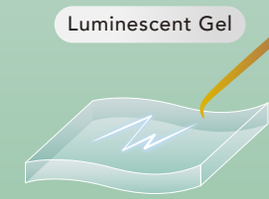


Now we will talk about a type of chemical reaction called a radical reaction. First, chemical bonds occur when two atoms each donate an electron to create an electron pair that is shared between the atoms. When a chemical bond breaks, it can break in two different ways. Either the bond is broken unevenly, and both electrons from the bond stay with one of the fragments, or the bond is broken evenly, with one electron going to each fragment. For the latter case, the result is the formation of two radicals, which are molecules or atoms that have an unpaired electron. Unpaired electrons are usually unstable and seek a bonding partner, thus radicals easily react with other radicals or molecules, and they can often trigger a chain reaction. When radicals react with other molecules, an electron pair is formed at the radical, stabilizing it. However, since the molecule supplied one of its electrons, there is now an unpaired electron on the molecule, turning it into a new radical. This new radical can then bond with another molecule, turning that bonding partner into a radical. This bond formation and transfer of the unpaired electron can repeat many times like falling dominoes, until two radicals react with each other to form a stable electron pair and end the chain reaction.

3. Commonplace radical reactions

All you need is the first domino and the force to knock it over in order to set off the rest of the dominoes to fall. For a radical reaction, that first domino piece is a molecule that easily forms radicals, called an initiator. The force that knocks over that piece is energy from heat, light, or mechanical force. Have you ever heard of the term "ozone depletion"? The ozone layer in the stratosphere keeps the amount of UV rays that reach the earth's surface at a suitable level, protecting the ecosystem. A pollutant called Freon, which was once commonly used as a coolant in refrigerators and a propellant in aerosol cans, forms chlorine radicals when hit by UV light. A single one of these chlorine radicals can destroy 100,000 ozone molecules through a chain reaction, so there are now regulations across the globe to abolish the use of Freon. In a more everyday example, UV light also provides the energy to initiate the radical reaction that hardens gel fingernails. The liquid gel consists of small molecules mixed with an initiator molecule. When exposed to a UV lamp, a radical reaction connects the small molecules together into large polymer molecules, which causes the gel to solidify.

4. Combining radicals and mechanochemistry



Nanoscale damage to the gel causes those areas to emit light via a radical reaction, making damaged areas visible.

ICReDD has developed unique technologies by combining mechanochemistry and radical reactions. In one case, a gel was developed that emits light in places where it was subjected to a strong force such as pulling or pressing. The damage this force induces at the nanoscale can lead to deterioration that cannot be seen with the naked eye, but the light emission from damaged areas could be used to contribute to the development of materials. In a separate project, ICReDD researchers discovered a method which uses a ball mill to initiate radical reactions using common plastic materials as the initiator. They were even able to use shredded up bits of a plastic grocery bag as a radical initiator and promote a reaction that can reduce the toxicity of hazardous chemicals. If we can reuse the plastic bag waste produced from our daily lives to help with the treatment of hazardous chemicals, we could tackle two environmental problems in one fell swoop!

Activation!

Quiz

Radicals are generated by:

- **A** one-to-one electron sharing that creates a bond
- **B** electron pairs splitting evenly when a bond breaks
- **C** a positive ion and a negative ion creating a bond
- **D** electrons pairs splitting unevenly when a bond breaks

Send us your answer!

Check our Instagram highlights for the answer to the quiz!
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ICReDD News

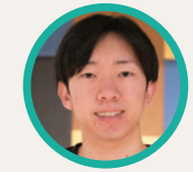
June 2024

New Researchers

Wataru Matsuoka
Computational chemistry, virtual screening

Kalipada Jana
Radical chemistry, asymmetric catalysis

Martin
Machine learning, drug discovery



Koki Tsuchiya
Photoacoustic imaging, organic synthesis

Chenghan Sun
Machine learning, catalysis

Tavinder Singh
Organic Synthesis

Kosaku Tanaka III
Organometallic chemistry, photocatalysis

Keisuke Wada
Host-guest chemistry, supramolecular chemistry

Balasubramaniyan Sakthivel
Computational chemistry, informatics

Selected Publications (from March 2024 to May 2024)

Bridging the Gap: From Frequent Molecular Changes to Observable Phenomena
(Y. Nagahata, M. Kobayashi, S. Maeda, T. Taketsugu, T. Komatsuzaki)
https://www.icredd.hokudai.ac.jp/research/11263

Artificial intelligence-based, on-the-fly Raman spectroscopy method shows promise for rapid medical diagnosis
(K. Tabata, J. E. Clement, T. Komatsuzaki)
https://www.icredd.hokudai.ac.jp/research/10794

Light stimulates a new twist for synthetic chemistry (Y. Harabuchi, S. Maeda)
https://www.icredd.hokudai.ac.jp/research/10644

Outreach

- Visit from National Chung Hsing University led by Prof. Kuan-Jiuh Lin
- Monthly Research Postcard
- The CATALYST Issue 15

Visit from National Chung Hsing University led by Prof. Kuan-Jiuh Lin

Award

- MEXT Minister's The Young Scientists' Award
(Harabuchi, Takahashi)

Monthly Research Postcard

The CATALYST 15th Issue

Researcher Profile

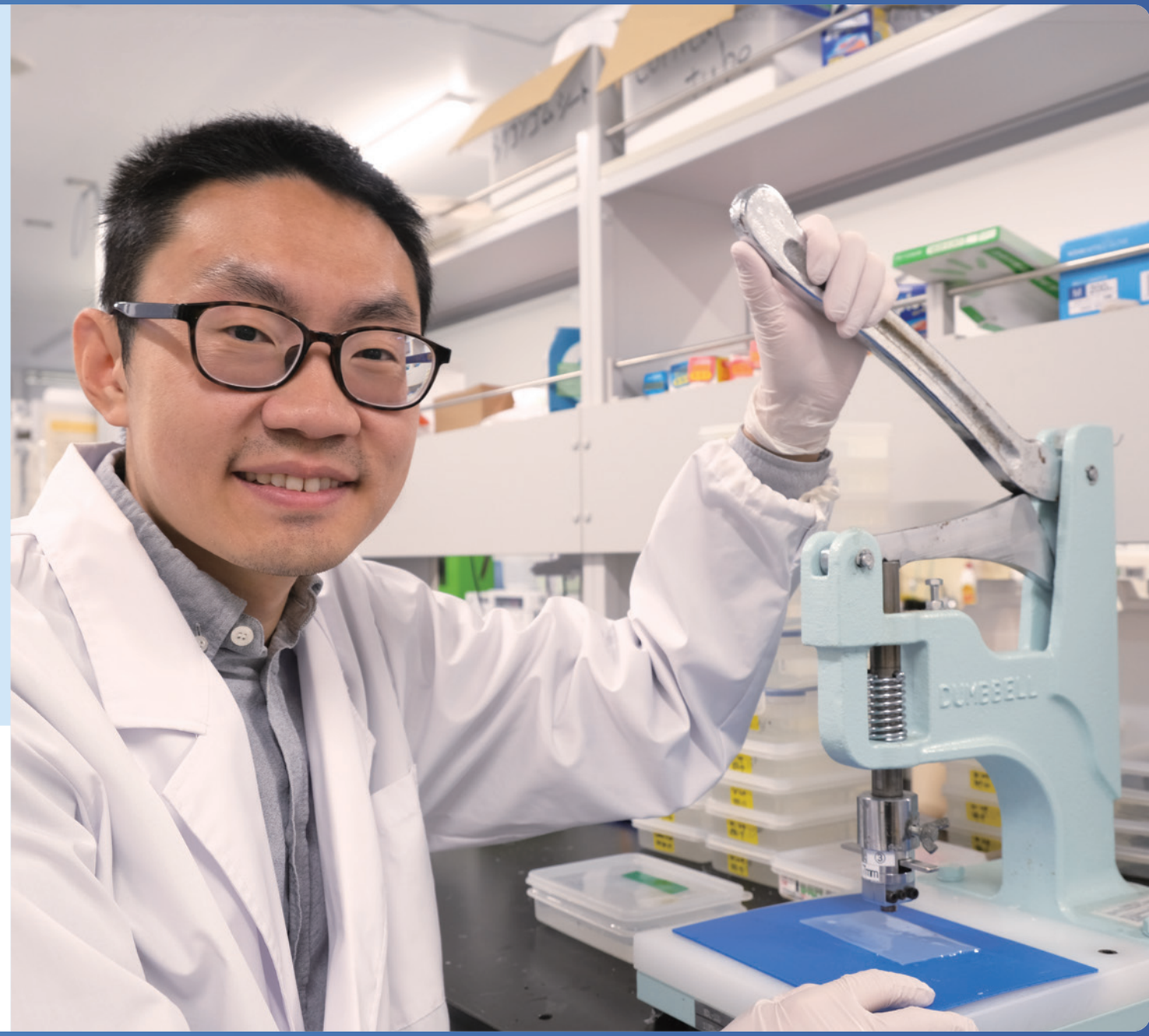
vol.16

Hailong Fan

Specially Appointed Associate Professor Hailong Fan's research focuses on the design and synthesis of functional hydrogels. He works on controlling the arrangement of building block molecules in polymers to achieve underwater adhesion of hydrogels.

Representative Papers:

Nat. Commun. 2019, 10, 5127.
Proc. Natl. Acad. Sci. U.S.A. 2022, 119, e2206685119.
Adv. Mater. 2021, 33, 2102983.



Short Biography

Dr. Fan received his Ph.D from Renmin University of China in 2017. He then joined Prof. Jian Ping Gong's group at Hokkaido University as a postdoctoral research fellow. He was promoted to assistant professor in 2020 and specially appointed associate professor in 2022. He received the Polymer Research Encouragement Award from the Society of Polymer Science Japan (SPSJ) in 2021.

About ICReDD

The development of new chemical reactions is intrinsically entangled with the prosperity of humanity and the preservation of the environment. A recent example of such transformative chemical reactions with profound impact is cross-coupling reactions, the discovery of which was awarded with the 2010 Nobel Prize in Chemistry. These reactions are used to produce approximately 20% of all medicinal reagents, and almost all liquid crystalline and organic electroluminescent materials. The industrial use of these chemical reactions contributes ~60 trillion yen per annum to the global economy. The development of new chemical reactions thus significantly affects the evolution of society.

ICReDD is the Institute for Chemical Reaction Design and Discovery, a WPI center at Hokkaido University where researchers from different disciplines combine their strengths to take full control over chemical reactions. The institute was born out of the realization that the purposeful design of chemical reactions requires cross-sectional collaborations at every step. Working on such a fundamental natural process, quantum-chemical computations, information technology, modern experimental techniques, and the development of advanced materials can no longer be separate fields if we want to achieve significant breakthroughs. Rather, they have to become part of a diverse toolbox for truly integrated research.

The Catalyst is inspired by catalysts used in chemistry to bring molecules together, to reduce reaction barriers, and to activate molecules—to make reactions happen faster. In this spirit, this poster series should enable its readers to make the connection between chemical reactions and the wellbeing of our society, and to look at the world in a new way, seeing how chemical reactions and chemistry shape the world around them. And if we can take this opportunity to introduce ourselves, too, this may also catalyze new friendships and opportunities. #ReactWithUs

React With Us!

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with what's happening at ICReDD,
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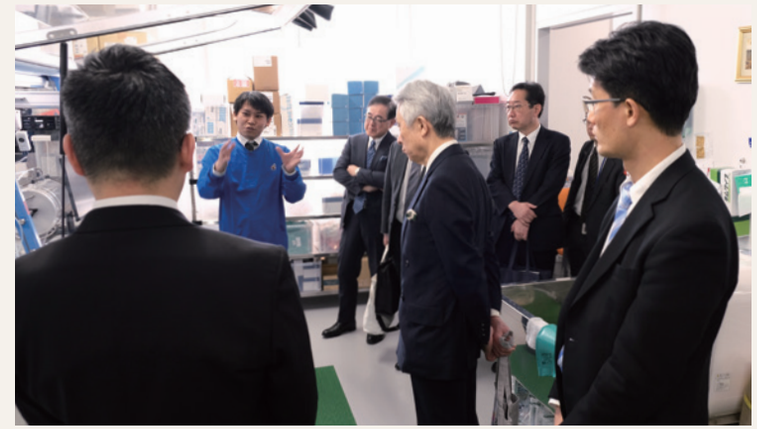

(Top) On April 6th, Minister Masahito Moriyama from the Ministry of Education, Culture, Sports, Science and Technology visited ICReDD. He was welcomed by Hokkaido University President Kiyohiro Houkin, and representatives of ICReDD including Director Satoshi Maeda and Administrative Director Koichiro Ishimori, and they held a discussion. (Bottom) During the subsequent tour of the facilities, Specially Appointed Assistant Professor Seiji Akiyama demonstrated the process of using an automated synthesis robot for chemical synthesis in ICReDD's Smart Lab.

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