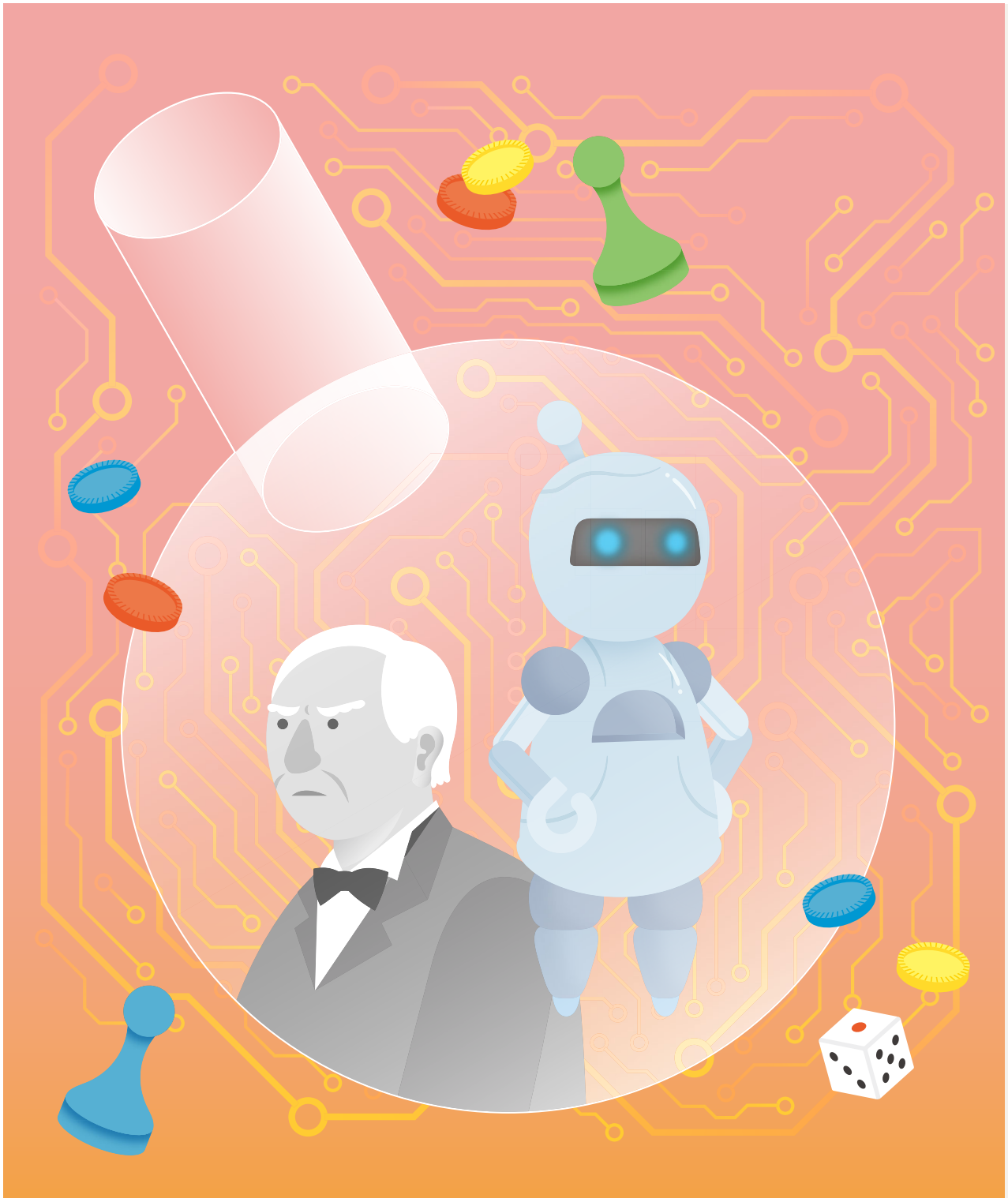


The CATALYST

Helping you react with chemical reactions

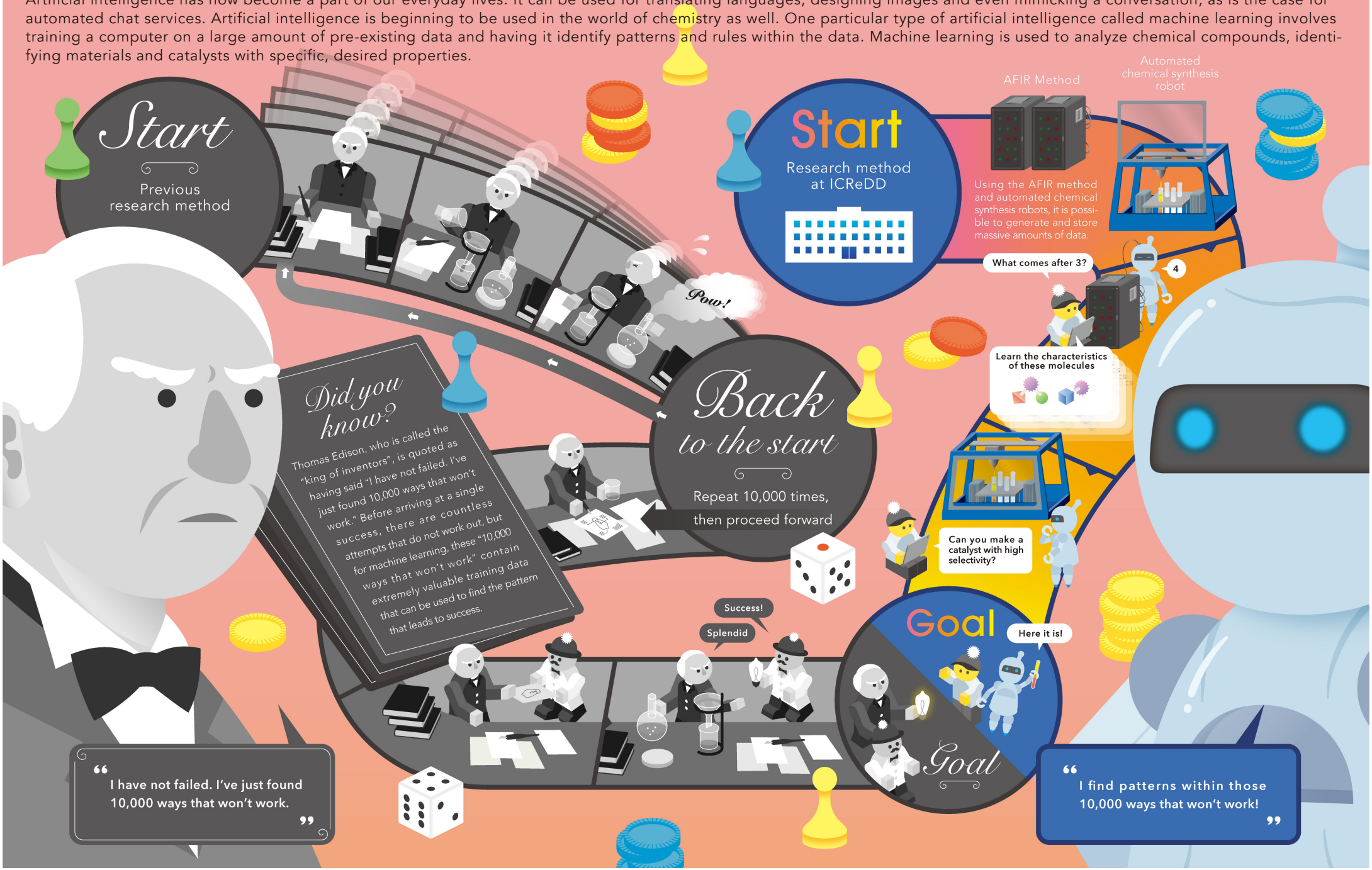
Issue 13
September 2023

Machine Learning for Chemical Reaction Design

ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY

Machine Learning for Chemical Reaction Design

Artificial intelligence has now become a part of our everyday lives. It can be used for translating languages, designing images and even mimicking a conversation, as is the case for automated chat services. Artificial intelligence is beginning to be used in the world of chemistry as well. One particular type of artificial intelligence called machine learning involves training a computer on a large amount of pre-existing data and having it identify patterns and rules within the data. Machine learning is used to analyze chemical compounds, identifying materials and catalysts with specific, desired properties.

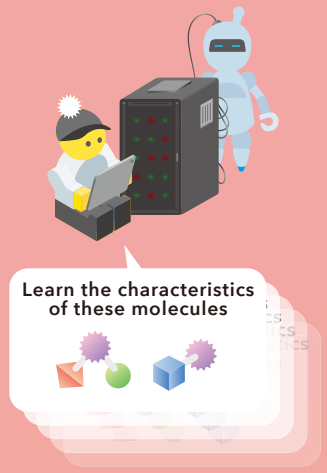


1. Recognizing Patterns

If you saw a list of numbers that read "1, 2, 3, 4…" and you were asked what is the next number in the list, what would be your guess? The natural answer would be "5". Human brains recognize a variety of patterns and learn how to predict future outcomes based on these patterns. As we gain more experience and encounter new situations, our expectations of the world around us change. For example, if a close friend has been consistently punctual in the past, but they suddenly start to be late, our brain will adjust our prediction from "they will be on time" to "they might be 5 minutes late". The more experience, or in other words, the more data we have regarding something, the better we can predict the outcome. However, there is a limit to the amount of data that the human brain can process, and this is where machines can be a huge help.

2. Training a Machine

While computers don't learn in the same way the human brain does, they can be taught to mimic learning. One common method for this is called supervised machine learning. For this, the computer is first given an adjustable equation for modelling outcomes based on given input information. The model is then "trained" on pre-existing sets of input and outcome data, where it is known which outcome corresponds to which input. During this training process, the computer makes small adjustments to its model so that its predictions more accurately fit the training data. This trained model is then tested on another set of pre-existing data to compare the model's predicted outcomes with the actual outcomes. Once an accurate model is obtained, it can be used to evaluate new data for which the outcome is unknown.

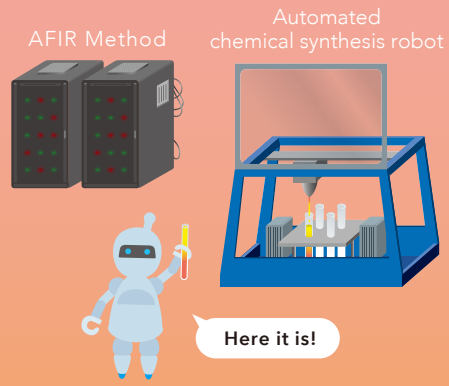


3. Machine Learning in Chemistry

Machine learning's ability to evaluate unknown data is beginning to be used in the field of chemistry for identifying molecules or materials with specific, desired properties. In this case, molecular structures are provided as the input data and the value of the target property is the outcome. As the model is trained on molecular structures and the corresponding experimentally measured target property values, it can identify patterns in the relationship between molecular structure and the target property. Once an accurate model is obtained, molecular structures that have promising values for the target property can be quickly identified. However, a large amount of training data is needed to obtain such an accurate model, and generating that much data through doing laborious experiments in the lab by hand is not realistic. The application of machine learning to chemistry has been limited due to the insufficient amount of data for training.

4. Towards Automated Discovery

At ICReDD we are working to address this lack of data in two ways. Firstly, researchers at ICReDD are utilizing an automated chemical synthesis robot to speed up the collection of experimental data to use for training machine learning models. This efficient data collection approach was used by researchers to make a model for identifying novel catalysts with high selectivity, which is an important property for designing new medicines and other functional molecules. Secondly, ICReDD is exploring ways of using machine learning to find patterns in the huge amounts of reaction path simulation data computed by ICReDD's AFIR method. By using machine learning to efficiently find patterns in both experimental and simulation data, ICReDD aims to further accelerate the design and discovery of new chemical reactions.



Activation!

Quiz

The process by which a machine learning model examines input and output data to improve the accuracy of its predictions is called _____.

Send us your answer!

- A memorizing
- B training
- C practicing
- D applying

Check our Instagram highlights for the answer to the quiz! #ReactWithUs

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ICReDD News

September 2023

New Researchers

Shun Zhou
Organocatalysis, asymmetric catalysis

Masashi Fujiwara
Equipment and data management

Akari Mukaimine
Chemical biology, photochemistry

Márton Nagyházi
Organic and organometallic chemistry, catalysis

Selected Publications (from June 2023 to August 2023)

Computationally guided catalyst design for low-temperature methane combustion
(MANABIYA program participant: S. Yasumura)
https://www.icredd.hokudai.ac.jp/research/9620

Reaching new heights: ultrasound-based microfluidic platform enables droplet control with high jumping ability
(Y. Nagata)
https://www.icredd.hokudai.ac.jp/research/9604

Virtual exploration of chemical reactions
(Y. Harabuchi, S. Maeda, K. Takahashi)
https://www.icredd.hokudai.ac.jp/research/9540

Identifying high-grade serous ovarian carcinoma-specific extracellular vesicles by polyketone-coated nanowires
(Y. Inokuma)
https://www.icredd.hokudai.ac.jp/research/9530

A blueprint for transforming indigos to photoresponsive molecular tools
(C.Y. Huang)
https://doi.org/10.1002/chem.202300981

Outreach

- Joint Open Campus (Interactive Activities and Public Lectures)
- Chemical Society of Japan hands-on lab experience
- Open Campus lab tour
- Science Eye lab tour
- Visit by Tosajuku Junior and Senior High School students
- Visit by European Union Ambassador to Japan
- Monthly Research Postcard
- The CATALYST Issue 12

Joint Open Campus

Science Eye lab tour

Monthly Research Postcard

The CATALYST 12th Issue

Special Event

- New ICReDD Building Opening Ceremony

Researcher Profile

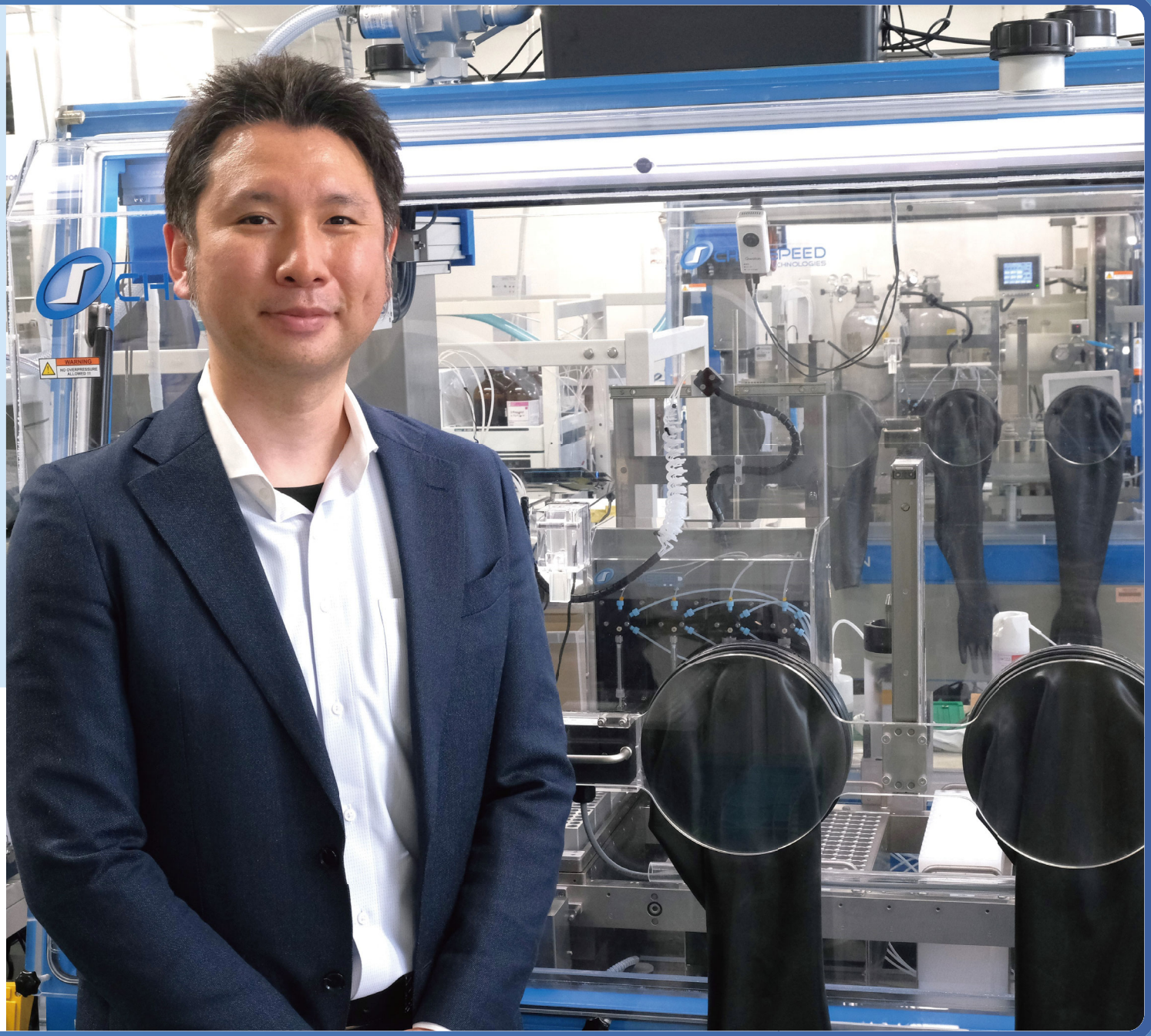
vol.13

Yuuya Nagata

Specially Appointed Associate Professor Nagata uses automated synthesis robots to develop new reactions and new materials. In particular, he pioneers new synthesis methods that combine automated synthesis technology with theoretical chemistry and information science.

Representative Papers:

Commun. Chem. 2022, 5, 158;
Angew. Chem. Int. Ed. 2023, 62, e20221865;
Org. Biomol. Chem. 2023, 21, 3132



Short Biography

Specially Appointed Associate Professor. In 2008, Professor Nagata received his PhD from the Department of Polymer Chemistry at Kyoto University. From April 2008, he was a postdoctoral researcher in the same department before becoming an Assistant Professor in the Department of Synthetic Chemistry and Biological Chemistry in May 2008. He continued there until December 2019, when he started his current position.

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!

To stay up to date
with what's happening at ICReDD,
follow us on our social media channels:

@ICReDDconnect

ICReDD participated in a number of outreach events for students this summer. (Top) Professor Yasuchika Hasegawa from ICReDD dressed up as a Gryffindor as he explained the magic of chemistry and luminescence. (Bottom) High school students participating in The Chemistry Society of Japan's 2-day hands-on lab experience made and tested hydrogel materials under the guidance of Associate Professor Tasuku Nakajima.

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