The CATALYST

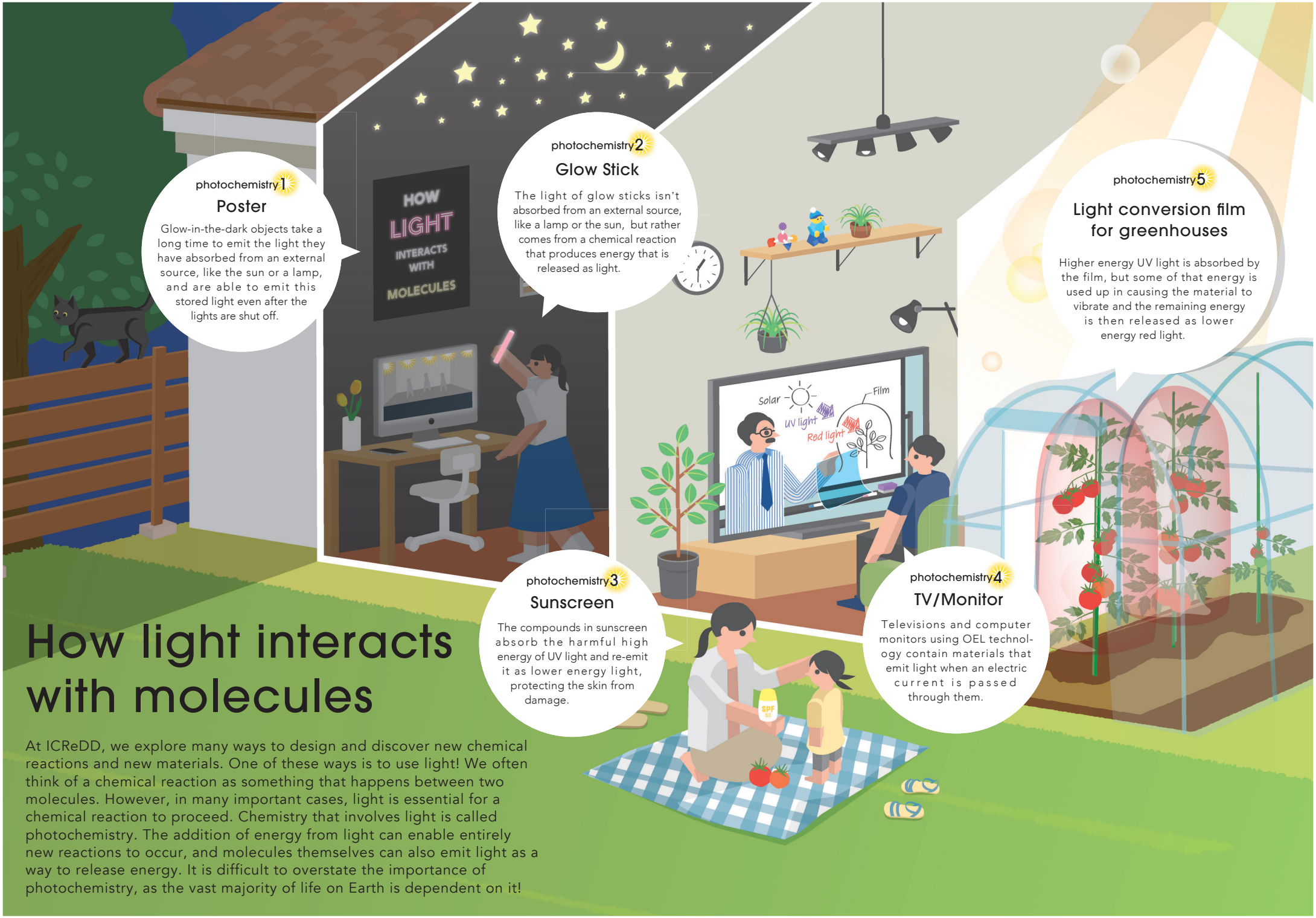
Helping you react with chemical reactions

Issue 8

June 2022

How light interacts with molecules

ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY



How light interacts with molecules

At ICReDD, we explore many ways to design and discover new chemical reactions and new materials. One of these ways is to use light! We often think of a chemical reaction as something that happens between two molecules. However, in many important cases, light is essential for a chemical reaction to proceed. Chemistry that involves light is called photochemistry. The addition of energy from light can enable entirely new reactions to occur, and molecules themselves can also emit light as a way to release energy. It is difficult to overstate the importance of photochemistry, as the vast majority of life on Earth is dependent on it!

1. The foundation of life

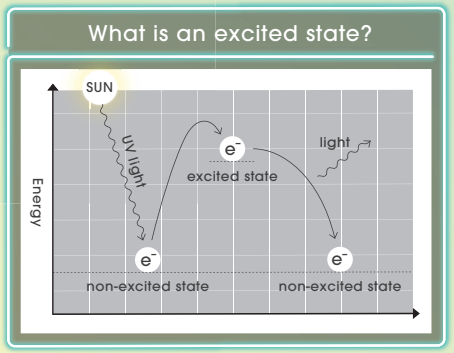
Here on Earth we are lucky to be surrounded by beautiful greenery, with many kinds of grains and vegetables to keep us nourished. However, these things would not exist without photochemistry! We mentioned photosynthesis in Issues 2 and 5 of the CATALYST, and photosynthesis is a photochemical process plants use to convert light energy from the sun into chemical energy they can use to grow. Photochemistry is also important in our bodies. It enables us to see with our eyes and is essential for our bodies to make Vitamin D, which helps keep our bones and teeth healthy. In addition to biological processes, photochemistry is at the heart of many modern technologies, including our computers and smartphones!

2. Power-packed light

To understand photochemistry, it is important to realize that light carries energy which can be transferred to molecules. Some light we can see, like red, green or blue light, and some we can't see, like infrared or ultraviolet light. These different kinds of light carry a different amount of energy depending on their wavelength and thus interact with molecules differently. Lower energy light, like infrared, only has enough energy to cause the molecules to vibrate more, raising their temperature. Small space heaters often work by this method. They emit infrared light that is absorbed by molecules in the surrounding air, warming up the room. Higher energy light, like visible light and ultraviolet light have enough energy to cause chemical reactions to happen. Sometimes the reaction can be helpful, like in photosynthesis, and sometimes it can be harmful, like when we get a sunburn from UV light.

3. Light interacting with molecules

For light to cause a chemical reaction, it must first be absorbed by a molecule. Some molecules are better at absorbing certain types of light more efficiently than others, so combining the right molecule with the right type of light is important. When a molecule absorbs light with enough energy, that light energy quickly bumps up an electron to a higher energy "excited" state that can't be reached by simply heating up the molecule. Molecules in such an excited state have different properties and can undergo different reactions compared to when they are not excited. The reverse process, in which an electron drops back down to its non-excited state, is also of interest because it can produce light. This ability to produce light can be used in many technologies, including computer and smartphone screens.



4. Developing new technology with photochemistry

At ICReDD we are utilizing photochemistry not only to discover new reactions, but also to create new materials useful to society. Our researchers have developed molecules that only emit a very specific type of light when exposed to UV rays. This property makes these molecules useful as security inks. The ink can be shined with UV light, and the specific light emission can be checked to verify important documents, like a passport. On a different project, researchers from ICReDD working with agricultural researchers at Hokkaido University have developed a thin film for use in greenhouses which promotes plant growth. Molecules in the film can convert ultraviolet light from the sun into red light, which plants can use in photosynthesis. This additional energy source especially has an effect on plants grown in winter. ICReDD is also working on predicting how molecules respond to light using computational methods, which could potentially help accelerate experimental scientists' search in for more interesting photochemical reactions and materials. Understanding and controlling how molecules absorb and emit light will lead to the discovery of new reactions and technologies.

Activation!

Quiz

A molecule can change to an excited state when it _____ light.

Send us your answer!

- **A** reflects
- **B** emits
- **C** transmits
- **D** absorbs

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

June 2022

New Researchers

Ryota Isshiki
Organometallic Chemistry and Mechanochemistry

Seiji Akiyama
Quantum chemistry and main group chemistry

Yusuke Kinoshita
Coordination Chemistry and Porphyrin Synthesis

Tomoko Akama
Quantum Chemistry and Electron Dynamics

Yoshihiro Matsumura
Physical Chemistry and Reinforcement Learning

Pan Gao
Mechanochemical Synthesis of Organic Molecules

Saeesh Mangaonkar
Synthesis of Heterocyclic Compounds

Nhan Van Thanh Do
Organocatalysis

Amit Jaiswal
Photocatalysis and Data Science

Sitanan Sartyoungkul
Organic synthesis of curved molecules

Selected Publications

(from March 2022 to May 2022)

Alkali Metal Ion Binding Using Cyclic Polyketones
(K.I. Shivakumar, T. Yoneda, Y. Ide, J. Pirillo, Y. Hijikata, Y. Inokuma)
DOI: 10.1039/d2cc00361a

Virtual Ligand-Assisted Screening Strategy to Discover Enabling Ligands for Transition Metal Catalysis
(Y. Harabuchi, S. Maeda)
DOI: 10.1021/acscatal.2c00267

Quantum Chemical Calculations to Trace Back Reaction Path for the Prediction of Reactants
(Y. Harabuchi, Y. Nagata, S. Maeda)
DOI: 10.1021/jacsau.2c00157

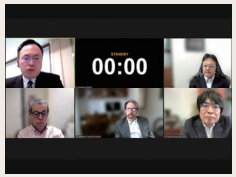
Virological Characteristics of the SARS-CoV-2 Omicron BA.2 Spike
(M. Tsuda, L. Wang, S. Tanaka)
DOI: 10.1016/j.cell.2022.04.035

Synthesis of a Möbius Carbon Nanobelt
(J. Pirillo, Y. Hijikata)
DOI: 10.1038/s44160-022-00075-8

Symposia

(invited and more)

- ICReDD 4th International Symposium
- Inaugural Akira Suzuki Awards Ceremony



ICReDD
4th International Symposium

Inaugural Akira Suzuki Awards Ceremony

Outreach

- Monthly News Postcard
- The CATALYST 7th Issue

Monthly News Postcard

The CATALYST
7th issue

Researcher Profile

vol.8

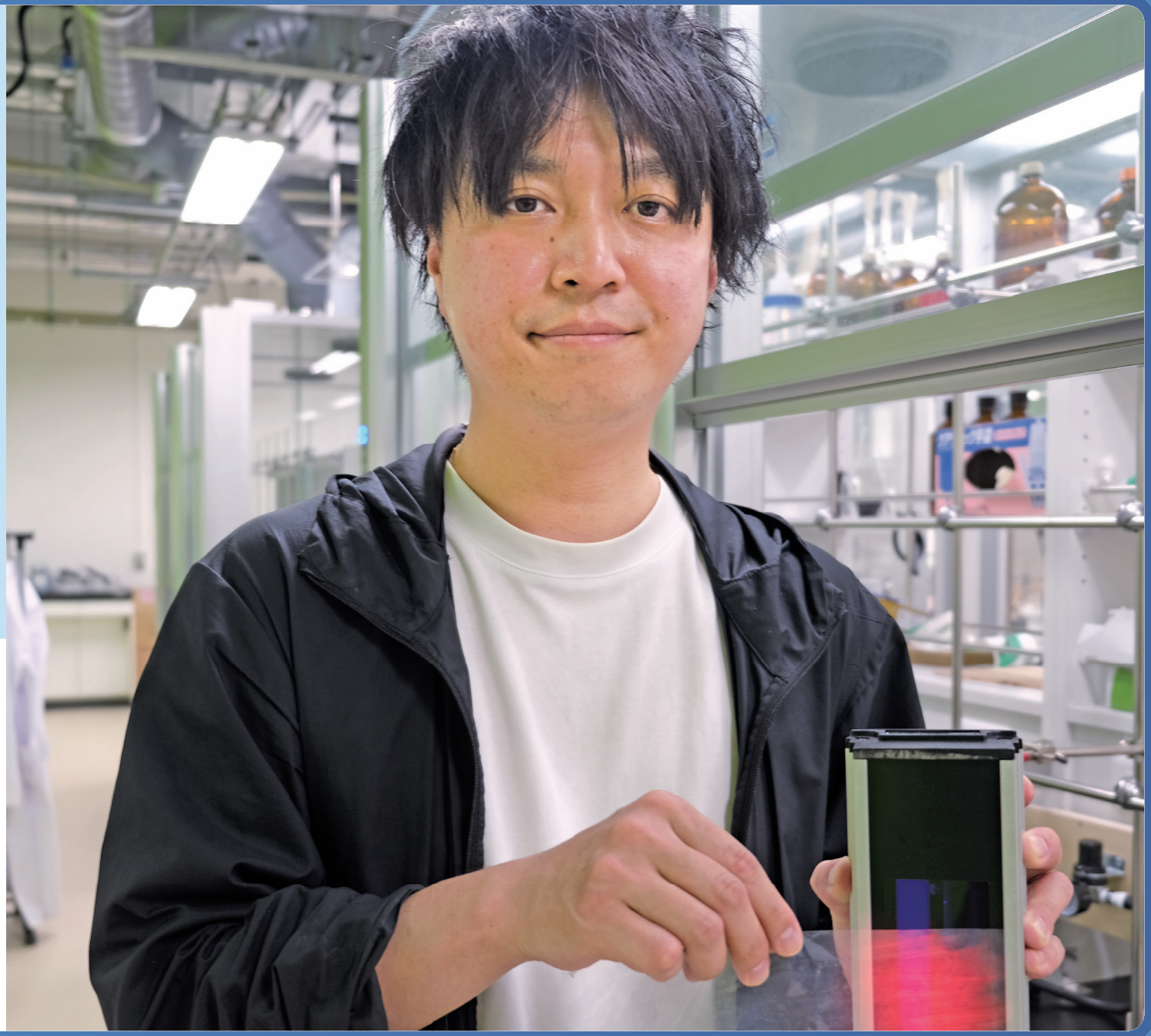
Sunao Shoji

Assistant Professor Shoji researches the structure and optical function of supramolecules that consist of multiple organic molecules. He freely creates nanotubes and nano sheets comprised of organic pigments. Recently, Professor Shoji has also been researching plant cultivation utilizing luminescent materials.

Representative Papers:
Chem. Lett. 2022, 51, 185–196; Sci. Rep. 2019, 9, 14006; Nano Lett., 2016, 16, 3650–3654.

Short Biography

Assistant Professor at ICReDD and Hokkaido University (HU) Graduate School Faculty of Engineering. Professor Shoji received his PhD from Ritsumeikan University in 2014, graduating six months early. He continued there from 2014 under the JSPS Research Fellowship for Young Scientists and then from 2016 was a postdoctoral researcher at the Ritsumeikan University Research Organization of Science and Technology. In 2019, he joined the HU Graduate School Faculty of Engineering as a postdoctoral researcher before starting his current position in January 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!

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

@ICReDDconnect

The Inaugural Akira Suzuki Awards ceremony was held on March 12th, 2022. The purpose of the awards is to recognize outstanding contributions to research in the discovery of chemical reactions, defined in the broadest sense, and to contribute to the advancement of science and technology. The awards are given to researchers who have achieved remarkable results, regardless of age or nationality. We look forward to their continued contributions to the development of new fields and new chemical reactions.

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