The CATALYST

Helping you react with chemical reactions

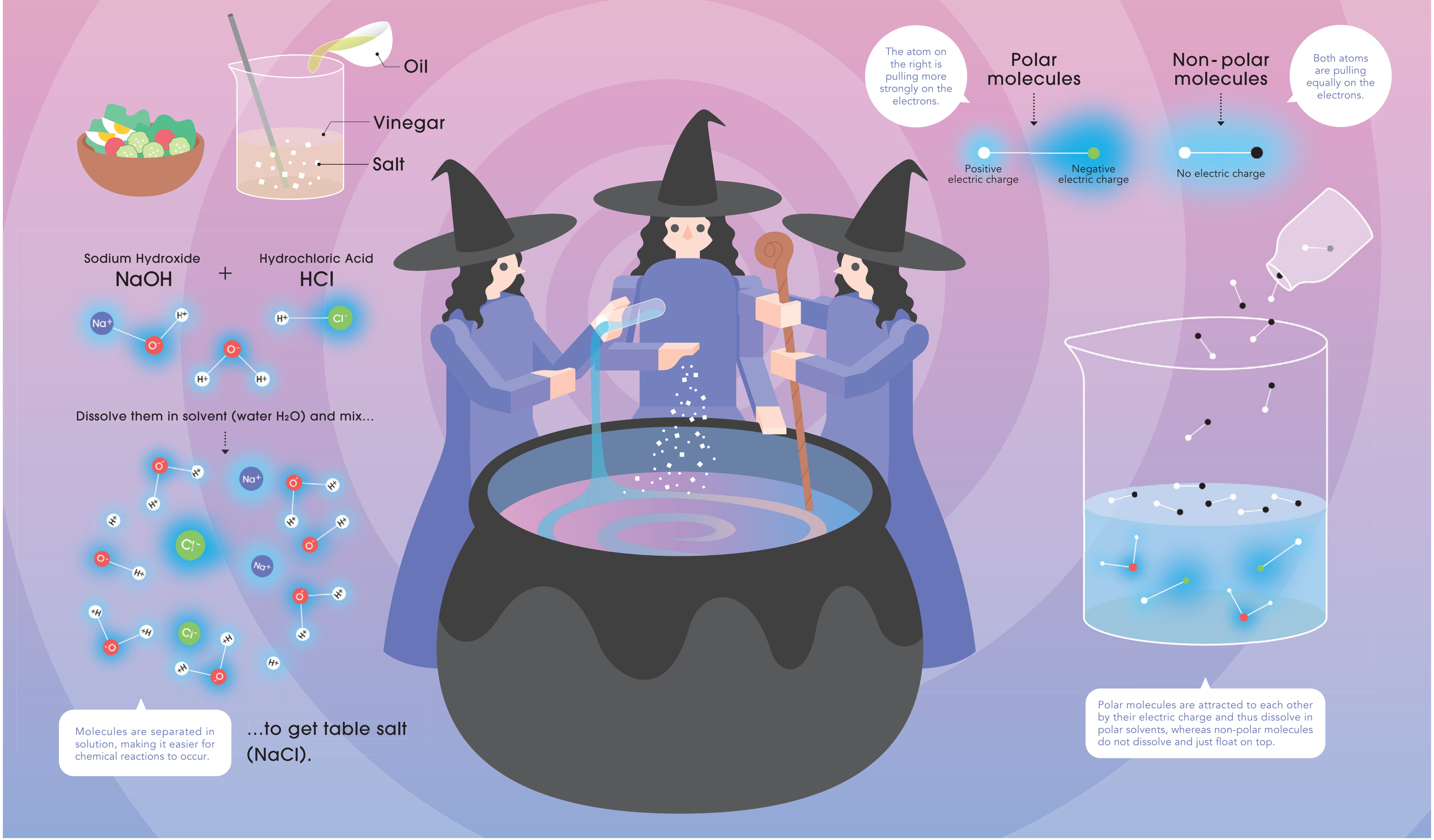
Issue 7
March 2022

How mixing affects chemical reactions

ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY

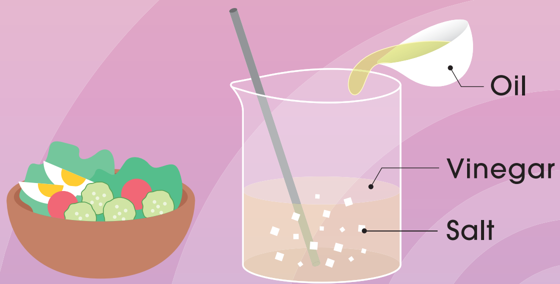
How mixing affects chemical reactions

Solutions are an essential concept for our daily lives. If you've ever had a carbonated beverage or done any cooking or baking, then you've had first-hand experience with a solution! Most chemical reactions in the lab and in nature take place in a solution, and thus rely on solubility, a measure of how well a substance dissolves into a given liquid. Solubility affects what substances can and cannot be mixed together in solution, which can sometimes prevent scientists from trying reactions with certain combinations of chemicals. Researchers at ICReDD are developing new methods to overcome the limitations that solubility can impose!



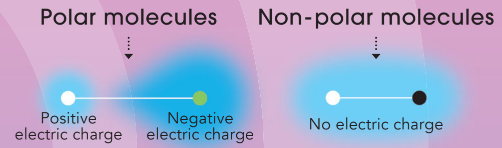
1. Solutions around us

It's not hard to find examples of solubility around us. In the kitchen, when we mix different ingredients together to make sauces, solubility plays an important role. However, some ingredients do not like to mix because they have low solubility with each other. For instance, when making salad dressing, if you mix the ingredients in the wrong order, they won't dissolve. If you add salt directly to the oil, the salt won't dissolve no matter how much you stir. The correct order is to first dissolve the salt into the vinegar, and then add the oil. This is because the solubility of salt in vinegar is different from in oil.



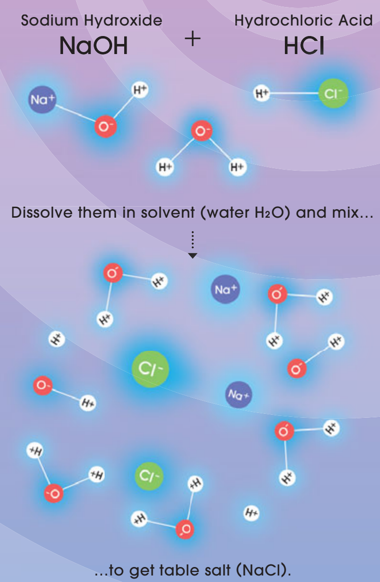
2. Solutions at the molecular level

In molecules, atoms share electrons in bonds, but not all bonds are the same. How electrons are shared between atoms in a molecule determines how well a molecule dissolves in different substances. Each atom involved in a bond pulls on the electrons they share, kind of like a game of tug of war. Sometimes the two atoms pull with similar strength, and they share electrons nearly equally. This is called a non-polar bond, and there isn' t much of an electrical charge on either atom. Other times, in what is called a polar bond, one of the atoms pulls more strongly than the other and keeps the electrons closer to themselves. Here, the "stronger" atom has a more negative electric charge, and the "weaker" atom has a more positive electric charge. Positive and negative charges are attracted to each other, so the positive and negative charges in a polar bond will be attracted to the charges in other molecules that have polar bonds. In contrast, they aren' t attracted to non-polar molecules that don' t have any positive or negative charges. Thus, polar molecules dissolve well into solvents made of polar molecules and non-polar molecules dissolve well into solvents made of non-polar molecules, but both don' t dissolve well into solvents made of the opposite type of molecule.



3. Solubility in chemical reactions

Dissolving molecules into a solvent is important because it gives molecules more opportunities to interact with other molecules, which increases the efficiency of the reaction. Dissolved molecules can move individually rather than being clumped together when they are in solid form. Additionally, compared to molecules in gas form which are very spread out, dissolved molecules are more densely packed and have a greater chance to interact. Due to this advantage of increased interaction, most chemical reactions in the lab, and even in nature, are performed in solution. However, when developing a new reaction, sometimes there isn't a solvent that will dissolve both of the molecules the scientist wants to react. This can occur when trying to react a polar molecule with a non-polar molecule, and it puts a limit on the chemical reactions we can discover.



4. Breaking the limitations of solubility

Here at ICReDD, we are carrying out chemical reactions in new ways that overcome the restrictions of solubility. ICReDD researchers have developed methods for using a machine called a ball mill to provide mechanical force to mix two chemicals well enough that they will react with each other while in the solid state. This can greatly reduce or eliminate the need for dissolving molecules into a solvent. If we can perform reactions without the need for solvents, it opens up a world of new chemical reactions that were not possible due to solubility problems! Such solid-state methods also reduce solvent usage and potentially hazardous solvent waste, resulting in more environmentally friendly reactions!

For more details

Tackling Solubility Issues in Organic Synthesis: Solid-State Cross-Coupling of Insoluble Aryl Halides

Activation!

Quiz

Molecules in which electrons are shared evenly between individual atoms are called ________ molecules.

Send us your answer!

- **A** Solute
- **B** Polar
- **C** Solvent
- **D** Non-polar

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

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ICReDD News

March 2022

Introducing ICReDD's Junior PIs

Mingoo Jin

Molecular rotors in solid state with photo-functions

Pavel Sidorov

Artificial neural networks and quantitative structure-property relationship modeling

Dennis Chung-Yang Huang

Transition metal catalysts and photo-responsive materials

Selected Publications

(from Decenmber 2021 to February 2022)

- Electrochemical Dearomative Dicarboxylation of Heterocycles with Highly Negative Reduction Potentials. Journal of the American Chemical Society.
  (Y.You, H.Takano, H. Hayashi, S. Maeda, T. Mita)
  DOI: 10.1021/jacs.1c13032
- Attenuated fusogenicity and pathogenicity of SARS-CoV-2 Omicron variant
  (W. Lei, M.Tsuda, S. Tanaka)
  DOI: 10.1038/s41586-022-04462-1
- Photoinduced Copper-Catalyzed Asymmetric Acylation of Allylic Phosphates with Acylsilanes
  (Y. Masuda, J. Hasegawa, M. Sawamura)
  DOI: 10.1021/jacs.1c11526
- Facile preparation of cellulose hydrogel with Achilles tendon-like super strength through aligning hierarchical fibrous structure
  (T. Nakajima, K. Cui, J.P. Gong)
  DOI: 10.1016/j.cej.2021.132040
- Anthraquinodimethane Ring-Flip in Sterically Congested Alkenes: Isolation of Isomer and Elucidation of Intermediate through Experi-mental and Theoretical Approach
  (Y. Harabuchi, S. Maeda)
  DOI: 10.1246/bcsj.20210355

Symposia

(invited and more)

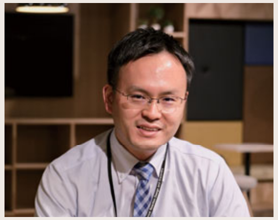
- 24th Chem-Station Virtual Symposium (N. Tsuji)

24th Chem-Station Virtual Symposium

Awards

- 74th Chemical Society of Japan Award (J.P. Gong)
- 39th Academic Award of the Chemical Society of Japan (S. Maeda)
- Inaugural Nagakura Saburo Award for 2021 (S. Maeda)

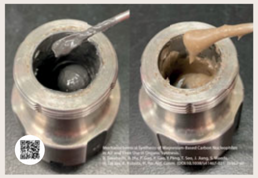
J.P. Gong



S. Maeda

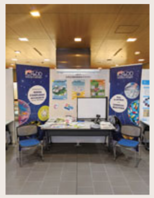
Outreach

- Monthly News Postcard
- The CATALYST 6th Issue
- Booth at 10th WPI Science Symposium
- NHK Science Zero TV Program Appearance (N. Tsuji)



Monthly News Postcards

The CATALYST 6th issue



Booth at 10th WPI Science Symposium

Researcher Profile

vol.7

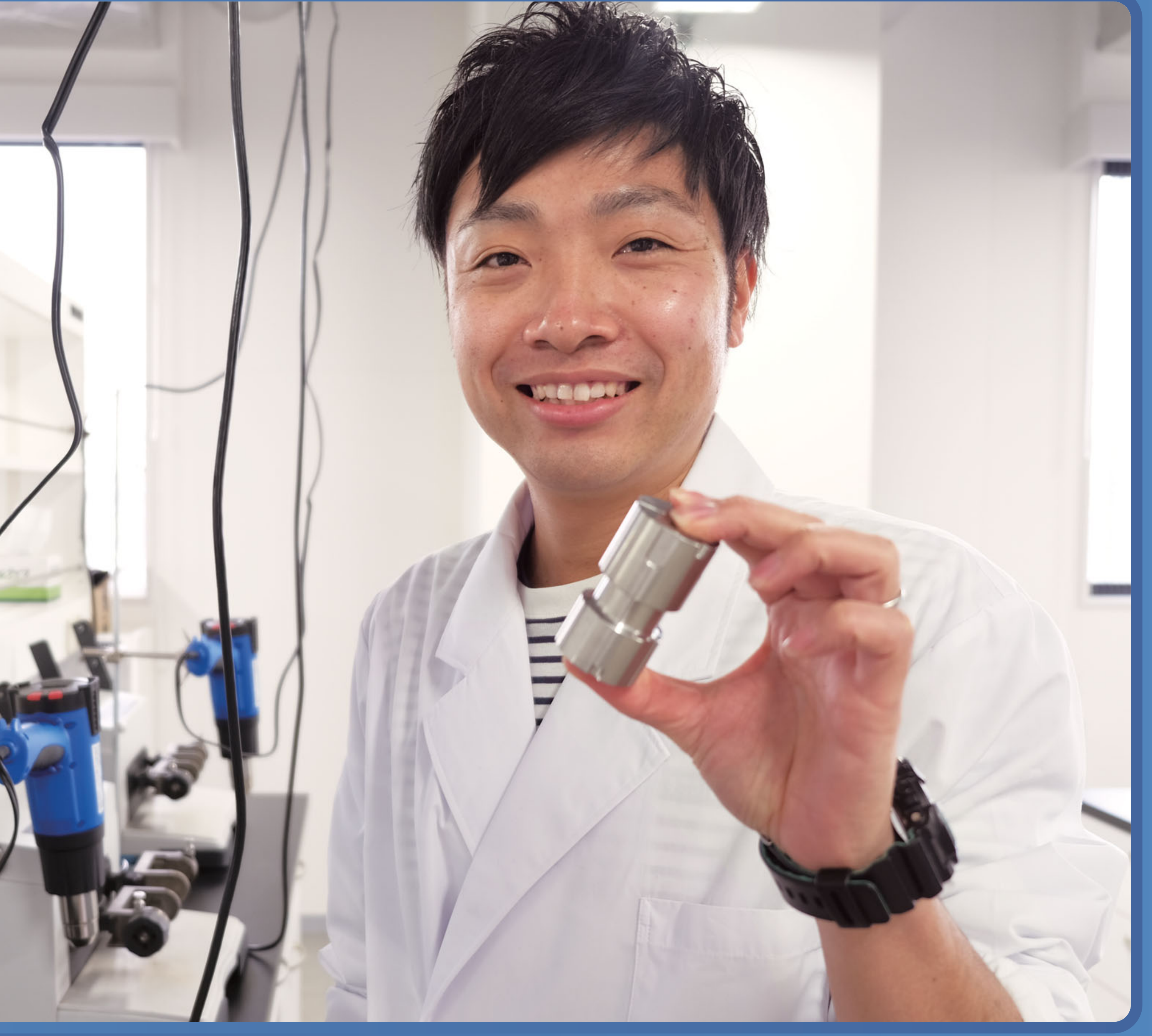
Koji Kubota

Associate Professor Kubota develops mechanochemical reactions using a ball mill machine. His research focuses on solid-state reactions and organic transformations driven by mechanical force.

Representative Papers:
Nature Commun. 2021, 12, 6691; J. Am. Chem. Soc. 2020, 142, 9884-9889; Science 2019, 366, 1500-1504.

Short Biography

Associate Professor at ICReDD and the Hokkaido University Faculty of Engineering. Professor Kubota received his PhD from the Hokkaido University Graduate School of Chemical Sciences and Engineering in 2016. He was then a postdoctoral researcher at the University of California Berkeley (2016) and the Massachusetts Institute of Technology (2017). In 2018, he joined the Hokkaido University Faculty of Engineering as a Specially Appointed Assistant Professor and started his current position in April 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.

ICReDD is excited to be expanding into a dedicated new building in the north campus of Hokkaido University! The groundwork started this winter and the building will be completed in 2023! Can't wait to see all the new chemical reactions that will be discovered there!

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:

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