The CATALYST

Helping you react with chemical reactions

Issue 1

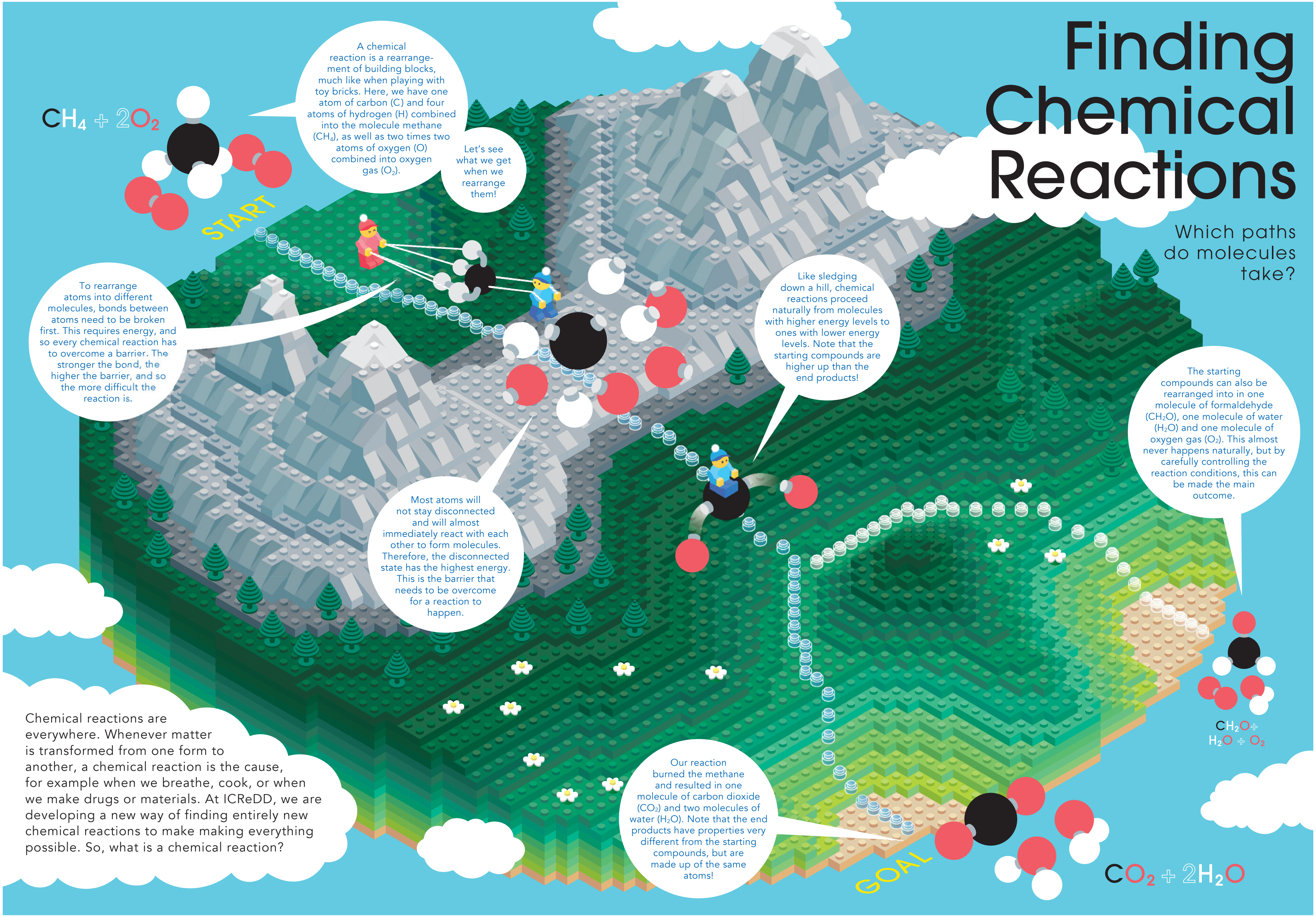
August 2020

Finding Chemical Reactions

ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY

Finding Chemical Reactions

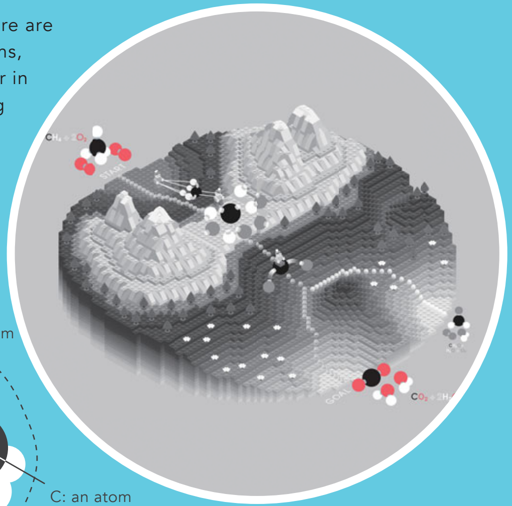
Which paths do molecules take?

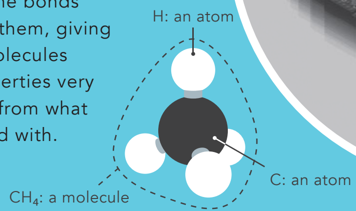


Chemical reactions are everywhere. Whenever matter is transformed from one form to another, a chemical reaction is the cause, for example when we breathe, cook, or when we make drugs or materials. At ICReDD, we are developing a new way of finding entirely new chemical reactions to make making everything possible. So, what is a chemical reaction?

Level 1 Rearrangements

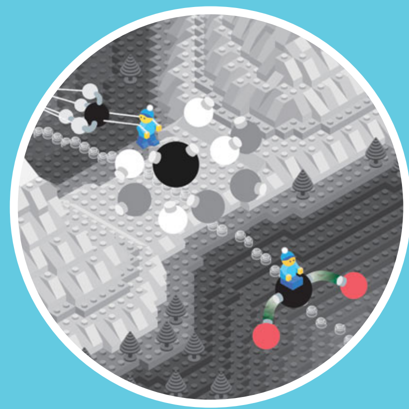
All things are made of atoms. There are a limited number of different atoms, but they can bond with each other in infinitely many ways. The resulting structures, called molecules, have properties that depend on the arrangement of the atoms they are made of. A chemical reaction is a rearrangement of atoms through forming or braking the bonds between them, giving rise to molecules with properties very different from what we started with.





Level 2 Activation Energy

To explain why some chemical reactions happen almost spontaneously while others don't, we assign a property to each molecule that we call "chemical energy". A chemical reaction proceeds naturally if it transforms a molecule of higher energy to one of lower energy, whereas energy has to be put into a reaction to proceed from molecules of lower to higher energy. But before they can happen, all chemical reactions first need a little extra energy, because the chemical bonds need to be broken before they can be rearranged. The crucial point of all chemical engineering is how to transfer the right amount of energy to the right place in a molecule so that specific bonds can be broken and formed.

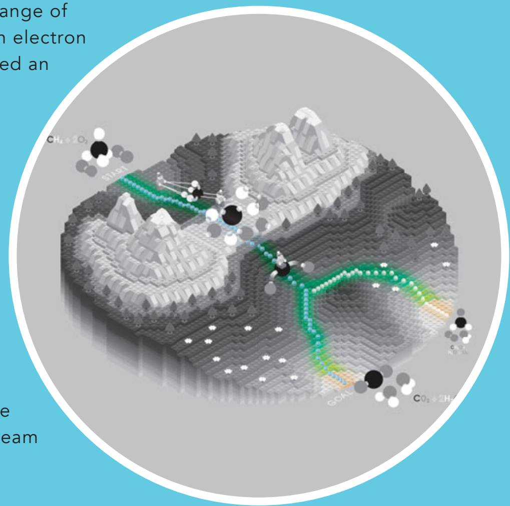


Level 3 Breaking Bonds

The right placement of the right amount of energy is so crucial because the bonds between atoms are maintained by electrons that are held in place by a balance of attraction to the atoms' nuclei and repulsion by other electrons. If atoms need to be rearranged, the repulsion between specific electrons needs to be overcome. Only then can chemical reactions be realized purposefully.

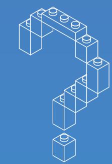
Level 4 Potential Energy Surface

Every little change of the state of an electron can be assigned an energy. Therefore, all rearrangements of electrons are chemical reactions. And if we can calculate all energy levels of all electronic rearrangements, it should be possible to know exactly how much energy is needed where to make every chemical reaction possible—and to produce everything. This is the dream of ICReDD.



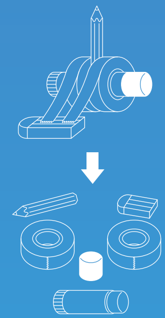
Activation

Quiz



What is the oldest chemical reaction used by humans? Send us your answer.

Challenge



Arrange the things on your desk to make something. Try to combine the same objects into two or three different things. What did you make?

Share your answer on social media!

#ReactWithUs
@ICReDDconnect

NEWS

New Researchers

IDE Yuki

Rapid evaluation of molecular interactions using image diagnosis

TAKANO Hideaki

Development of new reactions by AFIR

TANIKAWA Satoshi

Development of biomaterials for neural regeneration

PANG Yadong

Development of new reactions using mechano-chemistry

HASEGAWA Jun-ya

Catalysis Theory and Catalysis Principle (ICReDD research collaborator)

Selected Publications

(out of 14 papers from April to June)

Discovery of a Synthesis Method for a Difluoroglycine Derivative Based on a Path Generated by Quantum Chemical Calculations

(T Mita, Y Harabuchi, S Maeda)

DOI: 10.1039/D0SC02089C

Theoretical and Experimental Studies on the Near-Infrared Photoreaction Mechanism of a Silicon Phthalocyanine Photoimmunotherapy Dye: Photoinduced Hydrolysis by Radical Anion Generation

(M Kobayashi, T Taketsugu)

DOI: 10.1002/cplu.202000338

Fabrication of Bioinspired Hydrogels: Challenges and Opportunities

(H Fan, JP Gong)

DOI: 10.1021/acs.macromol.0c00238

Supramolecular Conformational Control of Aliphatic Oligoketones by Rotaxane Formation

(T Yoneda, Y Inokuma)

DOI: 10.1021/acs.orglett.0c01010

Symposia

- 1st Chem-Station Virtual Symposium: “Advanced Organic Chemistry” (H Ito)
- 3rd Chem-Station Virtual Symposium: “Young chemists talk about their experiences abroad” (N Tsuji)

Awards

- Commendation for Science and Technology by MEXT (Y Nagata, T Seki)
- Ube Industries Foundation Prize (T Mita)

Outreach

- Social media flyer “ICReDD Word Reactor”
- Educational resource “Periodic Pen Stand”

React With Us!

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

@ICReDDconnect

Researcher Profile

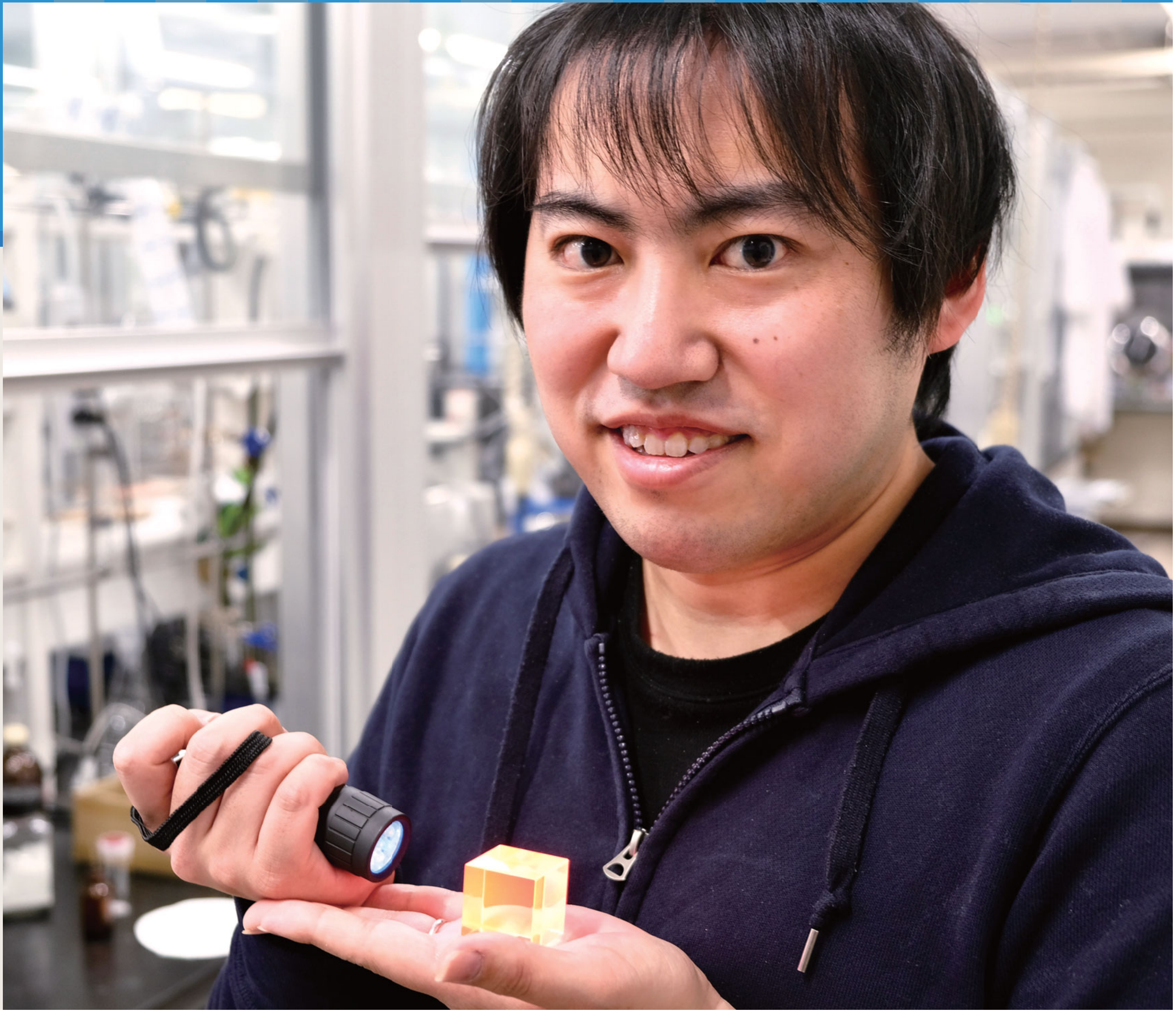
Yuichi KITAGAWA

This is Yuichi Kitagawa.
He works on
Europium complexes that
can emit very bright red light
when illuminated with
UV or blue light.

Short biography

Specially Appointed Lecturer at ICReDD and Faculty of Engineering, Hokkaido University

After his Ph.D. from the University of Tokyo in 2013, a JSPS Research Fellow at Ritsumeikan University. From May 2014, a Specially Appointed Assistant Professor at the Faculty of Engineering, Hokkaido University. Current position since April 2019. He specializes in photochemistry.

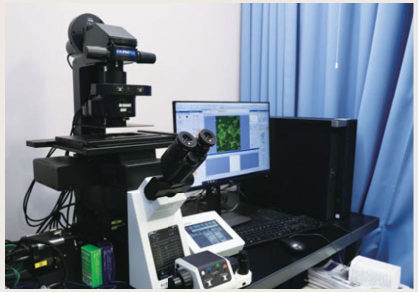


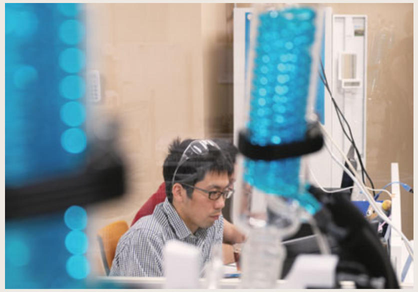
About ICReDD

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





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