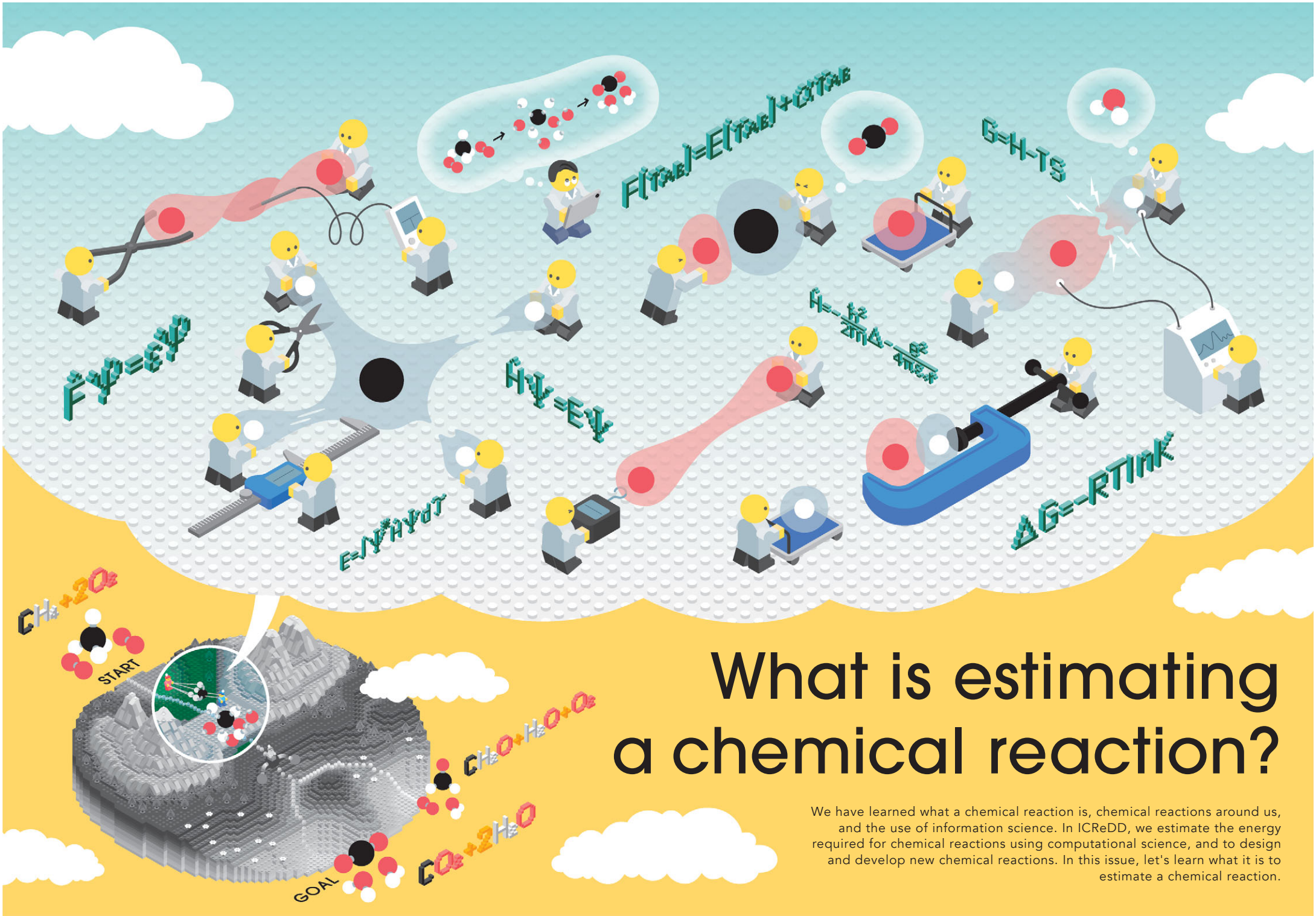
The CATALYST

Helping you react with chemical reactions

Issue 4
June 2021

What is estimating a chemical reaction?

ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY



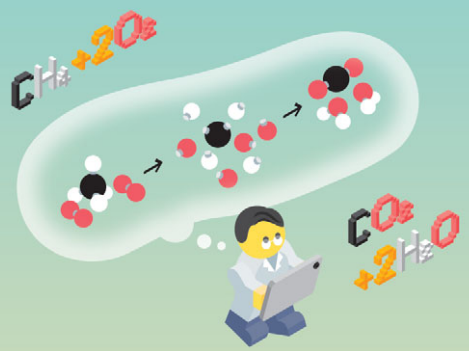
What is estimating a chemical reaction?

We have learned what a chemical reaction is, chemical reactions around us, and the use of information science. In ICReDD, we estimate the energy required for chemical reactions using computational science, and to design and develop new chemical reactions. In this issue, let's learn what it is to estimate a chemical reaction.

Level 1

What is a chemical reaction?

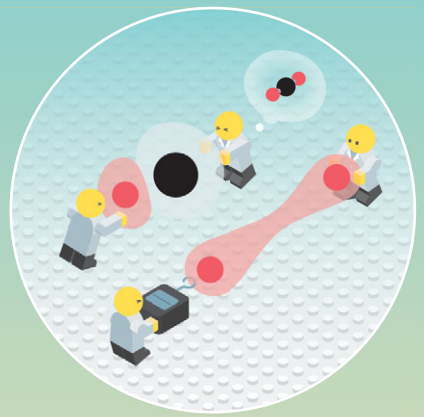
We have learned that a chemical reaction changes the structure of molecules by cleaving and bonding, just as methane and oxygen react to form carbon dioxide and water. However, actual chemical reactions are very complicated. To change the structure of molecules that exist stably at ordinary temperature and pressure by reacting with each other, energy from outside such as heat, pressure, and light, or catalysts are required. In addition, it is not easy to study the detailed reaction pathways, such as which part of the molecule is first cleaved and how it bonds with which atom or molecule.



Level 2

The energy of a molecule

In a stable molecule, the distance between atoms is kept constant. If it is increased, an attractive force works to bond the atoms. If it is shorter than this distance, repulsion occurs. The forces between the atoms are balanced within the molecule. To change the structure of a molecule, the bonds between atoms have to be cleaved. In other words, it is necessary to pass through a high-energy state.



Level 3

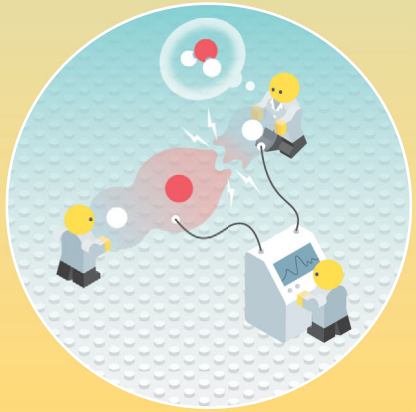
Estimating the energy of a reaction

Quantum chemistry is to understand the behavior of atoms and molecules with equations based on the electron distribution and coordinates of atoms. With the rapid advancement of computer, it has become possible to calculate complex equations of their electron distribution, and to analyze and predict the structure and physical properties of molecules. If we can find the pathway with the lowest energy from the starting material to the desired product, that will often be the actual reaction pathway.

Level 4

Artificial force induced reaction method

The Artificial Force Induced Reaction (AFIR) method estimates the energy required for a reaction by pulling bonds in a molecule to cleave them, or by pushing atoms or molecules to bond them. In this way, several new stable structures can be estimated from the starting structure. At ICReDD, we use this method to design and develop new chemical reactions.



Activation

Quiz

Quantum chemistry is the understanding of the behavior of atoms and molecules by _____.

Send us your answer!

1) intuition
2) equation
3) model
4) experiment

Challenge

Send us if you find an equation that helps you understand chemical bonding.

Share your answer on social media!

#ReactWithUs
@ICReDDconnect

NEWS

New Researchers

Wang Lei

Development of new cancer stem cell therapies and innovative regenerative medicine using biomaterials

Ammathnadu Sudhakar, Amrutha

Prediction of innovative chemical reactions by combination of AFIR and combinatorial optimization

Kilingaru Ishwara, Shivakumar

Investigation of structural, physical and functional properties of aliphatic polyketones a.k.a. carbonyl ropes

Symposia (invited and more)

- 3rd ICReDD International Symposium
  (S. Maeda, H. Ito, T. Taketsugu, J. P. Gong, A. Varnek)
- Open Lecture for Citizen by the Cancer Professional Development Plan and Faculty of Medicine, Hokkaido University
  (S. Tanaka)
- Joint Symposium of Engineering & Information Science & WPI-ICReDD in Hokkaido University
  (T. Mita, K. Kubota, I. Takigawa, A. Lyalin)
- Organic Chemistry -the next generation- (Y. Shimizu)
- Symposium on Theoretical Chemistry, Japan (Y. Harabuchi)
- Chemical Record Lecture 2021 by CSJ and Wiley-VCH (B. List)

Selected Publications

(out of 29 papers from February 2020 to April 2021)

Rapid Reprogramming of Tumour Cells into Cancer Stem Cells on Double-Network Hydrogels
(M. Tsuda, L. Wang, J. P. Gong, S. Tanaka)
DOI: 10.1038/s41551-021-00692-2

Combined Graph/Relational Database Management System for Calculated Chemical Reaction Pathway Data
(T. Gimadiev, S. Maeda, P. Sidorov, A. Varnek)
DOI: 10.1021/acs.jcim.0c01280

Tackling Solubility Issues in Organic Synthesis: Solid-State Cross-Coupling of Insoluble Aryl Halides
(K. Kubota, H. Ito)
DOI: 10.1021/jacs.1c00906

Awards

- The 33rd Award of the Society of Rubber Science and Technology, Japan (J. P. Gong)
- The Rare Earth Society of Japan Award (Shiokawa Award) (Y. Hasegawa)
- Awards for Science and Technology (Research Category) of the Commendation for Science and Technology by MEXT (M. Sawamura)
- The Young Scientists' Award of the Commendation for Science and Technology by MEXT (T. Nakajima)

Outreach

- Monthly news postcards
- Quarterly news poster The CATALYST 3rd issue

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with what's happening at ICReDD,
follow us on our social media channels:

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Researcher Profile

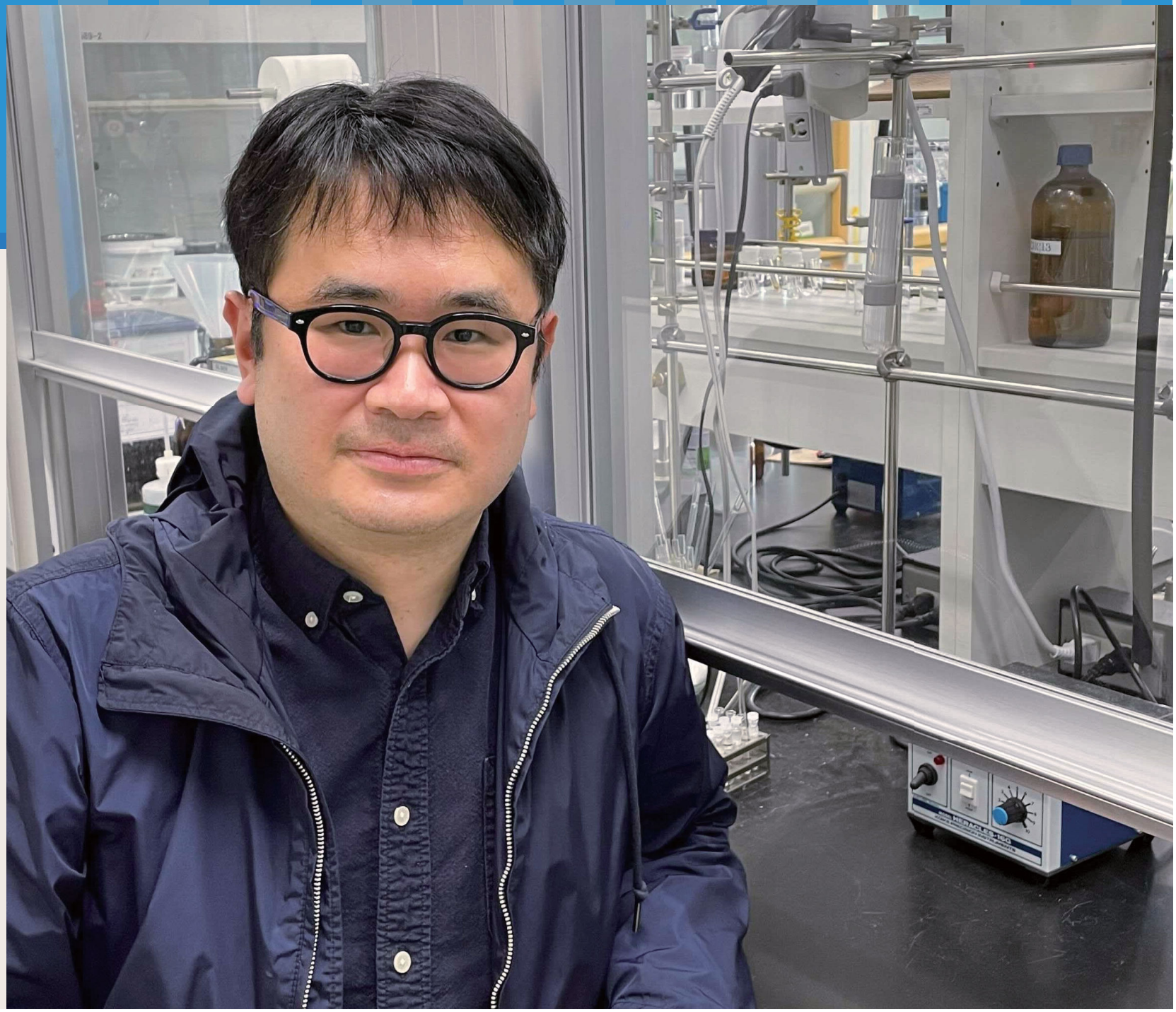
Tsuyoshi Mita

Tsuyoshi Mita is developing new chemical reactions based on quantum chemical calculations. His group recently achieved α,α-difluoroglycine synthesis and its application guided by the Artificial Force Induced Reaction (AFIR) Method

(Chem. Sci. 2020, 11, 7569 & Chem. Eur. J. 2021, DOI: 10.1002/chem.202100812).

Short biography

Specially Appointed Associate Professor at Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University.
Ph.D. from the University of Tokyo in 2007. Postdoctoral fellow at Department of Chemistry & Chemical Biology, Harvard University in 2007-2009. Assistant Professor at Faculty of Pharmaceutical Sciences, Hokkaido University in 2009-2019. Current position since 2019. Project Associate Professor in organic synthesis group of "MAEDA Artificial Intelligence in Chemical Reaction Design and Discovery Project (JST, ERATO)" since 2019.
His current interest is in the areas of synthetic organic chemistry, organometallic chemistry, medicinal chemistry, and computational chemistry.



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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