The CATALYST

Helping you react with chemical reactions

Issue 11

March 2023

Controlling chemical reactions with temperature

ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY

Controlling chemical reactions with temperature

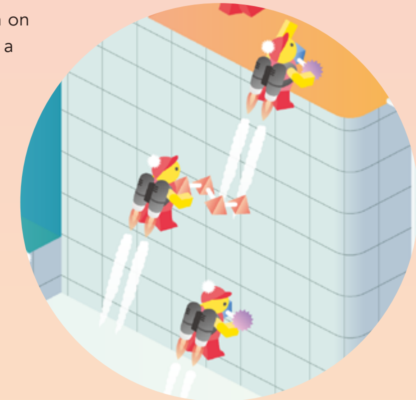
Temperature is very important for chemists to consider when developing new chemical reactions. The temperature at which a reaction is performed can alter not only the speed of the reaction, but it can also change the product that is formed! Temperature is closely related to energy, influencing molecular vibrations or the speed of a molecule's motion. Additionally, calculating the energy of molecules can help chemists better predict whether a reaction is possible and what products will be produced.

1. Heat and temperature

We often experience the sensations of hot and cold in our daily lives. Similar to everyday objects around us, the temperature of a molecule is raised by heating it. Heat is a form of energy, and when a molecule absorbs heat it gains energy and moves with a greater speed. The more quickly molecules move, the more they collide into each other. This creates more chances for a reaction to occur, speeding up the overall rate of reaction.

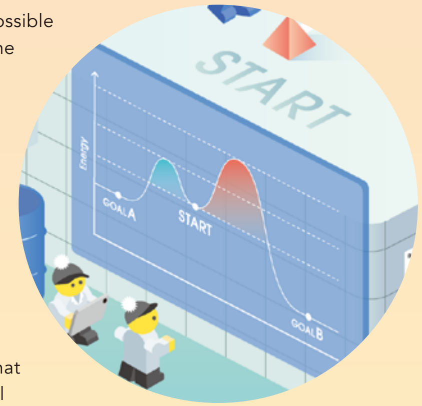
2. Energy Barriers

In principle, chemical reactions do not begin on their own. For example, when starting a fire, a spark is needed to get the combustion reaction going. All chemical reactions require some amount of external energy to get started, and this is called activation energy. Activation energy acts as a barrier, preventing the reaction from happening on its own. However, if enough energy is supplied to the starting molecules, this barrier can be overcome, and the reaction can proceed. Every reaction has a different activation energy barrier, and reactions with higher barriers require more energy to get started.



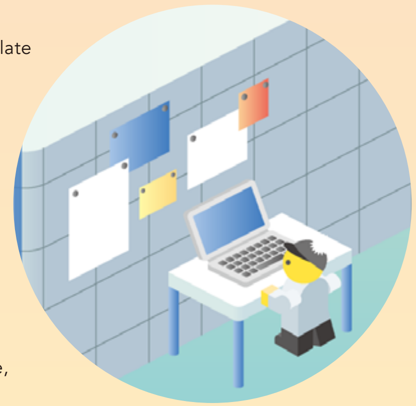
3. Controlling reactions with temperature

For some chemical reactions, it is possible to obtain a different product from the same starting materials by changing the temperature at which the reaction is performed. In chemistry, lower energy molecules are more stable, so reactions naturally proceed toward the lower energy product molecules (GOAL B instead of GOAL A). However, sometimes the activation energy barrier is high and the starting molecules don’t have enough energy to overcome that barrier. In that case, the reaction will proceed along an alternate path with a lower activation barrier (path A). By heating the reaction and providing enough energy to climb the taller barrier, the reaction can be controlled to follow path B.



4. Optimizing reaction conditions with computational chemistry

At ICReDD, computational chemists use mathematics and quantum chemistry to calculate the height of the energy barrier and the energy of the product molecules. Using the Artificial Force Induced Reaction (AFIR) method developed at ICReDD, researchers can automatically search for and compute all possible paths for a reaction. This can inform scientists of situations when multiple products might form. Scientists can then use the calculated energies of the products and energy barriers of the different paths to help them optimize experimental conditions, such as temperature, to get only the desired product. In this way, computations enable scientists to find suitable reaction conditions more quickly, speeding up new chemical reaction discovery!



Activation!

Quiz

Heating a molecule makes it ________.

Send us your answer!

- **A** stop vibrating
- **B** move more quickly
- **C** less reactive
- **D** lose energy

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

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ICReDD News

March 2023

New Researchers

Chandu Gopalakrishnan

Photoresponsive Asymmetric Catalysis and Radical Transformations

Selected Publications

(from December 2022 to February 2023)

- Red-light photoswitching of indigos in polymer thin films" Chem. Sci. 2023
  (C.Y. Huang)
  https://www.icredd.hokudai.ac.jp/research/8687

- Automated chemical reaction prediction: now in stereo
  (T. Mita, H. Hayashi, H. Takano, Y. Harabuchi, S. Maeda)
  https://www.icredd.hokudai.ac.jp/research/8491

- Graph neural networks accelerate AFIR-based automated reaction path search
  (Y. Harabuchi, S. Maeda)
  https://www.icredd.hokudai.ac.jp/research/8594

- Robots and A.I. team up to discover highly selective catalysts
  (N.Tsuji, P. Sidorov, Y. Nagata, T. Gimadiev, A. Varnek, B. List)
  https://www.icredd.hokudai.ac.jp/research/8645

- It Takes Two: cooperating catalysts provide new route for utilizing formate salts
  (S.R. Mangaonkar, H.Hayashi, H. Takano, S. Maeda, T. Mita)
  https://www.icredd.hokudai.ac.jp/research/8676

Outreach

- Visit by delegation from the UK Embassy in Tokyo led by Deputy Head of Mission Helen Smith
- Monthly Research Postcard
- The CATALYST Issue 10

Monthly News Postcard

The CATALYST 10th issue

Visit by delegation from the UK Embassy in Tokyo led by Deputy Head of Mission Helen Smith

Symposia

- The 2nd Akira Suzuki Awards Ceremony and 5th ICReDD International Symposium

The 2nd Akira Suzuki Awards Ceremony

Awards

- 17th Annual HPC Innovation Award
  (A. Lyalin)
- 72nd Annual Chemical Society of Japan Award for Young Chemists
  (K. Kubota)
- 2023 Thieme Chemistry Journals Award (N. Tsuji)

Researcher Profile

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Min Gao

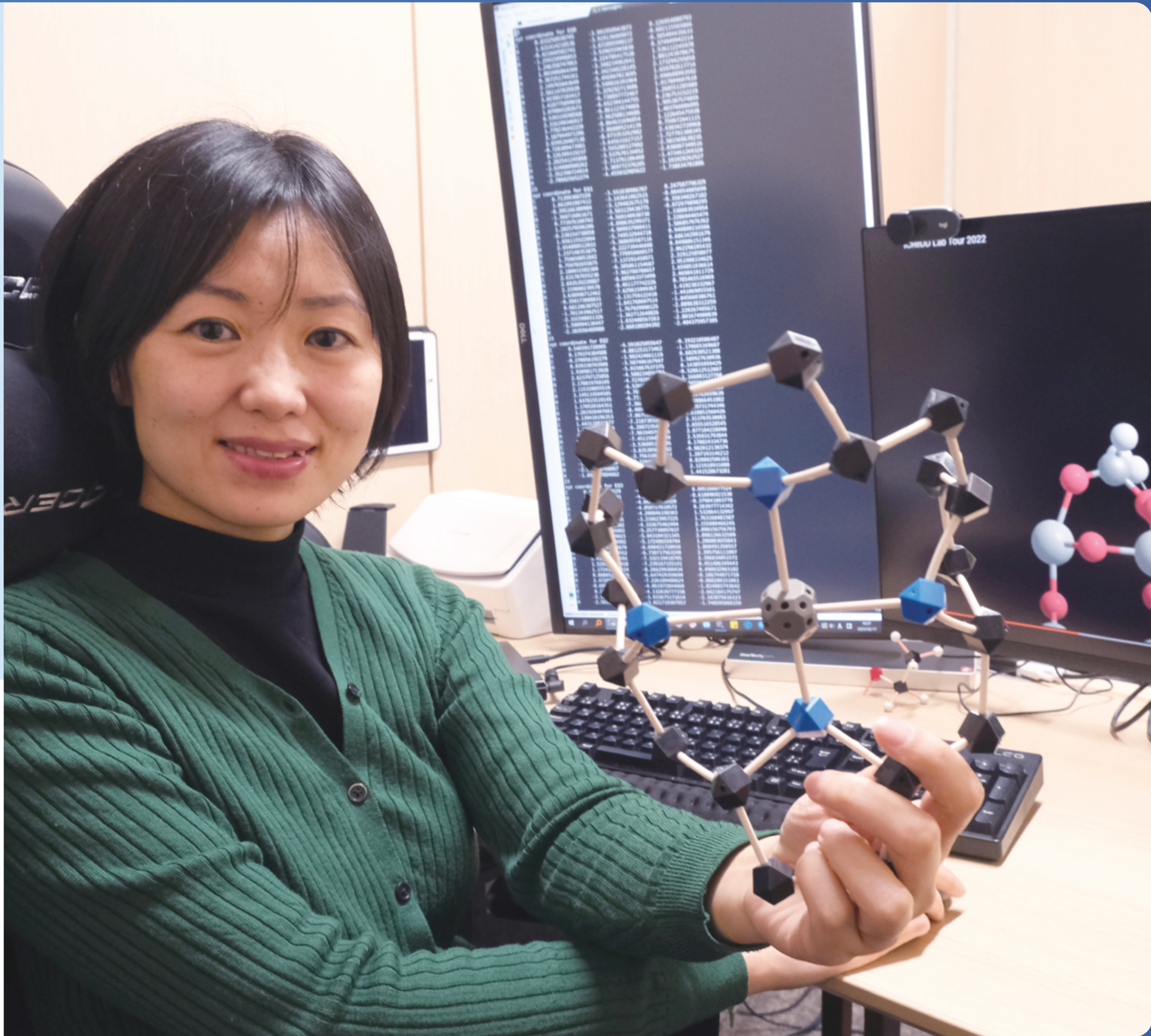
Associate Professor Gao is working on computational catalysis. Her research focuses on understanding and developing catalytic reactions at the atomic level by using computers.

Recently, she is also doing experiments based on the results of her theoretical calculations.

Representative Papers:
J. Phys. Chem. C, 2021, 125, 19219-19228.
J. Phys. Chem. C, 2021, 125, 1334-1344.
J. Chem. Theo. Comp., 2014, 10, 1623-1630.

Short Biography

Associate Professor, Junior PI at ICReDD, Hokkaido University
Prof. Gao received her PhD from the Graduate School of Science in Hokkaido University in 2012. She continued her research work as a postdoc and joined the Institute for Catalysis in Hokkaido University as an assistant professor in 2018. She started her current position in August 2022.



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 held The 2nd Akira Suzuki Awards Ceremony and 5th ICReDD International Symposium on January 11th, 2023. The 2nd Akira Suzuki Award was presented to John F. Hartwig, the Henry Rapoport Professor of Chemistry at the University of California, Berkeley. The 2nd ICReDD Award was presented to Kendall N. Houk, Distinguished Research Professor at the University of California-Los Angeles.

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!

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with what's happening at ICReDD,
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Published in March 2023

Published by the Institute for Chemical Reaction Design and Discovery (WPI-ICReDD)

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