The CATALYST

Helping you react with chemical reactions

Issue 17

September 2024

Designing crystals that spin

ICReDD
Institute for Chemical Reaction Design and Discovery
HOKKAIDO UNIVERSITY

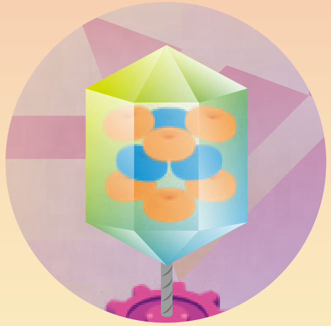
Designing crystals that spin

Crystals can be found all around us. Sugar and salt are crystals, and so are gemstones such as diamond and quartz. The word crystal means something that is made up of atoms, ions or molecules arranged in an orderly, repeating pattern. You probably imagine a crystal to be something hard and brittle, so it would make sense for the atoms and molecules inside the crystal to be stiff and unmoving, right? Well in this issue of The Catalyst we will touch on movement can happen in crystals and molecules.

1. How crystals are formed

Particles can be formed when atoms, ions or molecules start to stick together due to changes in the temperature or amount of the gas or liquid they are dissolved in. Particles that can no longer stay dissolved form a very small bit of solid material. More particles attach to this small solid at the center, which is called a nucleus, and a crystal is one of these solids that has grown large enough to see. Snow is a crystal which forms when water vapor cools and ice particles in the air stick together and become big enough to be a snowflake. Salt (sodium ions and chloride ions) dissolved in water can form salt crystals when the water is evaporated. Component molecules of quartz that were dissolved underground also gradually gather and crystallize over long periods of time. The crystals of snow, salt, and quartz are different shapes, and this is due to differences in the three-dimensional arrangement of particles in the crystal.

2. The shape of crystals

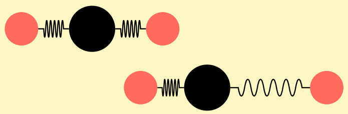


The orderly structure of a crystal can be described by the smallest repeating arrangement of atoms, ions or molecules. This repeating pattern extends in three dimensions to make a large crystal. The shape of this pattern affects the shape of crystal. Snowflakes are hexagonal, salt is cubic, and quartz is a hexagonal pillar. The same atoms, ions or molecules can be arranged in different repeating patterns to produce very different materials. Both diamonds and the lead in your pencil are made of carbon atoms, but because of their different crystal structure, pencil lead is soft and its layers can be easily separated, while diamonds are extremely hard.

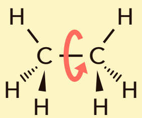
3. Movement of atoms in molecules

We naturally imagine that molecules in crystals are stiff and do not move, but in reality the molecules are just packed together so tightly that there is no space for them to move. Atoms within individual molecules, however, have more freedom of movement. For example, two bonded atoms can move toward and away from each other, with the bond stretching and compressing like a spring. Atoms can rotate freely around a single bond but cannot rotate around double or triple bonds. While atoms in molecules can move freely, they move in a way that they don't collide with each other and don't give the molecule a distorted shape. By skillfully bonding atoms together, it is possible to design molecules that exhibit a desired type of motion.

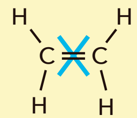
Chemical bonds stretch and compress like a spring.



Atoms can rotate depending on the type of chemical bond.



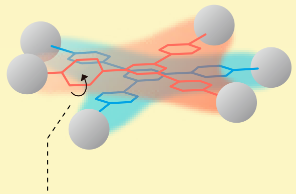
Atoms can rotate around a single bond.



Atoms cannot rotate around a double bond.

4. Movement in crystals

At ICReDD, we successfully designed a molecule that can move even in a crystal! The molecule has 3 rotatable benzene rings, and the researchers designed and made the molecule based on what they imagined its crystal structure would be. They designed the molecule so that when a benzene ring on one molecule rotates it pushes on the rings of the neighboring molecules above and below, causing those rings to rotate, much like gears that rotate together. After making a crystal of this molecule, the researchers observed the molecules moved just as they had designed. With this sort of gear-like molecular design, ICReDD succeeded in doing what was thought to be impossible, enabling molecules in a crystal to move!



Space between the molecules and its structure are designed so that the benzene rings can rotate in a crystal.

Activation!

Quiz

In general, molecules in a crystal structure cannot move because:

- **A** all the chemical bonds become stiff
- **B** they are frozen
- **C** they packed together so tightly that there is no space for them
- **D** all the chemical bonds are broken

Send us your answer!

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

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ICReDD News

September 2024

New Researchers

Gumi Wei
Hydrogel, Mechanochemistry

Selected Publications (from June 2024 to August 2024)

New avenue towards widely applicable indigo photoswitches – Combining experimental, computational and data-science approaches –

(Amit K. Jaiswal, Kimichi Suzuki, Satoshi Maeda, Chung-Yang Dennis Huang)

https://www.icredd.hokudai.ac.jp/research/11996

Development of a New Method for the Chemical Synthesis of Diphosphine Ligands from Strained Small Molecules

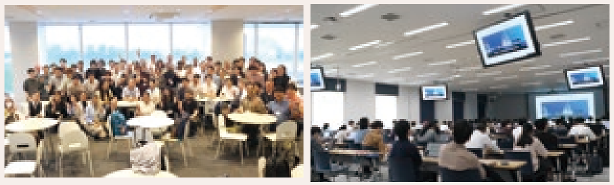
(Chandu G. Krishnan, Hideaki Takano, Hitomi Katsuyama, Hiroki Hayashi, Tsuyoshi Mita)

https://www.icredd.hokudai.ac.jp/research/12044

Event

- 2024 joint open campus event, Hokkaido University
- WPI-SKCM² & WPI-ICReDD Joint Research Symposium
- WPI online seminar for educators-8, "Tackling environmental issues with the help of Chemistry"

WPI online seminar for educators-8



WPI-SKCM² & WPI-ICReDD Joint Research Symposium

Visitor

- The Industry/Academia Exchange Committee from the Chemical Society of Japan
- Yuei Fukuji, Executive Vice President, Ryukyu University
- Akio Fujiwara, MEXT Vice Minister
- Hisao Eguchi, President and CEO, Tosoh Finechem Corporation
- Prof. Shan-hui Hsu (National Taiwan University) from National Science and Technology Council

Delegates from National Science and Technology Council

Outreach

- Monthly Research Postcard
- The CATALYST Issue 16

Monthly Research Postcard

The CATALYST 16th Issue

Award

- 2024 Royal Society of Chemistry Horizon Prize (Gong, Rubinstein)

Researcher Profile

vol.17

Mingoo Jin

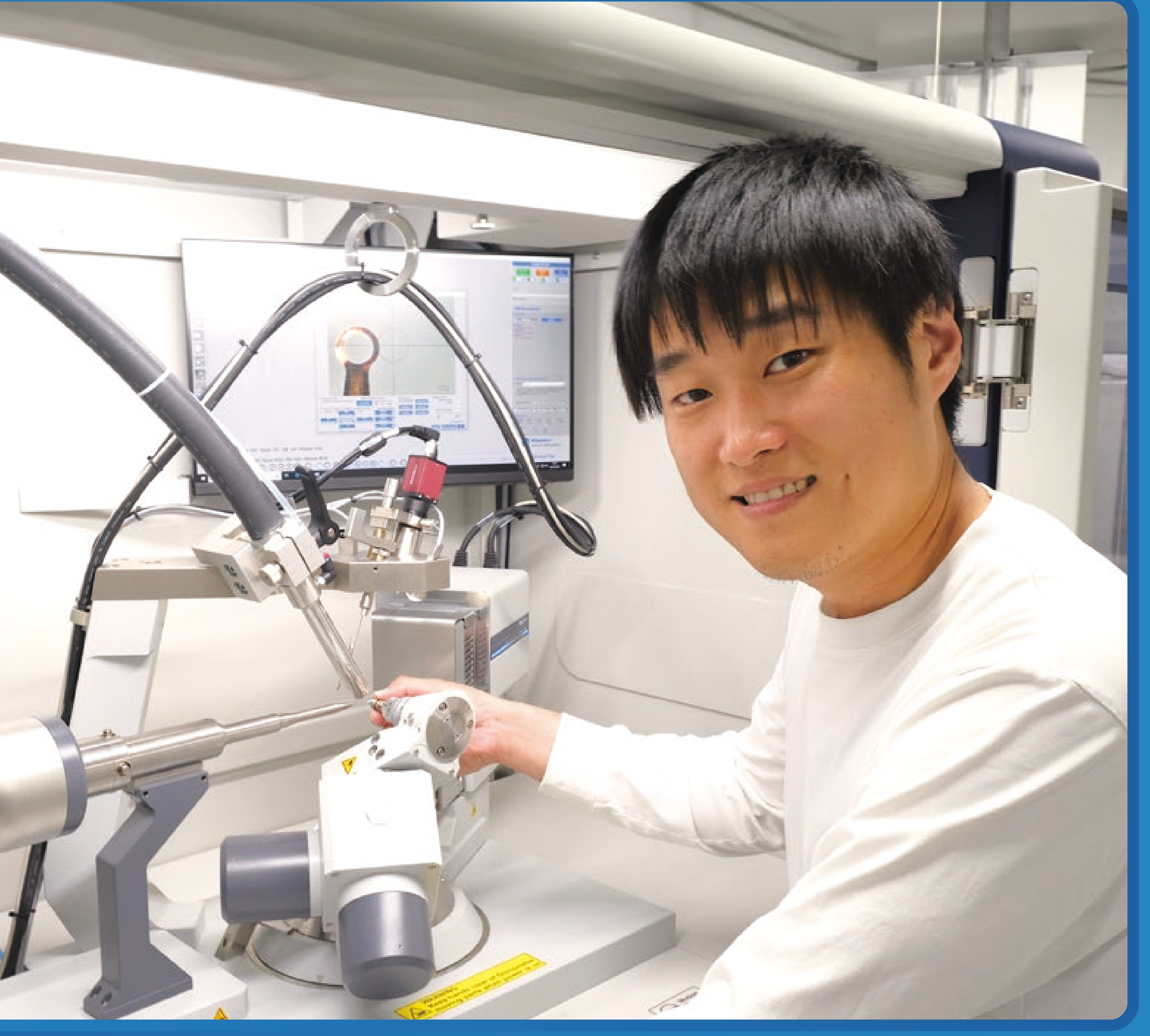
Associate Professor Mingoo Jin's research focuses on developing methods for enabling molecular gears to operate within solid, crystalline materials. His goal is to develop materials with unique properties and functions by controlling the motion of molecular gears.

Representative Papers:

J. Am. Chem. Soc. 2023, 145, 27512–27520.
Angew. Chem. Int., Ed. 2023, 62, e202309694.
J. Am. Chem. Soc. 2021, 143, 1144–1153.

Short Biography

ICReDD Associate Professor and Junior-PI of the Jin group at ICReDD. He completed his Ph.D. studies at Hokkaido University's Graduate School of Chemical Sciences and Engineering under the supervision of Professor Hajime Ito. After his graduation, he joined as postdoctoral researcher in the laboratory of Professor Miguel A. Garcia-Garibay at the University of California, Los Angeles. From 2019, he joined ICReDD as a Specially Appointed Assistant Professor in the laboratory of Professor Hajime Ito, and in 2022 he was promoted to Associate Professor in ICReDD as a Junior-PI, establishing his own research group.



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.

At the Joint Open Campus event held on June 8 (Sat.), ICReDD participated in the hands-on corner (slime making, molecular simulation) and science talks, as we did last year. Top About 240 people participated in the hands-on corners, which were big hits again this year! Bottom At the Science Talk, Specially Appointed Assistant Professor Yuki Ide gave his lecture introducing the latest research with a quiz under the title of "AI to distinguish between sugar and salt –Guess which are these crystals!?"

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,
follow us on our social media channels:

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