FY2013

Innovative Molecular Structure Analysis Based on Self-Assembly Technology

A once-in-a-century revolution — resolving the bottleneck of X-ray structural analysis

The creation of new materials has made our lives more convenient. Identifying a new material requires an analysis of its molecular structure. X-ray diffraction technique* is a reliable analytical method for determining molecular structure, but is requires crystallization of the sample, which takes a large amount of both the sample and time.

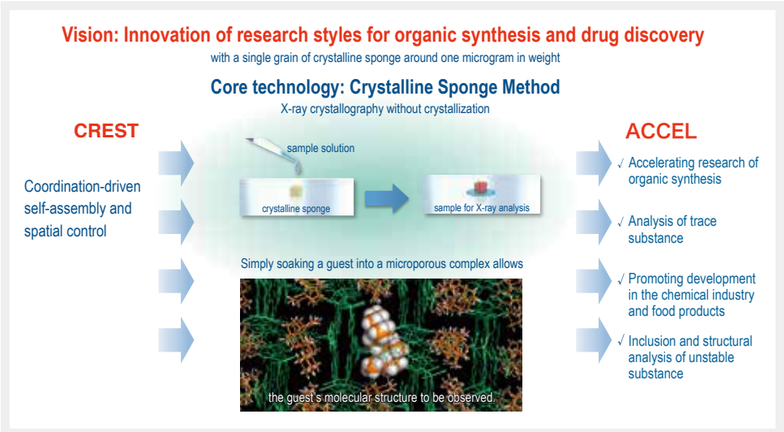
Hence we developed a **crystalline sponge method** that does not need sample crystallization, solving a long-standing problem. The crystalline sponge method allows a chemical compound to be structurally analyzed even if it is a liquid at room temperature, as well as allowing analysis with a sample of around five micrograms, or roughly a thousandth of the previous amount. To date, we have developed the epoch-making LC-SCD method, used to analyze the molecular structure of a trace of some constituent material extracted from an animal or a plant, and succeeded in identifying the structure of more than a hundred different chemicals.

* A method of analyzing structure where molecules are aligned in an orderly fashion (periodic sequence) by using the characteristics of X-ray transmission that bends around behind the molecules. Even gigantic molecules can be observed and their 3D structure visually imaged.

Research to analyze more diverse materials is in progress

In the ACCEL project, we seek a way to commercialize the crystalline sponge method based on our previous research results. We are developing several types of crystalline sponge, which we estimate can handle 20 to 30 % of all organic molecules. From now on, we would like to expand the applicable range of molecules and also develop crystalline sponges focused on capturing specific rare molecules.

Widespread use of our crystalline sponge will contribute to fostering innovation in many fields: from drug discovery, where the period of new drug development can be shortened, to chemicals and foods. With help of those engaged in commercialization, we shall contribute to society.



Crystalline sponge method

The crystalline sponge is a hollow chemical with a structure similar to a basket made up of numerous micropores between 0.5 and 1 nanometers in diameter. Soaking a liquid sample into the crystalline sponge permits the molecules to be introduced in the basket and be automatically aligned in an orderly fashion, stabilizing them and allowing X-ray analysis without crystallizing samples.

Research Director

Makoto Fujita

Distinguished Professor, The University of Tokyo, and Distinguished Professor, Institute for Molecular Science, National Institutes of Natural Sciences

I majored in organic synthesis as a young man, and then gained experience on briefly working on inorganic materials, allowing me to acquire a cross-sector, comprehensive way of thinking which brought me to my current research. What triggered me to study X-ray structural analysis was the discovery of *self-assembly*, the spontaneous construction of unprecedented structures by mixing organic molecules and metallic ions. My inspiration that these structures could perhaps be used to analyze molecular structures turned out to be the solution for a long-standing problem.

In the ACCEL project, the researchers are trying to find what sorts of application frameworks should be offered to society, with Dr. Ezaki, the Program Manager, teaching them about commercialization, not a field they have much expertise in. Our short-term task is to develop various types of crystalline sponges and increase the number of analyzable molecules. We are currently preparing types for hydrophilic and acidic molecules as well as for the current type for analysis of molecules which are reluctant to mix with water.

The fundamental research is a challenging task. After a half century since I started, my research is about to be ready for applications, and so I am eager to make this happen.

Program Manager

Atsuo Ezaki

ACCEL Program Manager, Japan Science and Technology Agency

I have experience in being the person responsible for product development and commercialization, and have always wished to commercialize superior research in the academic sector for use in industry, making my contribution to society. The fundamental research has high purity as science, but has a long way to go to achieve commercialization. That requires hard effort, but solving daily problems is rewarding as well as fascinating.

I have talked with many from industry who are interested in this research, and also asked them what sort of social contribution their companies each wish to make. Through this program, I will polish this technology to make it into "technology that can contribute to social value," within the overall ecosystem composed of industry, academia, and other related organizations. Working in concert with the stakeholders, I would like to transform this innovative fundamental research outcome into socially-applicable products.

I want to create the "axle" that connects the two wheels of science and technology, and have this research roll on to our goal of social contribution.

The crystalline sponge that solved the "100-year-problem" of X-ray structural analysis will bring about innovative research styles in the organic-synthesis-related industry.

PROFILE MAKOTO FUJITA

1982: M.S. (Engineering), Chiba University. Joined Sagami Chemical Research Institute; 2002: Professor, School of Engineering, The University of Tokyo after successively Chiba University, the Institute for Molecular Science and Nagoya University; 2018: appointed concurrently to Distinguished Professor, Institute for Molecular Science, National Institutes of Natural Sciences. Field of expertise: Self-assembly of molecules. Ph.D. (Engineering)

PROFILE ATSUO EZAKI

1980: M.S. (Engineering), Tokyo Metropolitan University. Joined Konishiroku Photo Industry Ltd. (currently Konica Minolta, Inc.). Engaged in product R&D, business start-up, and technical strategy promotion through the development of photographic material and launching businesses for inkjet printer systems and Organic LEDs.