【Grant-in-Aid for Specially Promoted Research】

Science and Engineering (Chemistry)

Title of Project： Self-assembled porous coordination networks as crystalline molecular flasks

Makoto Fujita
(The University of Tokyo, Graduate School of Engineering,
Professor)

Research Area：Coordination chemistry, Organic chemistry
Keyword：Self-assembly, Porous coordination network

【Purpose and Background of the Research】

In solution, a wide variety of self-assembled coordination hosts are known to encapsulate guest molecules and to work as nano-sized reaction containers. Typically, such unique chemical events are limited only to solution, because molecules lose their mobility in the solid state.

We have recently synthesized networked molecular cages composed of an infinite array of self-assembled molecular cages. Surprisingly, the cage subunits encapsulate guest molecules as is in solution even in a crystalline state. This finding implies that we can transfer exhaustively studied solution chemistry into solid state by constructing the same molecular cavities both in solution and solid.

This research is aimed to bridge the gaps between solution and solid state chemistries by self-assembled porous coordination networks derived from molecular hosts and create a new field for academic research and practical application.

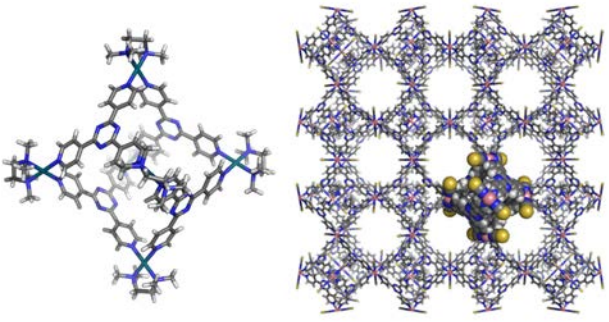

Figure 1 (left) Solution cage molecule and (right) crystalline networked cages. The nature of hollow host cage is preserved even in crystal.

【Research Methods】

The research begins by networking discrete molecular hosts to make single crystalline hosts as “crystalline molecular flasks”. To develop crystalline state reactions, we first use discrete solution hosts that are isostructural to the building unit of crystalline hosts and suitable reaction conditions will be fully optimized in solution. We then transfer the well-examined solution reactions into crystalline state, which allows us accurate design of solid-state reaction at the molecular level. Another benefit of crystalline molecular flasks is that we can easily determine the structures of substrates, products, and even labile intermediates by X-ray single crystallography. The obtained outcome will be fed back to the design and fine-tuning of host molecules in solution.

【Expected Research Achievements and Scientific Significance】

Use of pseudo-solution state in porous coordination network crystals for heterogeneous reaction system will be a breakthrough in scientific technology. Since porous coordination networks are macroscopically crystals but microscopically solution, they can cover the shortcomings of both solution and solid state chemistry. It is no doubt that this project will open a door to new academic field, and that expected research outcome will cause a paradigm shift from solution to solid.

【Publications Relevant to the Project】

[1] "Crystalline molecular flasks" Y. Inokuma, M. Kawano, M. Fujita, *Nat. Chem.* **2011**, 3, 349-358.
[2] "Networked molecular cages as crystalline sponges for fullerenes and other guests" Y. Inokuma, T. Arai, M. Fujita, *Nat. Chem.* **2010**, *2*, 780-783.
[3] "X-ray observation of a transient hemiaminal trapped in a porous network" T. Kawamic Haneda, M. Kawano, M. Fujita, *Nature* **2009**, *461*, 633-635.

【Term of Project】 FY2012-2016

【Budget Allocation】 304, 500 Thousand Yen

【Homepage Address and Other Contact Information】

http://fujitalab.t.u-tokyo.ac.jp/
mfujita@appchem.t.u-tokyo.ac.jp