文部科学省ナノテクノロジープラットフォーム

第19回ナノテクノロジー総合シンポジウム

JAPAN NANO 2021

"Platforms strengthening material innovation force in a new era"

Proceedings

Nanotechnology

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Venue: **Tokyo Big Sight, Conference Tower(Tokyo)**
※Online

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National Institute for Materials Science,
National Institute of Advanced Industrial Science and Technology,
The University of Tokyo, Tokyo Institute of Technology,
Waseda University, Shinshu University,
National Institutes of Natural Sciences Institute for Molecular Science,
Nagoya University, Nagoya Institute of Technology,
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NanotechJapan
Nanotechnology Platform

文部科学省ナノテクノロジープラットフォーム

第19回ナノテクノロジー総合シンポジウム

JAPAN NANO 2021

「マテリアル革新力強化のための次世代プラットフォーム」

Nanotechnology

講演予稿集

開催日：2020年12月11日（金）
※オンライン併用開催 LIVE

会　場：東京ビッグサイト
会議棟1階レセプションホール（東京都江東区有明）

主　催：文部科学省ナノテクノロジープラットフォーム
国立研究開発法人物質・材料研究機構ナノテクノロジープラットフォームセンター

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December 11th (Fri.), 2020, Reception Hall
2020年12月11日（金）　会議棟1階レセプションホール

10:00-10:10【Opening Remarks/ 開会挨拶】

10:00- **Kazuhito Hashimoto** (President, National Institute for Materials Science, Japan)
橋本 和仁（物質・材料研究機構理事長）

10:05- **Ministry of Education, Culture, Sports, Science and Technology**
文部科学省

10:10-12:00【Session 1】

Form of new era platforms based on big data / データを基軸とした次世代プラットフォームのあり方

10:10-10:20【Message to new era platforms. / 次世代プラットフォームへのメッセージ】

Makoto Gonokami (The University of Tokyo)
五神 真（東京大学総長）

10:20-10:55【Special Lecture / 特別講演】

Maki Kawai (Institute for Molecular Science)
川合 眞紀（自然科学研究機構 分子科学研究所）
“Strategy Towards the Realization of Society 5.0:
Strengthening Research Infrastructure and Development of Human Resources”
「Society 5.0 の実現に向けて、人材育成および研究基盤の強化」

11:00-12:00【Overseas Invited Lectures / 海外招待講演】

11:00- **Lynn Rathbun** (Cornell University, USA)
“The (U.S) National Nanotechnology Coordinated Infrastructure (NNCI) and ACCELNET :
Global Quantum Leap; Models for International Collaboration and Cooperation.”
「米国における国際協調・協力モデル：NNCI と ACCELNET、量子技術の飛躍的進展における世界協力」

11:30- **Gian-Marco Rignanese** (Université catholique de Louvain, Belgium)
“OPTIMADE : a REST API for querying materials databases”
「OPTIMADE : マテリアルデータベースを操る REST API の開発」

12:00 - 13:10　Lunch / 昼食

13:10-13:45【Plenary Lecture / 基調講演】

Nobuyuki Osakabe (Hitachi)
長我部 信行（株式会社日立製作所）
“Transformation of Research Platform to create Future Society”
「研究現場のトランスフォーメーションによる研究力強化と未来社会創造」

13:50-15:05【Session 2】

A Year After Coronavirus: Leave No R&D Behind / ニューノーマル時代の研究開発を考える

13:50- **Keisuke Takahashi** (Hokkaido University)
髙橋 啓介（北海道大学）
"The Rise of Catalyst Informatics: Concepts and Applications"
「触媒インフォマティクスの基本概念と実例」

14:15- **Toshiaki Taniike** (Japan Advanced Institute of Science and Technology)
谷池 俊明（北陸先端科学技術大学院大学）
"Data-driven materials science based on high-throughput experimentation"
「ハイスループット実験を基盤としたデータ駆動型材料科学研究」

14:40- **Kazunori Arifuku** (JEOL)
有福 和紀（日本電子株式会社）
"Remotely utilization in the instrument for research (In Jobsite) : The current situation and the going forward"
「研究機器（現場）における遠隔利用の現状と今後」

15:05 - 15:25 Coffee Break / 休憩

15:25-15:50【Session 3】

nanotech 2020 award lecture / nano tech大賞 2020 講演

Masato Masuda (TORAY)
増田 正人（東レ株式会社）
"Innovative Conjugate Spinning Technology NANODESIGN®"
「革新複合紡糸技術 NANODESIGN®」

15:55-17:10【Session 4】

Topics and future perspectives of nanotechnology platforms / ナノテクノロジープラットフォームの成果と将来展望

15:55- **Ministry of Education, Culture, Sports, Science and Technology**
文部科学省
"Digital transformation of materials research and development"
「マテリアル研究開発の DX 化について」

16:10- **Takahisa Yamamoto** (Nagoya University)
山本 剛久（名古屋大学）
"Nano-scale analysis for development of materials"
「マテリアル開発につながる微細構造解析技術」

16:30- **Ryuji Yokokawa** (Kyoto University)
横川 隆司（京都大学）
"MICROFLUIDIC DEVICES FABRICATED BY FOUNDRY SERVICE AND THEIR APPLICATIONS TO LIFESCIENCE RESEARCHES"
「受託代行サービスにより作製した微小流体デバイスとそのライフサイエンス研究への応用」

16:50- **Takaaki Mitsuhashi** (Institute for Molecular Science)
三橋 隆章（分子科学研究所）
"Structure Elucidation Support by the Crystalline Sponge Method"
「結晶スポンジ法による構造解析支援」

17:10-17:15【Closing Remarks / 閉会挨拶】

Yasuo Koide (Chairperson of the Organizing Committee of JAPAN NANO 2021 / Director, Center for Nanotechnology Platform, National Institute for Materials Science, Japan)
小出　康夫（JAPAN NANO 2021 組織委員長、物質・材料研究機構ナノテクノロジープラットフォームセンター長）

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Session 1
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【Special Lecture / 特別講演】

"Strategy Towards the Realization of Society 5.0 : Strengthening Research Infrastructure and Development of Human Resources"

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「米国における国際協調・協力モデル：
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Lynn Rathbun (Cornell University, USA)

"OPTIMADE : a REST API for querying materials databases"

「OPTIMADE : マテリアルデータベースを操るREST APIの開発」

Gian-Marco Rignanese (Université catholique de Louvain, Belgium)

Prof. GONOKAMI Makoto
President
Professor GONOKAMI Makoto became the 30th President of the University of Tokyo on April 1st, 2015, with a six-year term. Prof. Gonokami was previously the Dean of the School of Science. He became a full professor in 1998 having joined UTokyo as an academic staff in 1983. He has held several appointments in UTokyo including the positions of Vice President (2012-2014), Director of Photon Science Center (2008-2014), and the Director of Institute for Photon Science and Technology (2013-2014). He is a member of the Science Council of Japan, and a Fellow of the American Physical Society (2012) and Optical Society of America (2013).
Professor Gonokami is well-known in the field of photon science, and has established world leading photon research centers in the School of Science and School of Engineering.

Strategy Towards the Realization of Society 5.0: Strengthening Research Infrastructure and Development of Human Resources
Society 5.0 の実現に向けて、人材育成および研究基盤の強化

[1]Maki Kawai

[1]Institute for Molecular Science,
Myodaiji, Okazaki, Aichi 444-8585, Japan

Abstract

Materials Science has made a tremendous progress during last several decades. Triggered by the invention of high Tc superconductors, a series of metal oxides representing strongly corelated electron systems emerged. Synthetic chemistry has also developed during these decades. Synthesis based on "non-covalent bond formation" has greatly expanded by connecting molecules with non-covalent bonds for example via metal atoms. Technology of measurement has developed significantly as well. Fundamentals to support the development of both material synthesis and technique for measuring function of matter have to be continuously supported and encouraged.

As a result of repeated reform charged, our traditional University system has changed. Research resources are centralized to several research universities, while others emphasis their peculiar character as their foci. In order to sustain the quality of research in Japan, utilization of the shared facility system has to be further encouraged. Especially experience and knowledge integrated through Nano-Platform project is of great importance. For mature society of S & T, acquisition of existing data and to utilize towards further development is of crucial importance. Shared facility could play an important role for the data acquisition as well.

Japan is facing a serious decrease in population. We have to be prepared for the expecting decrease which is crucial at present. Globalization is an indispensable measure, while preparation for accepting none Japanese to majority of our society is imperfect. Covid-19 brought us some positive effect as to promote borderless environment between countries. We have to be open minded and prepare for providing equal opportunity to people coming from other countries. Job market will become truly globalized.

<CV>
Director General, Institute for Molecular Science, Japan
Member, Science Council of Japan
Professor Emeritus, The University of Tokyo,
Honorary Scientist, RIKEN
Honorary Fellow, Royal Society of Chemistry
Fellow, American Physical Society

Degrees:

B. Sc. 1975	Department of Chemistry, University of Tokyo
M. Sc. 1977	Graduate School of Science, University of Tokyo
Dr. Sc. 1980	Graduate School of Science, University of Tokyo

Awards
Saruhashi Award, for Woman Scientist (1996), Japanese Surface Science Society Award (2005), The Commendation for Science and Technology by the MEXT (Research Category) (2008), The Chemical Society of Japan (CSJ) Award (2008), Mukai Award (2012), The IUPAC 2015 Distinguished Women in Chemistry / Chemical Engineering (2015), Gerhard Ertl Lecture award, Fritz-Haber Institute der Max Plank Society (2015), AVS Medard W. Welch Award (2016), Humboldt Research Award (2017), Medal with Purple Ribbon (2017), Honorary Fellow, Royal Society of Chemistry (2019), L'Oreal-UNESCO Women in Science (2019), Japan Academy Prize (2020).

Professional Experience

1980-85	Postdoc period: Contract Researcher at RIKEN, JSPS Fellow at The University of Tokyo, Assistant, Osaka Industrial Research Institute of MITI, Contract Researcher at Osaka Gas Co.,
1985-88	Researcher, Catalysis Lab., RIKEN
1988-91	TDK Professor, Tokyo Institute of Technology
1991-10	Chief Scientist, Director of Surface Chemistry Laboratory, RIKEN
2004-17	Professor, Department of Advanced Materials Science, The University of Tokyo
2010-15	Executive Director, RIKEN
2016 --	Director General, Institute for Molecular Science
2018-20	President, Chemical Society of Japan

The (U.S) National Nanotechnology Coordinated Infrastructure (NNCI) and ACCELNET: Global Quantum Leap; Models for International Collaboration and Cooperation.

米国における国際協調・協力モデル：
NNCI と ACCELNET、量子技術の飛躍的進展における世界協力

Lynn Rathbun, Ph.D.

Cornell Nanoscale Science and Technology Facility
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The National Nanotechnology Coordinated Infrastructure (NNCI, 2015-present) and its predecessor the National Nanotechnology Infrastructure Network (NNIN, 2004-2015) are the US counterparts to the Nanotechnology Platform Japan. NNCI/NNIN and the Platform/NIMS have had highly successful cooperative student programs since 2008. I will describe the history, development, and future of these programs. I am most appreciative of the long-term support of these programs by NIMS management.

In addition, members of NNCI have been recently funded by the National Science Foundation to form an international "network of networks", ACCELNET: Global Quantum Leap. This five-year program is focused on international cooperation and collaboration in the area of quantum information devices and materials. The Nanotechnology Platform Japan is one of our partners in this program along with several quantum networks in Europe. The program will support cooperation and collaboration between quantum research groups and the international nanotechnology user facilities-with particular emphasis on training and support for graduate students, post-docs, and young faculty. This will be accomplished through international student exchanges, short courses, conferences, and workshops as well as one to one faculty research collaborations. This program began Oct. 2020. Due to COVID-19, initial activities will be virtual, hopefully transitioning to in-person training and exchanges in 2022. We are open to suggestions from our network partners for effective activities and look forward to your full participation.

Lynn Charles Rathbun, Ph.D.

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Lynn Rathbun is a member of the senior management team of the Cornell Nanoscale Science and Technology Facility (CNF). In his capacity as Laboratory Manager he is responsible for daily management of one of the most advanced nanofabrication user facilities in the U.S. He has been at Cornell for over 40 years. He is most proud of his contributions to research training for undergraduate students through our REU program and for the international student training activities he has developed with Japan as well as several European countries.

Professional Preparation

1971	B.S. Physics	The Ohio State University, Columbus Ohio
1973	M.S. Physics	University of Illinois, Urbana-Champaign, Illinois
1979	Ph.D Physics	University of Illinois, Urbana-Champaign, Illinois

Appointments and Employment

1990-Present	Laboratory Manager, Cornell Nanoscale Facility, Cornell University
2016-2020	Assistant Director of User Program, PARADIM, an NSF MIP user facility at Cornell
2012-2015	Deputy Director, National Nanotechnology Infrastructure Network (NNIN), Cornell University
1994-2012	Program Manager, National Nanotechnology Infrastructure Network (NNIN), Cornell University
1985-1990	User Program Manager, Cornell Nanoscale Facility, Cornell University
1979-1985	Research Staff, National Research and Resource Facility for Submicron Structures/ National Nanofabrication Facility, Cornell University

OPTIMADE: a REST API for querying materials databases
OPTIMADE: マテリアルデータベースを操るREST APIの開発

Gian-Marco RIGNANESE

UCLouvain, Institut de la Matièere Condensée et des Nanosciences (IMCN),
Chemin des Ètoiles 8, Louvain-la-Neuve 1348, Belgium

Abstract

The Open Databases Integration for Materials Design (OPTIMADE) consortium aims to develop a common application programming interface (API) to make materials databases accessible and interoperational. In this talk, I will outline the latest released specification that is supported by leading databases such as AFLOW, the Materials Cloud, the Materials Project, NOMAD, OQMD, ... I will illustrate the API through some examples on materials databases that have implemented and made the API publicly available. I will discuss the challenges that were faced and the opportunities that it offers.

I. INTRODUCTION

In the last decades, a number of materials databases have become available online (see e.g. Ref. [1] for an extensive, yet inevitably incomplete, list). In many cases, these can be accessed via a graphical web interface which targets a "low-throughput" human usage but that is not very well suited for a systematic "high-throughput" computational approach. In fact, in order to take full advantage of modern data-analytics techniques, it is essential that these databases also become accessible through an application programming interface (API) as it is already the case for some of them [2-5].
It would actually be even more beneficial to have access to information originating from multiple databases as they often cover different material families and properties. Nonetheless, retrieving data from multiple databases is difficult since the available APIs are different from one database to another.

II. OPTIMADE

In order to overcome these difficulties, the OPTIMADE API was developed by the participants of the workshop "Open Databases Integration for Materials Design", held at the Lorentz Center in Leiden, Netherlands in October 2016, the CECAM in Lausanne, Switzerland in June 2018, June 2019, and June 2020. It is designed so that it can be implemented without significant changes to the established back-end code, and, furthermore, adopting the API is straightforward for the end user. The OPTIMADE API is queried through URLs, and the response adheres to the JSON API specification [6].
The OPTIMADE specification version 1.0.0 was released on 1 July 2020. The latest *stable* version is found in the master branch in the OPTIMADE GitHub repository [7]. The latest *development* version is found in the develop branch of the same repository. The databases that support the OPTIMADE API and the corresponding endpoints is published as an OPTIMADE Index Meta-Database [8].

The wider usage of the OPTIMADE API being a key goal for the consortium, two open libraries [9,10] are currently available to help users of the OPTIMADE API. Both libraries offer tools that aid the implementation of the API for materials databases, and the latter also contains tools to help a high-throughput tool compose queries.

In order to illustrate the differences between the current generation of APIs, I provide the queries that need to be used to request the records on the exemplar system of SiO_2 for AFLOW, COD, and the Materials Project, respectively:

http://aflowlib.duke.edu/search/API/?species(Si,O),nspecies(2)
http://www.crystallography.net/cod/result.php?formula=O2\%20Si
http://www.materialsproject.org/rest/v2/materials/SiO2/vasp/structure?API_KEY=YOUR_API_KEY
The three queries vary not only in format, but moreover differ in the fundamental philosophy behind the specification of the number of elements and species. AFLOW returns all structures with both Si and O present, COD returns those with 2 O and an Si, and Materials Project delivers systems containing SiO_2. The wide range of query formats that will deliver non-overlapping structures significantly complicates access to all available data for SiO_2. The distinction between the requests, that are different for each database, requires the user to become expert in many different APIs. This only again re-emphasises the need for a single well-designed and standardized API to access all materials databases, which is provided by the OPTIMADE API.

In contrast, the OPTIMADE API provides a holistic tool to access information any compatible materials database. Starting from the base URL that serves the OPTIMADE API (for example http://example.com/optimade/), the exemplar case of SiO_2 is accessed by appending
structures/?filter=chemical_formula_hill="SiO2"
The philosophy of the OPTIMADE query is to enable the structural formula to be specified in a straightforward and intuitive manner. A benefit of the OPTIMADE API is that the structure of the response is common to all materials databases. The responses differ only in the optional and database specific information preceded by the database name.

III. SUMMARY

The OPTIMADE API offers full access to leading materials databases providing researchers with an easy access to over 10,000,000 results for different materials. This opens new benchmarking opportunities whilst reducing repetition of calculations between databases and offers a huge opportunity for screening and machine learning studies. The ability of the OPTIMADE API to search databases, expose links between databases, and deliver multiple results makes it well-positioned to significantly enhance the impact of preexisting data silos. This should empower researchers to scan through new and unexpected material families, and train models from all available data that can understand deep correlations.

The OPTIMADE API is flexible and will be extended going forward. Proposed developments include the addition of more material properties, experimental results, and extensions beyond electronic structure calculations. The future development of APIs, including OPTIMADE, should herald an era of effective use of data-analytics techniques in the materials science.

References
[1] J. Hill *et al.*, MRS Bulletin **41**, 399-409 (2016).
[2] R.H. Taylor *et al*., Comput. Mater. Sci. **93**, 178-192 (2014).
[3] S.P. Ong *et al.*, Comput. Mater. Sci. **97**, 209–215 (2015).
[4] F. Rose *et al.*, Comput. Mater. Sci. **137**, 362–370 (2017).
[5] L. Talirz *et al.*, Sci. Data **7,** 299 (2020).
[6] http://jsonapi.org
[7] https://github.com/Materials-Consortia/
[8] https://providers.optimade.org/ ; https://www.optimade.org/providers-dashboard/
[9] https://github.com/Materials-Consortia/OPTiMaDe-Filter
[10] https://github.com/Materials-Consortia/optimade-python-tools

Gian-Marco RIGNANESE is Professor at the Ecole Polytechnique de Louvain (EPL) and Research Director at the F.R.S.-FNRS. He received his Engineering degree from the Université catholique de Louvain in 1994 and Ph.D. in Applied Sciences from the Université catholique de Louvain in 1998.
During his Ph.D., he also worked as a Software Development Consultant for the PATP (Parallel Application Technology Project), collaboration between CRAY RESEARCH and Ecole Polytechnique Fédérale de Lausanne (EPFL) in the group of Prof. Roberto Car. He carried his postdoctoral research at the University of California at Berkeley in the group of Prof. Steven Louie. In 2003, he obtained a permanent position at the Université catholique de Louvain.
In 2019, he was named APS Fellow for original efforts developing free license software in the field of electronic structure calculations, and high-throughput calculations in a broad range of materials types.

Gian-Marco RIGNANESE is especially active in high-throughput approaches collaborating to the Materials Project, computing:

- electronic and optical properties (bandstructure, band gap,…),
- vibrational properties (phonons, entropy,…),
- transport properties (effective masses, Seebeck coefficient,…).

Furthermore, he exploits machine learning to predict the properties of materials.

His group plays an active role in the development of different softwares (Abinit, Abipy, PyMatGen, FireWorks) and pseudopotentials through the PseudoDojo.

【Plenary Lecture / 基調講演】

“Transformation of Research Platform to create Future Society”

「研究現場のトランスフォーメーションによる研究力強化と未来社会創造」

Nobuyuki Osakabe (Hitachi)
長我部 信行（株式会社日立製作所）

Transformation of Research Platform to create Future Society
研究現場のトランスフォーメーションによる研究力強化と未来社会創造

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I. INTRODUCTION

There are strong concerns over the current capability in Science and Technology of Japan[1]. The growth rate of the number of scientific and technological publications and citations are said to be not enough and getting less predominate among those countries growing rapidly. Nevertheless, Nanotechnology is one of the area that Japan still has its leading position and also the very noticeable domain in science[2]. To keep its leading position, transformation of research platform in nanotechnology is mandatory for more productive research.

II. TRANSFORMATION OF RESEARCH PLATFORM

There are many argument why Japanese material R&D and industry has been in good position globally. One may think that the education in this field has been very successful as theoretical science and engineering to actually produce materials are well balanced and each researcher has deep scientific insight to develop new material of expected properties. One may also argue that devoted work of postdoctoral fellows and students enable the thorough investigation of materials around targeted composition. But these advantages has been becoming less dominant under the current demographic situation and global competitiveness. Thus, innovative approach to transform research methodology is required.

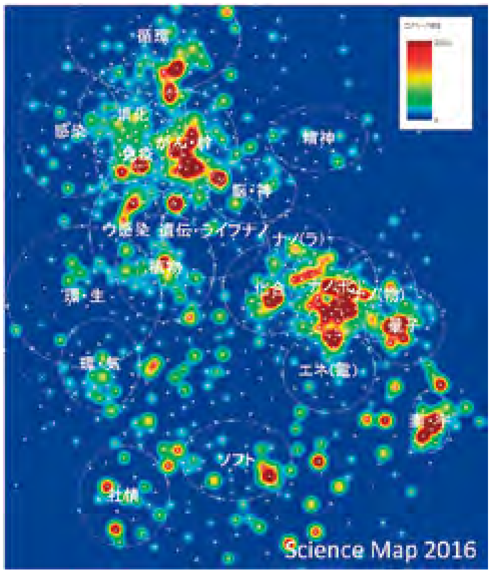

Fig. 1 Science Map 2016
Middle right red cluster shows nanotechnology .
Cited from reference[2].

JST-Mirai Program Common Platform is one of those trials to transform research platform. Some activities are presented in the lecture together with the global bench marking.

III. SUMMARY

Recent research in JST-Mirai Program shows that the whole potential material space so far explored is only a small portion of the total space, so that we still have plenty of uncovered area that may create better future society. We should strongly promote to construct competitive material research platform to fully utilize historically developed strength of this field.

References

[1] MEXT, "White Paper on Science and Technology 2020", (Nikkei Printing Inc., Tokyo, 2020).
[2] NISTEP, "Science Map 2016", NISTEP REPORT **178** (2018).

Dr. Nobuyuki Osakabe is currently CSO of Smart Life Business Management Division of Hitachi, Ltd. He also serves as Program Officer of JST-Mirai Program of Japan Science and Technology Agency. Prior to his current position he had been working as CSO and CTO of Healthcare Business unit in Hitachi, Ltd. He is also active in promotion of healthcare industry and is currently a Vice Chairman of Forum for Innovative Regenerative Medicine(FIRM).
Osakabe had been General Manager of Advanced Research Laboratory and Central Research Laboratory of Hitachi, Ltd. for 10 years, managing Basic Research and R&D closely related the business. Osakabe joined Hitachi in 1980 as a researcher specializing in holography electron interferometry, working with the late Hitachi Fellow, Dr. TONOMURA Akira. Verification of Aharonov-Bohm effect has been their representative achievement. He succeeded Tonomura as Acting Principle Investigator of the FIRST Project, which is designed for the top 30 scientists in Japan. Osakabe also serves on 7 committees of the MEXT, METI, and Cabinet Office of Japanese Government.

Session 2
【A Year After Coronavirus : Leave No R&D Behind ／ ニューノーマル時代の研究開発を考える】

“The Rise of Catalyst Informatics : Concepts and Applications”

「触媒インフォマティクスの基本概念と実例」

Keisuke Takahashi (Hokkaido University)
髙橋 啓介（北海道大学）

“Date-driven materials science based on high-throughput experimentation”

「ハイスループット実験を基盤としたデータ駆動型材料科学研究」

Toshiaki Taniike (Japan Advanced Institute of Science and Technology)
谷池 俊明（北陸先端科学技術大学院大学）

“Remotely utilization in the instrument for research (In Jobsite) : The current situation and the going forward”

「研究機器（現場）における遠隔利用の現状と今後」

Kazunori Arifuku (JEOL)
有福 和紀（日本電子株式会社）

The Rise of Catalyst Informatics: Concepts and Applications
触媒インフォマティクスの基本概念と実例

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DATA-DRIVEN MATERIALS SCIENCE BASED ON HIGH-THROUGHPUT EXPERIMENTATION
ハイスループット実験を基盤としたデータ駆動型材料科学研究

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Abstract

High-throughput experimentation (HTE) means to implement experiments in a highly automated and parallelized fashion. It is powerful in the field of materials science, where combining different atoms and molecules is a basic strategy for desired structures and properties. It also plays a pivotal role in materials informatics (MI), as materials data that are sufficient in size, distribution, and consistency (i.e. appropriate for machine learning) are often not present. Here, I deliver our recent efforts to exploit HTE for data-driven materials science.

I. INTRODUCTION
An effort to improve the throughput of experimental research starts from identification of rate-limiting steps from a set of relevant processes (e.g. synthesis, purification, property evaluation). An efficient protocol or instrument is introduced to resolve the rate-limiting factors. Such “KAIZEN” is continued while balancing with cost performance and a tradeoff between the accuracy and the throughput. Our group recently developed experimental protocols/instruments for HTE and applied them to the field of polymer and catalysis[1–4].

II. POLYMER STABILIZATION[1]
A potential solution for the plastic pollution problem is to limit the variety of used plastics and to maximize their reuse/recycle. For this, degradation of the plastics needs to be minimized by means of novel stabilizer combinations. However, such research has been hardly feasible due to a low throughput of polymer lifetime measurements and the problem of combinatorial explosion. We developed a high-throughput chemiluminescence imaging instrument that enables simultaneous lifetime determination for 100 samples in thermo-oxidative degradation. Using the said instrument, stabilizer combinations were successfully explored for polypropylene (PP). The research scheme is shown in Fig. 1. Briefly, 10 stabilizers were selected from a stabilizer library, and they were melt-mixed with PP at a fixed content. The performance of different combinations was determined based on the chemiluminescence imaging, and combinations were evolved through a genetic algorithm so as to elongate the lifetime of PP. The evolution over 6 generations produced the data corresponding to 5.5 years, which were used to extract rules of designing stabilizer combinations.

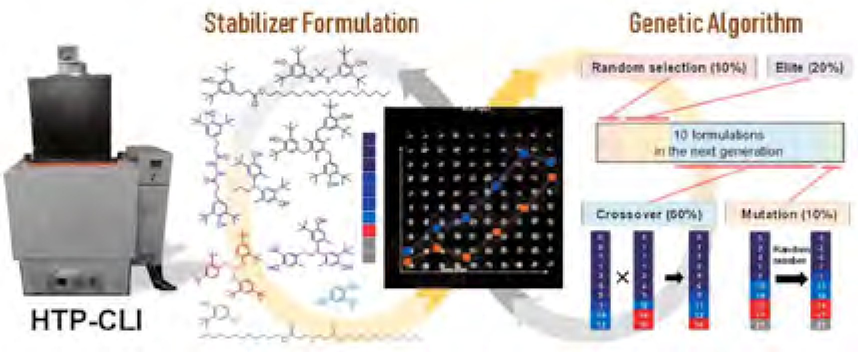

Fig. 1. Machine learning-aided stabilization of polymer.

III. CATALYST INFORMATICS FOR OXIDATIVE COUPLING OF METHANE[3]

One fundamental problem of implementing MI is the lack of a proper dataset. Data accumulated in the past largely reflect research interests and protocols of the corresponding ages and/or individual researchers. Hence, unrestricted correction of these data results in an unevenly distributed and inconsistent dataset, and vice versa. The said problem becomes the most impactful when MI is employed for catalysts, as they are generally sensitive to employed processes. In a recent publication, we have successfully developed a high-throughput screening instrument for enabling an automatic performance evaluation of 20 catalysts at a programmed series of conditions. The instrument was used to acquire the performance of 59 catalysts for oxidative coupling of methane (OCM) at 216 conditions, thus affording a total of 12708 data points within three successive operations. Analyzing the big data, important insights into catalysis and catalyst design were successfully manifested in a very short period of time (Fig. 2).

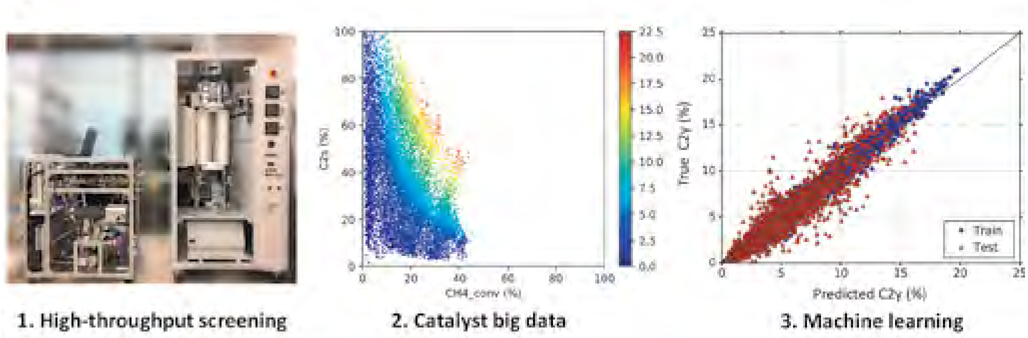

Fig. 2. Catalyst informatics base on high-throughput experimentation.

References

[1] T. Taniike, T. Kitamura, K. Nakayama, K. Takimoto, N. Aratani, T. Wada, A. Thakur, and P. Chammingkwan, *ACS Appl. Polym. Mater.* 8 (2020), pp. 3319-3326.

[2] A. Thakur, T. Hamamoto, T. Ikeda, P. Chammingkwan, T. Wada, and T. Taniike, *Appl. Catal. A Gen.* 595 (2020), 117508 (pp. 1-9).

[3] T.N. Nguyen, T.P.N. Tran, K. Takimoto, A. Thakur, S. Nishimura, J. Ohyama, I. Miyazato, L. Takahashi, J. Fujima, K. Takahashi, and T. Taniike, *ACS Catal.* 10 (2020), pp. 921-932.

[4] P. Chammingkwan, M. Terano, and T. Taniike, *ACS Combi. Sci.* 19 (2017), pp. 331-342.

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Remotely utilization in the instrument for research (In Jobsite) : The current situation and the going forward

研究機器（現場）における遠隔利用の現状と今後

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We can mention the working remotely as one of the requirement which is required to the research and analysis site on new normal generation. At that time, the issues are the security for instrument and operation for sample transportation or other. We have provided "The Screen sharing System" and "Working Remotely System" as way of solution for these issues. "The Screen sharing System": The instrument joins to the WEB meeting.

"Working Remotely System": Operating the instrument by remotely. And, we have expanded "WEB Contract and Sharing (Fig.1)" using these techniques in fact.

We introduce the concrete case in this session. And, we plan to expand to "WEB training and support" business or other by these technique in near future.

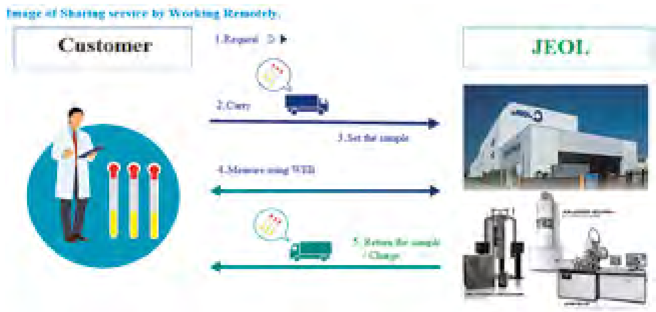

Fig. 1
The image of WEB Sharing in JEOL

Analysis technique is classified the qualitative analysis and the quantitative analysis roughly. The quantitative analysis is able to stylize and the automatize is fitted to it, but the qualitative analysis is not stylized and the Automize is very difficult to fitted to it. In analysis site, they are working the Preprocessing/Measurement/Processing the data to each analytical purpose for variously sample, therefore it's very difficult to be "Working remotely" and "Automize" of all process. When considering about research style in future, the directivity for open innovation becomes important, not self-sufficiency. We consider that the establishing the base which specialize in research and it needs the next step for "stylized" "Working remotely" "Automize". Analysis style is in a similar manner, we consider that doing "Method/Stylized " is the short cut to "Working remotely" and "Automize"

We have been convinced that "Working remotely" is the technique which connects to analysis base and it's high possibility to contribute to improve "Analisis productivity" and "Speed" as discussion tool for researcher and analst, not just network on instrument. (Fig.2)

In this session, we would like to suggest the current situation and going forward of the direction for the research and analysis site.

We hope that it will continue to be useful to you in the future.

Fig. 2
The going forward style of connecting to base of research and analysis site

Kazunori Arifuku, General Manager
Service Planning Promotion Division Field Solution Business Operations JEOL Ltd.

Session 3
【nanotech 2020 award lecture / nano tech大賞 2020 講演】

“Innovative Conjugate Spinning Technology NANODESIGN®”

「革新複合紡糸技術NANODESIGN®」

Masato Masuda (TORAY)
増田 正人（東レ株式会社）

Innovative Conjugate Spinning Technology NANODESIGN®
革新複合紡糸技術NANODESIGN®

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Abstract

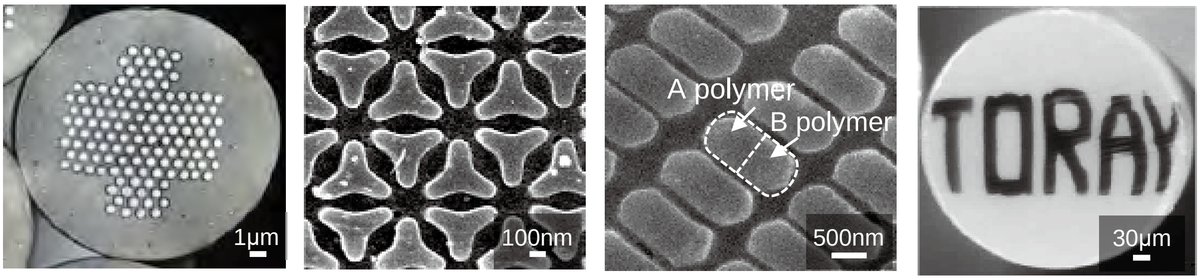
NANODESIGN® is an innovative conjugate spinning technology which produces fibers consisting of two or more different polymers while enabling to design the fiber cross-section with nano-scale. In this innovative conjugate spinning technology, polymer is divided into an enormous number of fine flows, and subsequently discharged and converged. It is thus possible to design the cross-section of conjugate fiber far more precisely than a conventional technology. This precise control of polymer flows can be applied not only to the nanofiber productions but also to the developments of a wide variety of fiber materials. We are advancing the development of highly functional apparel fabrics and high performance industrial products by this leading-edge technology.

I. Introduction

Fibers are used in a wide variety of products because of their useful thin and long shape. Especially, pursing the fineness of fiber is one of the most important subjects both academically and industrially. Nanofibers show nano-size effects that are not emerged in conventional fibers, because of their high specific surface area, nano-scale spaces between the fibers, etc. The sea-island conjugate spinning is one of the nanofiber production methods. We established this method in 1970's for producing continuous filament type ultrafine fibers[1)]. Ultrafine fibers consisting of island component can be obtained by removing the sea component from the sea-island conjugate fibers. In order to pursue the fineness of nanofibers by the sea-island conjugate spinning method, the number of the islands should be increased as large as possible, however, it was extremely difficult due to the processing limit of spinneret and the control of fine polymer flows divided in a spinneret.

II. Pursuit of ultrafine fiber technology

We were engaged in the research on the sea-island conjugate spinning and pursued the precise control of fine polymer flows to overcome above-mentioned technical issues. Finally, we attained the creation of innovative conjugate spinning technology NANODESIGN®, which can design the fiber cross-section with nano-scale. As a result, we succeeded in producing continuous filament type nanofibers which have 150 nm fiber diameter and homogeneous round cross-section[2)]. Furthermore, we also succeeded in controlling various cross-section shapes as shown in Fig.1. Therefore, we accomplished the world's first production of nanofibers with modified cross-sectional shape.



Fiber cross section with uniquely arranged islands | Fiber cross section with Y-shaped nanofibers | Fiber cross section with side by side nanofibers | Fiber cross section with Toray logo fiber

Fig.1 High precise conjugate fibers by NANODESIGN®

III. Developments and applications in NANODESIGN®

NANODESIGN® is a versatile spinning technology for advanced materials. This technology has so far been used to produce various fibers, such as “uts-FIT”: an ultra-fine side-by-side conjugate fibers [3], “Primeflex”: a stretch fabric with eccentric sheath-core conjugate fibers[4], “Nano-slit nylon”: a water-repellent nylon fibers in which microscopic slits run lengthwise on the fibers (Fig.2) [5], and “Kinari”: a light and airy silk-like texture with three-leaf clover shaped fibers conceived by natural silk (Fig.3) [6]. Furthermore, this technology can be used not only for clothing but also for medical applications.

Fig.2 Durable water-repellent textile “Nano Slit Nylon”

Fig.3 New feeling Polyester textile “Kinari”

References

[1] M. Okamoto, *Development of Advanced Fibers*, CMC Publishing Co., Ltd. (1988), pp213-222
[2] https://cs2.toray.co.jp/news/toray/newsrrs01.nsf/0/E5C87AF26F9490CA49257D0D0022E852
[3] https://cs2.toray.co.jp/news/toray/newsrrs01.nsf/0/CB1045BDA85268984925807B000B6CD6
[4] https://cs2.toray.co.jp/news/toray/newsrrs01.nsf/0/BD4F52C3AFCE9BAD492583450010471D
[5] https://cs2.toray.co.jp/news/toray/newsrrs01.nsf/0/B6BA4C8B14578E8B492583E40007CD30?open
[6] https://cs2.toray.co.jp/news/toray/newsrrs01.nsf/0/E22E649E8F10E229492584A3001E26B6?open

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Session 4
【Topics and future perspectives of nanotechnology platforms / ナノテクノロジープラットフォームの成果と将来展望】

“Digital transformation of materials research and development”

「マテリアル研究開発のDX化について」

Ministry of Education, Culture, Sports, Science and Technology
文部科学省

“Nano-scale analysis for development of materials”

「マテリアル開発につながる微細構造解析技術」

Takahisa Yamamoto (Nagoya University)
山本 剛久（名古屋大学）

“MICROFLUIDIC DEVICES FABRICATED BY FOUNDRY SERVICE AND THEIR APPLICATIONS TO LIFESCIENCE RESEARCHES”

「受託代行サービスにより作製した微小流体デバイスと
そのライフサイエンス研究への応用」

Ryuji Yokokawa (Kyoto University)
横川 隆司（京都大学）

“Structure Elucidation Support by the Crystalline Sponge Method”

「結晶スポンジ法による構造解析支援」

Takaaki Mitsuhashi (Institute for Molecular Science)
三橋 隆章（分子科学研究所）

Nano-scale analysis for development of materials
マテリアル開発につながる微細構造解析技術

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Abstract

So far, the nanotechnology platform for an advanced characterization branch at Nagoya University (hereinafter referred to as PF) have been working on various kinds of technical supports based on microstructure analysis using the equipment installed in the Ultra High Voltage Electron Microscope Center with full-time staffs of PF and the cooperation of technical personnel. The facilities installed at the center has characteristic equipment such as an environmental ultra-high-voltage electron microscope (HVEM), FIB-SEM and so on. HVEM can do in-situ observation and analyzation in various kinds of gas environment. FIB-SEM has a characteristic alignment of Ga ion and electron beams that enables us to do Cut & See observation easily. Here, we would like to briefly introduce the interesting two topics of the technical support we have done so far.

Devices that can decompose water with high efficiency using photocatalysts have attracted attention from the viewpoint of environmental conservation in recent years. Prof. Lippmaa's group at the University of Tokyo have succeeded in developing photoelectrochemical water splitting devices that can show high efficiency by incorporating characteristic Ir nanopillar structure in thin films. When $SrTiO_3$ thin film with the addition of Ir is homoepitaxially grown on $SrTiO_3$ substrate using pulsed laser deposition method, a nanoscale dot-like structure appears on the thin film surface. To confirm the inner structure of this dot-like structure, we were requested to analyze the structural analysis for their novel devices. As a method for preparation of thin foils for TEM observation, we adopted a thinning process by mechanical polishing using a precision polishing machine resulting in thickness about 10-20nm, and achieved the finish with Ar ion milling treatment of only about 5 minutes. Figure 1 show the cross-section and plane-view HAADF-STEM images of the sample. It's confirmed that a nano pillar is growing into the substrate vertically in $SrTiO_3$ film with 10nm in width. It can be seen that a nano pillar is growing slightly raised from $SrTiO_3$ thin film surface and its bottom contacts directly to the interface plane between thin film and substrate. Such characteristic structure had resulted in high efficiency of photoelectrochemical water splitting of this device. The results were reported in various media such as article of Nature Communication, Nikkei Technology and so on[1], and were selected as the top prize of the six selected best results of the nanotechnology platform in 2017.

There is another tectonic analysis support performed for lead-free solder material, which enabled the material to be on practical use as novel lead-free solder. In recent years, "lead-free solder" has been promoted from environmental problems, however, there is a major problem has been left in its durability. To overcome the issue, Napra Co., Ltd. have developed a new lead-free solder material using their intermetallic compound composite (IMCC) technology. The company has made to mix copper (Cu) etc. to Sn matrix at a fixed rate

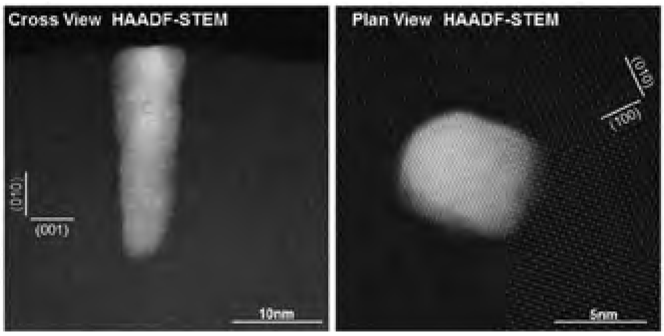

Fig. 1 HAADF-STEM images of Ir nanopillar grown in $SrTiO_3$ thin films.

using IMCC technique. In their lead-free solder, metallic Sn matrix particles are containing a functional particulate metal with a diameter of 10μm which forms the nano intermetallic compound. The IMCC particles have excellent thermal stability despite lead-free. Its functionality is characterized by surpassing the conventional lead solder. In this structural analysis support, Cut & See using FIB-SEM was carried out in order to clarify the reason for the thermal stability of IMCC particles. Figure 2 is an example of this. It was found that Sn-Cu intermetallic compounds present in β-Sn, and the compounds were localized with a bridge among Sn-Sn grains, alleviating distortions due to thermal shock. That Sn-Cu intermetallic compound was responsible for the "anchor effect" that suppresses structural changes from β-Sn to other phases with changes from low to high temperatures. The results of the technical support for microstructure analysis were reported in the Nikkan Kogyo Shimbun[2)] and selected as one of the six most excellent results of the nano platform in 2018.

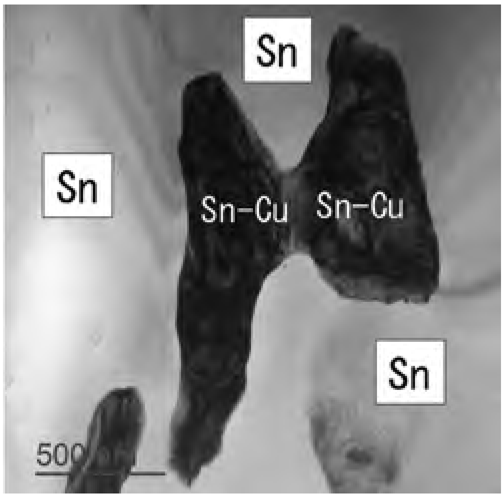

Fig. 2 TEM bright field image taken from IMMC lead-free solder.

Nine years have passed since the nanotechnology platform was launched as a national project by MEXT. It is a well-known fact that the state-of-the-art equipment for nano/sub-nano scale analysis has progressed rapidly, and the amount of capital investment has been increasing with the progress. Thus, it is clear that to keep a system sharing these state-of-the-art facilities and treating human resources with expert skills is an essential part of improving the research environment. The nanotechnology platform project, which was launched about nine years ago under this philosophy, is now widely recognized in Japan and overseas under the name of "nanoplat”. This attitude of "use of shared facilities" may suggest that it has begun to take root as a culture. We would like to cherish the word "nanoplat" as this brand.

References

[1] S. Kawasaki, R. Takahashi, T. Yamamoto, M. Kobayashi, H. Kumigashira, J. Yoshinobu, F. Komori, A. Kudo and M. Lippmaa, *Nature Comm*., 7 (2016), 11818.
[2] H. Ikeda, S. Sekine, R. Kimura, K. Shimokawa, K. Okada, H. Shindo, 2017 International Conference on Electronics Packaging (ICEP), pp. 171-176, (2017).

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MICROFLUIDIC DEVICES FABRICATED BY FOUNDRY SERVICE AND THEIR APPLICATIONS TO LIFESCIENCE RESEARCHES

受託代行サービスにより作製した微小流体デバイスとそのライフサイエンス研究への応用

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Nanotechnology platform at Kyoto University for nanofabrication has been providing many fabrication technologies for interdisciplinary researches. Compared to silicon-based micro/nano fabrications for MEMS applications, relatively simple structure and mechanisms are demanded in biotechnology applications. Foundry service at Kyoto University has accumulated experience to answer the demand through communication with lifescience researchers from various fields including biophysics, stem cell biology, developmental biology and biomedical engineering.

For the last couple of decades, micro/nano fabrication technologies have prevailed among many biological research disciplines. Expecting that micro/nano fabrications can be a powerful assay platform, many research groups have been focusing on applicability of fabrication technologies to multi-scale biomaterials from single molecule of RNA/DNA and proteins to cells and tissues. In this presentation, I will introduce the current status of foundry service at Kyoto University related to lifescience applications. Most of services have been initiated by a simple question from lifescience researchers such as “what if I can conduct a cell assay in a confined microenvironment?” and expansion of discussion about how staffs at nanotechnology platform realize it by fabrications.

My research group has been contributing to connect lifescience researchers and nanotechnology platform by conducting interdisciplinary researches. One of foundry service we used is a nanopatterning methods for motor proteins that contribute to their biophysical studies. We developed a molecular sorter to separate microtubules depending on their electro-mechanical properties [1,2], and to visualize motors and ATP at single molecule level [3]. More recently, nano-pillars were utilized to immobilize single individual motor proteins [4] and revealed that two different motor proteins behave differently [5].

Another example of foundry service is a simple PDMS microfluidic device fabricated by SU-8 mold, which was used to pattern endothelial cells for creating an on-chip vascular network that allows us to culture three-dimensional tissues. We developed an on-chip vascular network using human umbilical vein endothelial cells (HUVECs) and human lung fibroblasts (hLFs). The vascular network enables us to perfuse a spheroid for a long-term assay and evaluate angiogenic sprouts via applied shear stress [6]. The assay method was also applied to a tumor spheroid to evaluate the efficacy of an anti-tumor drug under a flow condition, which was not realized without the microfluidic device [7]. We have proposed several bioassays that create functional nanoscale systems and contribute to understanding of in vivo functions of motor proteins and endothelial cells. We keep exploring how micro/nano fabrications can deepen science both at molecular and cellular scale.

References
[1] N. Isozaki *et al*., ***Sci. Rep.***, 5, 7669, 2015.
[2] N. Isozaki *et al*., ***Sci. Robot.***, 2, 10, eaan4882, 2017.
[3] K. Fujimoto *et al*., ***ACS Nano***, 12, 12, 11975–11985, 2018.
[4] T. Kaneko *et al*., ***Nanoscale***, 11, 9879-9887, 2019.
[5] T. Kaneko *et al*., ***Sci. Adv.***, 6, 4, eaax7413, 2020.
[6] Y. Nashimoto *et al*., ***J. Vis. Exp.***, 134, e57242, 2018.
[7] Y. Nashimoto *et al*., ***Biomaterials***, 229, 119547, 2020.

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Structure Elucidation Support by the Crystalline Sponge Method
結晶スポンジ法による構造解析支援

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Abstract

The crystalline sponge (CS) method is a unique and powerful approach for the structure determination of molecules.[1] Since the structure determination is essential technique for the nanotechnology, the CS method would greatly accelerate the research and development in the field of nanoscience. In this presentation, I will talk about (i) an overview of the CS method, (ii) how we support researchers in the nanotechnology platform program, and (iii) future perspectives regarding the relationship between the CS method and the data-driven development of new materials.

I. What is the CS Method?

The CS method is a unique way to subject compounds of interest to the X-ray crystallography. The X-ray crystallography is known as one of the most reliable approaches to analyze the chemical structures of molecules. But, there is a serious limitation. Crystallization of the target compounds is required. Since there is no certain way to crystalize the molecules, the crystallization is laborious process, and takes a long time. However, by using the CS method, we can overcome this difficulty, because this method enables the "crystallization-free" X-ray crystallography (Figure 1). In the CS method, the molecules of interest are not crystalized but introduced into crystalline porous organometallic complexes. Since the introduced molecules can be neatly aligned in the porous complex, we can observe the structure of the introduced molecules by the X-ray analysis.

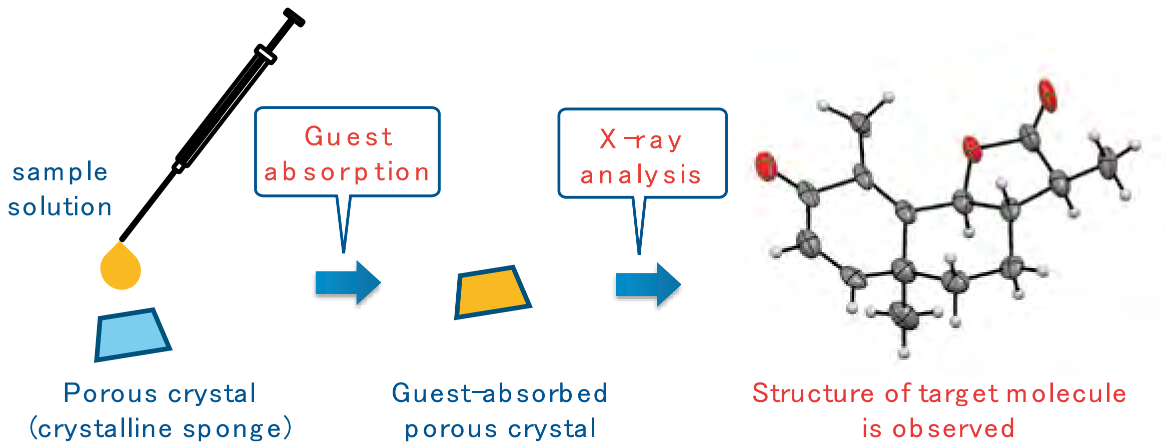

Fig. 1
The overview of the CS method.

II. Structure Elucidation Support by the CS Method in Nanotechnology Platform Program

We supported researchers (users of this program) from various research fields such as synthetic chemistry, natural product biosynthesis, and chemo-enzymatic synthesis, analyzing the structure of compounds, which they are interested in. Additionally, some users stayed our lab for several months and learned how to carry out the CS method.

III. Future Perspectives: Data-driven Approach would Improve the CS Method

It is worth noting that the porous organometallic complexes, which is used in the CS method, is a kind of materials. The most frequently used complex is composed of 2,4,6-tris(4-pyridyl)-1,3,5-triazine (**1**) and zinc halide (Figure 2). This complex has a great ability to neatly align the introduced molecules in its pore. However, for the further improvement of the CS method, development of new porous crystals is required. I believe that the data-driven approach using the big data and AI would be helpful for the development of the new porous crystals for the CS method.

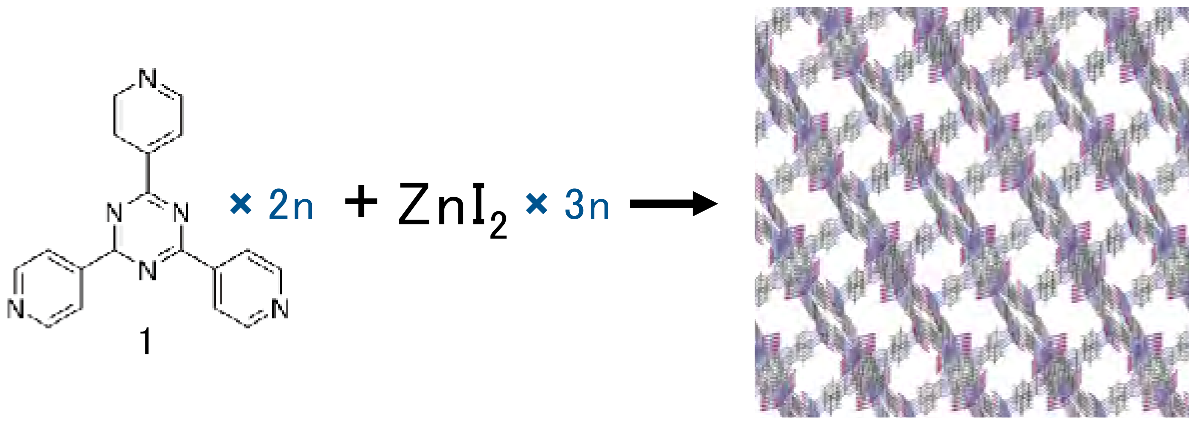

Fig. 2
Porous crystal, which is frequently used in the CS method.

References

[1] Y. Inokuma, S. Yoshioka, J. Ariyoshi, T. Arai, Y. Hitora, K. Takada, S. Matsunaga, K. Rissanen, M. Fujita, *Nature* **2013**, *495*, 461 – 466.

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電子情報通信学会	The Institute of Electronics, Information and Communication Engineers
ナノ学会	The Society of Nano Science and Technology
ナノテクノロジービジネス推進協議会	Nanotechnology Business Creation Initiative
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