Research area in the strategic objective "Creation of innovative catalysts using diverse natural carbon resources"

6.2.11 Science and Creation of Innovative Catalysts

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Overview

In the modern society, oil is the principal carbon resource in the production of feedstocks that can be converted into chemicals and energy. To make efficient use of resources other than oil, such as methane and the lower alkanes which form the main constituent of natural gas, the creation of highly advanced technologies based on new ideas will be required.

This research area aims to create innovative catalysts that efficiently convert methane and lower alkanes into chemical feedstocks and energy.

Specifically, this research area will conduct research leading to the design and creation of advanced catalysts in reactions that can efficiently convert methane and the lower alkanes. Research on a wide range of catalysts will be promoted in this research area. Catalyst types can be homogeneous, heterogeneous or microorganisms. Metals, oxides, metal complexes and organometallic complexes, molecules, proteins, and etc. can take various structures, such as nanoparticles, nanowires, nanosheets, porous materials, cage-types, core-shell types. Also, research into external reaction fields such as light, plasma, and electric fields can be included in the scope of this research area.

This research area aims to pioneer new methodologies in nanotechnology and materials research for catalysts, through the collaboration with fields such as computational science and evolving measurement technologies, and to promote original and challenging research that could become the new mainstream science and transform the chemical industry in the future.

Research Supervisor's Policy on Call for Proposal, Selection, and Management of the Research Area

1. Background

Modern society produces feedstocks that can be converted into basic chemicals, other chemical products, and energy with oil as the main carbon resource. But to improve the management of resource and energy, it is necessary to use low cost resources such as natural gas in addition to oil to produce feedstocks that can be converted into basic chemicals other chemical products, and energy.

However, in existing industrial processes that uses methane as a resource, which is the most abundant of natural gas, chemical feedstocks are produced indirectly via syngas ($CO+H_2$) . The production of useful basic chemicals and other chemical products directly from methane is extremely difficult, and industrial processes have not been developed. On the other hand, direct conversion of lower alkanes into useful chemical is easier compared to

methane. For this reason, it is predictable that only groundbreaking, innovative processes will become substantial candidates to replace the existing industrial processes. Many countries already started the development of new processes under the slogan “valorization of low value carbon”. The realization of innovative catalysts and processes that can directly convert methane and the lower alkanes into useful chemicals would have a very high international impact, but it will also require the development of highly advanced technologies. These advancements can lead to the dawn of a new “gas-based chemical industry” using natural gas resources, just as the Haber-Bosch process -that achieved the synthesis of ammonia- realized the nitrogen fixation, and the Ziegler-Natta catalyst for polymerization of olefins boosted the modern oil-based industry. In addition, it is expected that the development of innovative catalysts can contribute to a large energy reduction in existing chemical industrial processes. Furthermore, there is a high expectance from the society, regarding the establishment of industrial processes that can convert abundant natural resources other than carbon, such as air and water into basic chemicals.

2. Policy Concerning Selection and Screening

The target of this research area is not simply an extension of research to date, or a combination of existing research principles, or research towards improvements on existing technologies. Bearing in mind the background above, this research area will promote research leading to the design and creation of innovative catalysts based on original ideas and concepts with reactions that can efficiently convert methane and the lower alkanes to basic chemicals, other chemical products and energy. Research proposals which target reagents other than lower alkanes can be accepted, on the condition that they might generate high versatility, and can be applied to processes that involve lower alkanes in the future. In this way, this research area aims to pioneer new methodologies in the research of nanotechnology and materials for catalysis, and pursue unique, challenging research that could become the new mainstream science and, transform the chemical industry in the future.

While the types of catalysts and target reactions included in the scope of this research area are listed in the following, this research area will widely accept research proposals which do not fall into these lists, if they might contribute to the creation of innovative catalysts that can surpass the performance of existing catalysts. In addition, research proposals regarding actual systems based on measurement technologies and computational science are welcome.

1) Types of catalyst

This research area will accept proposals about all type of catalysts, whether homogeneous, heterogeneous or microorganisms. Research proposals about a wide range of catalysts including metals, oxides, metal complexes and organometallic complexes, molecules, proteins and other active substances, taking various structures such as nanoparticles, nanowires, nanosheets, porous substances, baskets, core shells are included in the scope of this research area.

In addition, considering catalysts in a broad sense, research proposals including processes and reaction fields that have not been used in the conventional chemical industry, such as light, plasma, electric fields, etc., will be pursued. Research approaches regarding plant engineering which can contribute to highly improve the efficiency of catalytic reactions are welcome.

Priority will be given to highly original research on nanotechnology and materials that has the potential to change the chemical industry in the future.

2) Target reactions

In this call for proposals, there are not restrictions concerning the type of reaction. This research area will welcome proposals concerning groundbreaking catalysts that can convert methane as a reactant directly and efficiently into useful basic chemicals and chemical products such as methanol, olefin and aromatics. On the other hand, ethane, propane and other lower alkanes show greater reactivity than methane, and their chemical activation have been widely investigated. Therefore, proposals concerning reactions using ethane, propane and other lower alkanes as reactants will be considered only if the activity and/or the selectivity of the reaction are innovatively high compared to the existing ones.

Proposals targeting reactants other than lower alkanes will be accepted under the condition that the proposal is innovative, can overcome existing concepts and technologies, and is expected to create high versatility and possibility of application into processes targeting lower alkanes in the future.

3. Selection policy

The target of this research area is not simply an extension of research to date, or a combination of existing research principles, or research towards improvements on existing technologies. It is expected that researchers will seek genuinely innovative new approaches to achieve the activation of methane and lower alkanes. For this reason, the applicant is asked to describe the trends in international research and indicate the superiority and originality of the research proposal compared with research to date.

It is expected that the researcher achieves the targets set for the PRESTO (“Sakigake”) research during the approximate research period of three years, but at the same time, it is expected that this PRESTO research can become an important foundation in the careers of the researcher. This research area is looking for research themes that could become the mainstream of new science, and the wellspring of science and technology innovation. Since it is expected that the researcher him/herself achieves a significant advance during the period of the PRESTO program, this research area will select only proposals that that strongly reflects the purpose of the PRESTO program. In other words, greater expectations will be placed on proposals containing new concepts developed by the individual researchers themselves, rather than the research concepts of the laboratories to which they were affiliated.

In 2016, a wide variety of catalyst types and reaction mechanisms were adopted based on the above selection policy. Especially we adopted several proposals based on advanced measurement methods modeling the real catalytic systems, theoretical approach, and process engineering. Such proposals are strongly expected to promote collaborative researches in this research area. For 2017, this research area will continue to welcome original and challenging proposals widely this year and especially expect proposals in the following subject:

・Challenges to extremely difficult conversion reactions such as methane direct reforming which can produces hydrogen and withdraws aromatic compounds or steam methane reforming which can contributes effective hydrogen production by lowering the reaction temperature.

・Catalyst creation based on measurement methods modeling real catalytic systems such as operando XPS using synchrotron radiation or XAFS study in the high pressure and high temperature environment.

・Catalytic property prediction based on advanced numerical simulation using kinetic theory or first-principle calculation and data-driven informatics.

・Innovative reaction system based on equilibrium shift such as separation technology or process engineering.

While it is desirable that research proposals regarding new catalyst substances or materials show preliminary experimental results, if the research proposal is still in the concept phase and lacks of experimental data, please provide information on the validity of the research proposal and how it complies with the purpose of this research area. For example, it is recommended that the research proposals include thermodynamic and kinetic considerations on the targeted reactions. In addition, please indicate how and when the applicant will verify the relevant catalytic function of the target substance or material. Moreover, if it is difficult for the researcher him/herself to verify the catalytic activity, it will be acceptable to the researcher to cooperate with another party, but it is a condition that the researcher him/herself conducts the experiment in accordance with the purpose of the program.

In this research area, cooperation with other researchers with the aim of maximizing the research output is recommended. Therefore, please state in the research proposal, the information on the cooperating researcher, the nature of the collaboration, and the expected results. However, please note that since this project aims to support individual researchers, there is no allocation of research expenses for other cooperating parties.

Although research proposals focused on the development of analysis and prediction methods of catalytic reaction using data science, theoretical calculation and measurement methods must also be established as individual research themes, the researchers in this area will be required to collaborate actively with other research themes selected in this research area.

Also, this research area will consider providing opportunities for discussion and collaborations with researchers participating of the PRESTO research area “Establishment of Basic Technology for Advanced Materials Informatics Integrating Theoretical, Experimental and Computational Science” starting in 2015. Moreover, active

collaboration will be promoted with the CREST research area “Innovative Catalysts and Creation Technologies for the Utilization of Diverse Natural Carbon Resources” undertaken under the same strategic goals.

Moreover, according to the progress in the research, collaboration and cooperation with research institutes and programs nationwide, such as the MEXT’s “Nanotechnology Platform Japan” will be promoted.

4. Research area management and fostering of young researchers

It is expected that the researchers who are selected for this research area will fully understand the social background of their research, and will develop their own PRESTO research, growing into researchers who are able to support future collaboration with industry. Consequently, the participating researchers are required to consider the acquisition of intellectual property during the research period.

In addition, over the six years that the research area will continue, it is expected that the participating researchers will be able not only to advance their own research significantly, but also, to contribute to the development of the research area through discussion and collaboration with researchers participating in the related PRESTO and CREST research areas.

No briefings on the call for proposals will be held on 2016. For more information on this year’s policy, download the renewed briefing material (PDF) from the following URL “ http://www.senryaku.jst.go.jp/teian.html “ (Japanese only)