Research area in the Strategic Objective “Creation of innovative catalysts using diverse natural carbon resources”

6.1.10 Innovative catalysts and creation technologies for the utilization of diverse natural carbon resources

Research Supervisor: Wataru Ueda (Professor, Department of Material and Life Chemistry, Faculty of Engineering, Kanagawa University)

Overview

This research area will promote the creation of innovative catalysts that can convert methane and other alkane gas resources to useful chemicals and energy, in order to progress towards the establishment of an industrial infrastructure that can make balanced use of diverse natural carbon resources. If new technologies can be used to convert methane, alkane and other natural gas resources easily into chemicals and energy, it will be possible to decrease our current dependence on oil, and to reduce carbon dioxide emissions. However, since it is difficult to convert methane and other alkane gas resources directly to chemicals, existing processes are indirect, for example *via* syngas ($CO + H_2$) generated by methane reforming.

The keynote object of this research area is to overcome this difficult task by pursuing new approaches to create advanced catalyst technologies. It is aimed to achieve a significant jump on the accumulated experience value on catalysts, by engaging with data-intensive science, computational science, and measurement technologies that have made advances in recent years.

This research area will focus on research themes using methane as a reactant. Research themes regarding reactions using ethane, propane and other lower alkanes as reactants will be promoted only if they show higher activity and/or selectivity compared to the existing ones.

It is aimed to promote genuinely world-leading catalyst researches that aim at pioneer new uses for resources such as natural gas in the future chemical industry, and lead to the establishment of a new industrial infrastructure.

Research Supervisor’s Policy on Call for Application, Selection, and Management of the Research Area

1. Policy Concerning Recruitment and Screening

(Background)

In the near future, it is anticipated that a new framework will emerge making balanced use of various carbon resources. Of these, alkane gas resources such as methane have the potential to become a major resource. The coasts around Japan are rich in methane hydrate, while neighboring Russia and China have locations with extensive natural gas and shale gas resources, but there are technical restrictions on their exploitation at present. If these alkane gas resources can be used at a similar level to oil, it will be possible for Japan strategically leverage a new carbon resource balance structure. Also, it can lead to new chemical industries, and permit to address environmental issues at a different level than before, by enabling the development of direct methane fuel cells, or by boosting the use hydrogen, for example.

What is now required is novel chemical technology that enables us to make the best use of alkane gas resources. Catalysts are the key, because catalysts are indispensable for the chemical processes for exploiting massive alkane gas resources that have low reactivity. However, adhering to conventional energy consumption processes such as steam reforming of methane alone will not be sufficient in the new age. Outstripping the conventional system is required. In order to replace old technologies, highly advanced and innovative catalysts should be developed that can be used in low-environmental-impact processes with the maximum efficiency using alkane gas resources, or that can make the reaction unidirectional (for example, direct synthesis of methanol from methane through low-temperature activation). It will be necessary to eschew earlier petrochemical catalyst technological deployment in favor of catalyst chemistry and technologies integration.

The methodologies for creating new states of matter from approaches such as nano-integration and hyper-nano-space structures have big potential to leads the development of solid or molecular catalysts with new functions. These approaches are anticipated to bring about the innovation of catalyst chemical technologies for the use of methane gas resources. In particular, in the reaction of methane, it is necessary for catalyst to activate the site which is made up of active element, and to activate molecule through a broad reaction field. It is essential to remove only product from reaction field, too. These can be seen from the enzyme reaction study. We need an aggressive effort to construct a reaction field with an artificial catalyst. At the same time, using innovative reaction process engineering is also an important initiative. However, it is also important to focus on approaches using new substances even in simple structures that can lead to unprecedented catalytic functions. The reason for this is that there are many materials that have yet to be considered for catalysts. It is aimed to achieve a significant jump on the accumulated experience value on catalysts, by engaging with data-intensive science, computational science, and measurement technologies that have made advances in recent years, to usher in a new age.

This research area will target the development of unconventional research concept leading to novel catalytic function domains. Four approaches are shown below as examples. It is imperative to use methane as the major reactant, and to present and design the catalyst with high potential after fully incorporating the characteristics of methane. In order to demonstrate the innovation of the concept, alkane gas resources such as ethane and propane should be used; at the same time, the prospects of using methane reaction should also be investigated.

Example 1. The creation of innovative catalysts through the establishment of new state of matter

The aim is to introduce new states of matter (unstable valence, three-dimensional atomic arrangement, complex structures, assemblies and so on) in substances (zeolite, complex or other element classes and their constituents) that already exist as catalysts, achieve catalytic reactions with alkane gases such as methane, and develop methods for synthesizing new substances and methodologies for conferring catalytic functions. This is the most important approach for creating innovative catalysts, and it is hoped that the researchers will actively apply themselves to the creation of catalytic functions with the original design concept of the catalyst.

Example 2. Creation of molecular assembly catalysts with superior functions

To create molecular assembly catalysts, such as complex, cluster, in order to establish a chemical process that can exploit massive alkane gas resources it will be necessary to establish a catalyst that mimics natural enzyme systems and that can outstrip the functions of enzymes. For this reason, in addition to activation functions already studied to date, creating new molecular assembly catalysts where reaction-promoting fields can be created by the formation of multiple interactions domains may be promising.

Example 3. Understanding the dynamism of catalytic reactions and using that for innovation in catalysts

Catalytic substances always possess dynamism, dynamically changing the reactants or products, involving phenomena that are not normally familiar in materials research other than catalysts. In particular, catalytic oxidation is one example that is strongly affected by this phenomenon. Controlling this dynamism is one of the greatest difficulties in creating catalysts, and it is one reason why the study of new substances as catalysts does not lead to immediate results. While it is necessary to pursue research into catalytic substances selected with a strong awareness of this important point, awareness alone is not sufficient to overcome this difficult challenge. What is required is academic development that clarifies the substance structures that ensure dynamism. This involves establishing computational science for dynamism, in-situ observation and measurement of dynamism, and the catalytic substance structure—dynamism correlation. Going further, it will be necessary to tackle computational science and measurement technologies, clearly targeting the methane catalyst chemistry mentioned above. Working with other groups by providing this information for other research, for example, into creating new states of matter, is expected to contribute to the realization and innovation of each catalyst.

Example 4. Search for new catalytic materials based on unexplored substances

It is aimed to break away from the conventional exhaustive material research approach that clings to existing catalyst configurations, and seek to develop technologies for creating innovative catalysts. Specifically, all of the substances and materials that have already been studied as catalysts from among the many research fields will be excluded, and then, new catalytic substances will be searched among the remaining unexplored materials and substances. In other words, continuous development based on existing knowledge will be precluded.

However, in order to search efficiently for new catalytic substances that are suitable as catalytic targets from among enormous groups of substances, it is essential to establish innovative research methods that eschew the research approaches of conventional catalyst chemistry. For example, research proposals in which measurement technologies and materials informatics, which have evolved in recent years, take the lead in the creation of innovative catalysts will be recommended.

To develop a catalyst construction methodology that can precisely control the local environment at the element and space levels, knowledge gained from other research fields is also required. Therefore, active participation by researchers of fields other than the catalyst is also desirable.

(Policy for this fiscal year)

In this research field, we invite research applicants who can help design an innovate catalyst for the chemical conversion of alkane gas resources, as represented by methane, under the above-mentioned research concept. Thus far, we have accepted two new challenges for creating an enzyme system and one challenge for creating complex catalysts, conducted four studies on creating innovative catalysts using solid based catalysts, and provided cross-cutting support to researches covering both this research field and the PRESTO area from the viewpoint of computational chemistry, thus establishing a system that ensures organizational deployment of the catalyst. To further extend the field of study for the use of methane gas resources in the current fiscal year, we have developed a policy that promotes studies on catalyst development, focusing on the creation of new catalysts and their methodologies.

The following are some examples of research topics: complex-based substances, zeolite functional materials, and functional porous materials such as MOF, composite oxides, hybrid structures, and cluster substances. Another research topic is the construction of a reaction field that can activate molecules to induce the reaction and helps in the effective mass transfer of the products and also provides necessary electrons or ions. In addition, we will call for proposals for research aimed at building a catalyst informatics program to create a new catalyst through development of materials informatics and the like. Furthermore, we will invite research proposals regarding an innovative catalyst creation method focused on the understanding, sophisticated analysis, and prediction of the dynamism of catalytic functions in an environment near that of a real catalyst and based on onsite observation and measurement using environmental TEM or radiation. It should be noted that, with this proposal, we expect a “team for catalyst measurement and evaluation” to be formed that is capable of transversely supporting the research from the perspective of measurement and evaluation in the present research area and PRESTO area.

We welcome ingenious researches with specialization in different fields, and not just limited to the field of catalyst, under an elaborate research strategy to help create innovative catalysts. In addition, applicants are expected to collaborate between various fields and to have strong research capabilities to be able to continue research in spite of the challenges.

In this research area, the keynote object will be research using methane. Research themes regarding reactions using ethane, propane, and other lower alkanes as reactants are desired that contain theories and objectives leading to the potential application of methane reaction.

This research area will be managed taking into consideration the cooperation with the related CREST and PRESTO research areas, so the applicant should keep that in mind when building the team.

2. Research area management policy

This research area will pursue high-level research aimed at cooperation with future industries under the leadership of a research director. Even during the research period, research cooperation with the industry that would lead to the creation of catalysts that can convert alkane gas into useful chemicals and energy will be recommended.

The management policy of this research area is to optimize the research plan for each research project through budget allocation, proper research team building and so on, based on international research and development benchmarking.

In addition, measures to enable cooperation with the PRESTO "Science and Creation of Innovative Catalysts" for the creation of innovative catalysts for methane and other alkane gas resources to be inaugurated at the same time, and the PRESTO "Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-centric Sciences" addressing materials research focused on calculation based on theory and data-intensive science will be considered.

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.

Notes

This research area is setting an upper limit for research expenses of three hundred million yen per research project.