Research area in Strategic Objective *“Precision control of bonding and decomposition for resource recycling"*

Precise Material science for degradation and stability

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Overview

In this research area, we will develop methods to freely decompose materials by external stimuli, develop materials whose decomposition can be easily controlled, research on the functionalization of these materials by controlling their hierarchical structures, and environmentally friendly methods to control degradation and stabilization of materials. The goal of this research area is to achieve precise control of decomposition, degradation, and stabilization of materials, as well as to establish precise materials science for the development of sustainable materials with freely controllable degradability and stability, which are the ultimate contradictory physical properties of materials.

Materials focusing on this project include polymers, organics, biomaterials, inorganics, metals, and their composites. For example, (1) method for reusing materials by transforming them into intermediate and substructures as well as atomic and molecular levels through external stimuli, a manufacturing process for materialization based on this method, and the design of sustainable materials whose decomposition products are environmentally friendly; (2) development of materials that combine decomposition functions with control methods for decomposition and degradation at multiple levels, including the molecular level and higher-order structure of materials; (3) development of visualization methods for material decomposition processes using spectroscopic methods, advanced separation methods such as chromatography, diffraction/scattering methods, microscopic methods, and computational science methods, and utilization of materials information through data accumulation; and (4) development of materials that combine the decomposition function with highly efficient self-healing of degraded areas.

We aim to systematize "materials science of decomposition, degradation, and stabilization" as a new academic area by understanding it from the molecular level to the macro level in a multilevel manner by fusing the collaboration of various research fields and the knowledge obtained from various materials, in order to develop sustainable materials that are indispensable for the realization of a sustainable recycling society.

<u>Research Supervisor's Policy on Call for Application, Selection, and Management of the Research Area</u>

1. Background

Polymers which include plastics and fibers, organic, biological, inorganic, and metallic materials as well as their composite materials are widely used and consumed in large quantities in all aspects of modern society. There is no doubt that these materials are extremely beneficial to our society. On the other hand, concerns about the environmental impact of chemical substances, whether intentionally or unintentionally released, such as plastic waste and microplastics, are becoming increasingly apparent. As a result of these social problems, there is a growing interest in reusing materials rather than disposing them. The development of materials that they can be decomposed into raw materials and intermediates after use is desirable. To develop such materials, it is critical to scientifically understand material decomposition, degradation, and stabilization, as well as to easily control decomposition and stability, which are the ultimate contradictory properties of materials. In Japan, the science of materials creation, as well as organic and polymer synthesis for bond formation, has traditionally been a strong research area, and knowledge in related fields is accumulated through related strategic basic research programs of JST and new academic area research as seed research. According to the white paper "Science to Enable Sustainable Plastics" compiled at the 8th Chemical Sciences and Society Summit in 2019, "understand the impact of plastics throughout their life cycles", "the development of new sustainable polymeric materials", "switching of polymeric material degradation", and "closed loop plastics recycling " have been identified as important challenging research issues for now on, and international attention in this field is increasing. In this research area, we aim to contribute to the realization of a resource-circular society by developing fundamental science of degradation, deterioration, and stabilization that transcend the boundaries of various material species.

2. Principle of invitation project and selection

(1) Basic principle

This research area aims to achieve precise control of material decomposition, degradation, and stabilization, as well as to establish precise materials science for the development of sustainable materials that enable flexible control of degradability and stability, which have the ultimate contradictory properties. Polymers, organics, biomaterials, inorganics, metals, and their composites are target material in the research areas. Also, the proposal based on surface chemistry, catalysis chemistry, environmental science, analytical chemistry, chemical engineering, adhesion science, and computational science are highly appreciated. We aim to systematize "materials science of decomposition, degradation, and stabilization" as a new academic field by focusing on hierarchical structures with different sizes from molecular to macro levels and on the time scales of decomposition and stabilization over short to long periods of time, by fusing the collaboration of various research fields and the knowledge obtained from various materials. Therefore, it is recommended that the research proposal outline your research strategy and plan for leading the materials science of decomposition, degradation, and stabilization of sustainable materials.

(2) Research fields assumed

This research area aims to achieve precise control of decomposition, degradation, and stabilization of materials, as well as to establish precise materials science for the development of sustainable materials that enable flexible control of degradability and stability.

a. Methods for reusing materials by transforming them into intermediate and substructures as well as atomic and molecular levels through external stimuli, a manufacturing process for materialization based on this method, and the design of sustainable materials whose decomposition products are environmentally friendly;

There is a need for materials that are as stable in use as existing commercial materials, and that can also be recycled after use, not only at the atomic or molecular level, but also into intermediate or substructures. Research proposals for materials that decompose in a short period of time when external stimuli are applied to the material, derived from sustainable raw materials and processes, are expected. Research proposals are also important for sustainable and efficient physical and/or chemical separation technologies involving homogeneous and heterogeneous interfacial stripping/separation methods, phase separation methods, and decomposition process methods.

b. Development of materials that combine decomposition functions with control methods for decomposition and degradation at multiple levels, including the molecular level and higher-order structure of materials;

Chemical bonds are cleaved during the environmental and mechanical degradation of materials. Amorphous regions are damaged if the material has a crystalline and amorphous molecular aggregation states, and easily degradable components or interface regions are damaged if the material has a multiphase structure. These phenomena are dependent on the presence or absence of UV light irradiation, which triggers decomposition and degradation, sorption of chemicals, action of enzyme, microorganism adsorption, and mechanical stimulation during degradation. Research proposals are expected to design materials with precisely controlled decomposition that take these factors into account using sustainable raw materials and non nontoxic degradation products. On the other hand, controlled decomposition of thermosetting resin and network polymer is important research field.

c. Establishment of visualization methods for material decomposition processes using spectroscopic methods, advanced separation methods such as chromatography, mass spectroscopy, diffraction/scattering methods, microscopy, and computational science methods, as well as utilization of informatics through data accumulation;

Recent remarkable advances in measurement technology have enabled in-situ observations in a variety of environments. Spatio-temporal multiscale, in-situ structural analysis during decomposition and degradation processes is particularly important for elucidating degradation and stabilization mechanisms. Research proposals are welcomed for the study of visualize decomposition and degradation process in a degraded environment with various impurities and contaminations, using infrared absorption spectroscopy, Raman scattering spectroscopy, X-ray scattering, scanning force microscopy, optical microscopy, etc., to hierarchically clarify chemical bonds to higher-order structures. It also covers research proposals for new observation methods, theoretical and computational methods related to actual phenomena, and data science.

d. Development of materials that combine the decomposition function with highly efficient self-healing of degraded areas;

It is critical to develop technology for healing degraded materials instead of disposing of them in resource circulation. Proposals for research on the development of materials that combine decomposition functions with technologies for efficient healing of degraded parts caused by external stimuli, etc., in polymeric, organic, biological, inorganic, and metallic materials and their composites are welcome. In particular, challenging research is expected to realize self-healing in a short time for systems with elasticity of -GPa and strength of -100MPa order.

It is recommended that the guidelines for material design, be developed based on theoretical grounds, and supported by mechanism elucidation, measurement, and evaluation techniques.

(3) Organizations for research implementation

Because CREST is a team-based research, the principal investigator, who is of high international standing, should organize the best research team that transcends the boundaries of industry, academia, and government boundaries in order to realize own challenging research concept. The team should be essential for the realization of the concept and sufficiently collaborative structure that can make a significant contribution toward achieving the research objectives. Please note that if collaboration with other research fields is useful, the research supervisor will ask you to change your research plan to promote joint research or rebuild the team structure.

For example, a research team that combines experiments, analysis, and theory in a specific material;

a research team that spans metallic, organic, polymeric and other materials to elucidate a certain decomposition or degradation phenomenon; or a research team that conducts fundamental measurements, simulations, and data scientific data analysis that can be applied to decomposition, degradation or stabilization. Cross-disciplinary research proposals, such as the development of common theories that are not limited to specific materials, or research themes that cannot be accomplished through existing research in a particular field, are encouraged.

(4) Selection policies

a. The output of the research such as "material decomposition methods for resource circulation," "guidelines for sustainable material design," and "creative analysis techniques for material decomposition processes," should be recognized on the proposal and the goals should be specific.

b. High academic or social value when the proposed goal is achieved.

c. Meaningful collaboration between researchers in different fields.

d. A challenging, attractive, and innovative proposal.

e. It is not just an extension of the traditional research.

3. Research periods and research funds

The budget for one research project at the beginning is 300 million yen at the maximum (direct expenses). The research period begins in fiscal year 2022 and ends in fiscal year 2027 (five and a half years or lesser).

4. Principle of research-area management

In order to maximize the results of the research area as a whole, networking will be promoted through information exchange and collaboration among researchers in different teams (including individual researchers in the PRESTO research area under the same strategic goal), industry, and other researchers inside and outside the research area. At the beginning of the research, we will visit to each research laboratory to check the research environment. In addition, progress report meetings will be held once or twice a year, and an interim evaluation will be conducted about three years after the start of the research, followed by a post evaluation at the end of the project. In addition, we plan to hold workshops and public symposia to disseminate the results of our research in the field, as well as workshops to foster young researchers. It is expected that the studies in this research area will contribute to the development of various academic fields as well as to the creation of a scientific theory of precise materials science for decomposition, degradation, and stabilization.