Research area in Strategic Objective *"Opening up of unexplored exploration space of materials with multi-element, composite, and metastable phases based on elements strategy"*

Creation of future materials by expanding materials exploration space

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Overview

The main aim of this research is to design new functional materials which will expand our fundamental knowledges in material science. These new materials are expected to be originated from simple but original ideas, and potentially prepared by using unconventional techniques. These new materials, together with the new designing principles, will help us solve challenges this society is currently facing, including but not limited to issues in areas of environment, natural resource, energy, medicine and health.

Specifically, the project will focus on the synthesis and characterization of materials strongly related to energy, electronics, medicine and environment. There are three perspectives regarding the research scheme: A scheme of 'multi-elements', in which materials containing different elements will be synthesized and investigated to understand how to combine the advantages of different elements; A scheme of 'functional composites' in which one will study how compositions/configurations of different elements in new materials affect the functionalities; A scheme of 'metastable phases', in which careful kinetic control will be employed to produce metastable materials.

In addition, the project aims to realize new synthetic pathways and designing principles (new theories) into 'future functional material'. Aim for research with a challenging approach backed up by a broad perspective, including the construction of principles by combining these with computational science, data-driven science such as machine learning, cutting-edge operand measurement techniques, and more, in order to establish technology for materials creation synthesis techniques and process control techniques.

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

1. Basic concept

In this research area, we aim to create future materials that express new and unexpected functions that change the nature of materials, and to explore unexplored material exploration spaces and the

fundamental technologies that support these explorations. By greatly expanding the scope of material creation to unexplored areas that have not been actively explored in the past, we expect to create future materials that can meet the demands for advanced materials, such as high performance and high functionality, coexistence of multiple functions, and compatibility of conflicting functions. In addition, we hope that logic/computational science, data science, and state-of-the-art measurement/evaluation techniques will serve as fundamental technologies necessary for clarifying the principles of their functional expression and synthesis processes, leading to feedback to experimental systems and the proposal of new material design guidelines.

The target research area is the creation of materials that are deeply related to various needs of society, including electronics, environment/energy, and medicine, etc. We seek proposals filled with curiosity to explore discontinuous concepts and concepts that differ from conventional technologies and to challenge the realization of simple and novel ideas.

We welcome dreamy and highly original research, but we also ask that you clearly state what kind of ideas, insights, and theoretical considerations you are basing your research on, as well as your views on materials and materials.

2. Assumed research fields

The policy of this research area is to seek simple and novel ideas that create new concepts and challenging approaches backed by the researcher's view of materials and materials. Therefore, research proposals that are simply an extension of the conventional route, such as the optimization of materials or improvement of existing processes, will not be considered.

Proposals are not limited to inorganic, organic, metallic, or composite materials, or to crystalline or non-crystalline materials, etc. The categories include multi-elements, functional composites, metastable phases, etc. Other unexplored areas of materials are also eligible. The material synthesis process is not limited to gas phase, liquid phase, or solid phase. In addition, we are also looking for proposals that take challenging approaches such as theoretical and computational science and measurement and evaluation techniques.

We welcome proposals that aim to contribute to solving social issues through the creation of future materials that express new and unexpected functions.

Specific research topics are shown below as examples:

1) Creation of multi-elements and functional complexes by combining elements based on the elucidation of synergistic effects between different elements, and creation of new materials and substances by utilizing metastable phases

・Development of materials consisting of multiple elements beyond the conventional mono, binary, and ternary element

Multi-element alloys, solid electrolytes, thermoelectric, high-entropy alloys, hetero-

element-containing polymers, etc.

・Development of materials that express functions by controlling the interface through complexation of different elements and structures

Hydrogenomics, mixed-anion, composite catalysts, etc.

・Development of materials utilizing thermodynamically unstable metastable phases, etc.

High-pressure superconductivity, power semiconductors, glassy polymers etc.

2) Establishment of fundamental technologies to support the creation of new materials

・Theoretical and Computational Science

Reaction pathway exploration and control, materials informatics, etc.

・Data science and high-precision processes

High throughput experiments, multi-element exploration systems (AI robots), process simulations, etc.

・Measurement and evaluation technology

Operand measurement, multi-scale and multi-modal measurement, atomic resolution observation, etc.

This year is the final call for proposals in this research area, and we will continue to follow the same policy, so please submit your proposals with a free spirit. In addition, since many synthetic research proposals were selected in the past two years' calls for proposals, we are expecting proposals especially from the theoretical/computational science and analysis fields.

3. Points to note when apply

While we expect applicants to achieve their research plans within the term of the PRESTO, we also expect ambitious research proposals that will lead to applications that will contribute to solving social issues in the near future, and that will pioneer new sources of science. Although PRESTO is an individual type of research, it is not necessary for one person to cover all research topics. If necessary, please describe the image of collaborative research. Especially for proposals for challenging approaches, please describe the image of the joint research in more detail. The proposal should be written in such a way that researchers and evaluators in other fields can understand the originality, feasibility, and scientific and social impact of the research. If you are reapplying to this research area, please be sure to include details of improvements from the previous year's proposal. In the selection process, consideration will be given not only to the period of the PRESTO research, but also to the possibility of further development of the research and the creation of new research fields.

In principle, the research period will not exceed three and a half years, and the total research budget will not exceed 40 million yen (direct costs).

4. Management Policies

In this research area, we will build an environment in which each researcher can carry out attractive research with original and advanced ideas full of curiosity, while making the most of his or her specialties and strengths. The time required to achieve research results varies depending on the goals and content of the research. While it is necessary to set and achieve research goals during the period of the preliminary research, it is also important to pursue what kind of development will take place beyond that point and what kind of new materials will be created. For this purpose, this research area will actively promote free and frank exchange of opinions among research supervisors, advisors, and adopted researchers through biannual meetings in principle and site visits to research sites. We will respect diversity in terms of research institutions, regions, gender, etc., to maximize the attractiveness of researchers and research themes, value synergy effects among researchers connected by "dreams," produce research from new perspectives and with flexible ideas, and support researchers to envision their own futures. We support researchers in the entire research field to create new perspectives and flexible ideas, and to enable them to envision their own future. Through the promotion of this research area, we hope to foster professionals (future human resources) in synthesis, theory, computation, measurement, and evaluation, who will become leaders in the creation of next-generation materials.

We will also actively promote academic exchanges with overseas research institutions and collaborate with CREST project " Exploring Innovative Materials in Unknown Search Space," which is being conducted under the same Strategic Objective, by holding workshops and symposiums. We hope that research in this research area will lead to the creation of new materials that express new functions beyond expectations, while spreading to various fields.