Research area in Strategic Objective *"Creating novel materials by controlling and utilizing fluctuations"*

Creation of functional materials through introduction/control of fluctuations

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Overview

This research area focuses on spatial and temporal fluctuations, which are critical factors in determining the functions and properties of materials. It promotes the creation of materials guided by the principle of controlling and utilizing these fluctuations. With the modern advancements in measurement technologies and computational science pertinent to materials science, we are now capable of visualizing and analyzing fluctuations in an advanced, multifaceted, and precise manner, which was previously unattainable. Leveraging these cutting-edge technological developments, our objective is to elucidate the intricate relationship between fluctuations and material functions, thereby utilizing this understanding to create groundbreaking materials. The scope of this research is comprehensive, encompassing a diverse range of materials, including metallic, inorganic, organic, polymeric substances, and their respective composites. The primary goal is to achieve a profound understanding of the spatial and temporal fluctuations inherent in these materials, to deliberately introduce and control these fluctuations to realize novel functionalities, and ultimately to develop revolutionary materials. A special emphasis is placed on avant-garde, strategic approaches that synergize advanced measurement techniques, computational science, data science, and state-of-the-art material synthesis processes.

In this research area, fluctuations encompass heterogeneities and irregularities in atomic arrangements, compositions, and orientations of atoms, ions and molecules, as well as non-equilibrium states and dynamic behaviors. Examples of such fluctuations include point defects, dislocations, interfaces, hierarchical structures, and molecular arrangements and orientations. However, the scope is not confined to these examples; fluctuations are examined from a comprehensive perspective. Additionally, through collaborative efforts across various research disciplines and the merging of insights derived from diverse material systems, we aim to deepen our understanding of currently unexplained fluctuations in materials and to establish fundamental principles that are applicable to a wide range of materials. Furthermore, our objective is to generate functionalities and develop novel materials that were previously challenging to achieve with existing materials.

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

１. Background

This research area aims to pioneer the creation of new materials with innovative functionalities and significantly enhanced performance by introducing and controlling spatial and temporal fluctuations, thereby contributing to the resolution of societal challenges. The recent rapid advancements in measurement technologies and computational sciences pertinent to materials have greatly enhanced our ability to capture and analyze fluctuations. Noteworthy advancements have been achieved in analysis and measurement technologies, such as operando measurements using large-scale facilities (e.g., SPring-8, SACLA, NanoTerasu, J-PARC), electron microscopy, and scanning probe microscopy, as well as in multiscale and multimodal measurement techniques. Furthermore, the remarkable progress in computing power and computational methodologies has profoundly contributed to materials research, enabling the modeling and simulation of materials that consider fluctuations, beyond the previous focus on uniform bodies and perfect crystals. In addition, various synthesis and processing technologies that allow for the precise design and high-level control of material composition, structure, and morphology across a spectrum ranging from nano to micro scales are continually advancing. Given the development of these diverse technologies, it is now imperative to establish scientific principles of materials science related to fluctuations and to develop design and process technologies that incorporate these fluctuations into materials and devices.

Therefore, this research area seeks original ideas for the development of new materials that exhibit novel functionalities and significantly enhanced performance by leveraging fluctuations to address societal challenges. We invite you to present your unique concepts and frameworks and to clearly articulate the research plan and expected outcomes needed to achieve these innovative ideas.

2. Expected Research Contents

By leveraging the extensive knowledge accumulated in materials science, along with advanced measurement techniques, computational science, and data-driven research, we aim to understand the relationship between fluctuations and material functions and establish processes to design and control fluctuations in materials. We seek proposals that aim to create groundbreaking innovative materials. To achieve this material creation, we promote technological innovation and interdisciplinary integration in the following research areas.

(1) Creation of New Materials and Devices Exhibiting Innovative Functions and Properties by Introducing and Controlling Fluctuations

- Construction of scientific principles of materials science relating to fluctuations.

- Establishment of design guidelines and processes for precisely introducing and controlling fluctuations in materials.
- Creation of new materials and devices that exhibit innovative functions and performance beyond the traditional concepts of material development.
- To achieve these goals, the following two items will be leveraged.

(2) Development and Advancement of Advanced Measurement Techniques to Capture Fluctuations

- Establishment of multiscale measurement techniques that capture fluctuations from nanoscale sizes of atoms and molecules to macroscopic element sizes and hierarchical structures.
- Development of measurement techniques to capture spatial and temporal fluctuations present during material generation processes, particularly process in-situ time-resolved measurements, non-destructive in-situ 4D measurements, and multimodal materials characterization methods.
- Establishment of operando measurement techniques to capture fluctuations present during the manifestation of material functions and properties.
- Advancement of measurement techniques to capture fluctuations at interfaces and grain boundaries between different materials and phase states
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(3) Development of Computational Science and Data Science for Handling Fluctuations

- Development of computational science techniques such as first-principles calculations and molecular dynamics simulations that consider spatial and temporal fluctuations to predict the physical properties of substances and materials, based on the motion of electrons in individual elements and the forces acting on each atom.
- Development of computational simulations that combine multiphysics to describe physical properties from nano to macro scales.
- Establishment of modeling techniques for fluctuations and construction of machine learning models through integration with mathematical sciences.
- Establishment of data-driven research incorporating the concept of fluctuations.
- Construction of a database of material functions and properties related to fluctuations, and proposal of material design hypotheses based on fluctuations.

This research area envisions a diverse array of material systems, including inorganic, metallic, organic, polymeric, and inorganic-organic composite materials. These systems encompass a wide range of properties, sizes, and forms, such as crystalline, amorphous, solid solutions, soft materials, nanomaterials, and colloids. We seek challenging research proposals that embody a deep understanding of the relationship between fluctuations and material functions, using such insights to create innovative materials. We encourage proposals that present novel ideas and strategies to realize them, liberating themselves from conventional thinking.

3. Organizations for research implementation

From the perspective of spatial and temporal fluctuations inherent in materials, this research area broadly encompasses the construction of scientific principles of materials science, the introduction and control of fluctuations, and the creation of innovative materials. To achieve the creation of new materials with novel functions, we welcome team compositions that include groups responsible for material synthesis as well as groups focusing on physical property research, measurement science, computational science, and materials informatics. In such team compositions, particular emphasis is placed on the planning of organic collaborative relationships centered around the material synthesis group. Furthermore, if the research involves advanced technical developments, themes specialized in the individual research elements mentioned above are also considered. However, in such cases, it is crucial to clearly indicate the pathway by which the research and development will be linked to material creation. We expect the creation of new functions and materials that go beyond a mere extension of conventional research on spatial and temporal fluctuations.

4. Research periods and research funds

The maximum budget for a research project is 300 million yen (direct expenses). We expect the principal investigator to take responsibility for the overall project and to appropriately set the budget plan, rather than uniformly distributing the budget to each group and applying for the maximum amount.

The research period should not exceed five years and six months (2025 - 2030).

5. Principle of research-area management

- After the adoption of the project, a site visit will be conducted to confirm the research environment and the setup status of the research team, and to share the research plan and concrete achievement images. Similar site visits may be conducted as needed in the second year and beyond to check the progress.
- Research Area meeting will be held once a year, with all selected teams participating, to confirm the progress of the research.
- In the fourth year, a mid-term evaluation will be conducted to assess the progress of the project and the feasibility of achieving its goals.
- In the final year of research, a post-project evaluation will be conducted to discuss the progress

of the project, the achievement of goals, and the policy for developing results.

- after the end of the research period. We also plan to hold public symposia and other events to promote the results of the CREST research to external parties and the industry.
- Collaboration within and outside the research area will be considered, especially with the PRESTO program, which is set under the same strategic goals "Materials innovation through understanding and controlling fluctuations".