Research area in Strategic Objective *"Precise arrangement toward functionality"*

Precise Arrangement of Atoms and Molecules and Its Properties and Functions

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Overview

The purposes in this Research Area are to spur innovation in basic science and to construct a new paradigm for materials science that contributes to more affluent daily life and social infrastructure, by creating unique structures from the viewpoints of dimensionality, hierarchy, homogeneity and heterogeneity, isotropy and anisotropy, symmetry and asymmetry, and complexity by fully utilizing techniques for intentional combination, arrangement and assembly of atoms and molecules and extracting the novel chemical, physical, biological and mechanical properties and functions that those structures bring about.

Concretely, the aim is to create new materials and new structures overflowing with originally based on novel concepts and strategies, on the foundation of chemical synthesis, atomic manipulation and molecular assembly techniques, which have achieved dramatic progress in recent years. We also intend to develop those unique materials and structures to the expression of unparalleled properties and functions by utilizing a combination of chemical structure analysis, crystal structure analysis, nano-array structure analysis and atomic-level precision analysis techniques, all of which have evolved remarkably, together with precise structural, chemical property and physical property prediction/analysis methods utilizing large-scale calculation.

In addition to chemistry focusing on the synthesis, conversion, organization and arrangement of materials and structures consisting of atomic/molecular constituent elements and their analysis, we also hope to pioneer science and technology that contributes to the achievement of the SDGs (United Nations Sustainable Development Goals) by performing comprehensive new manufacturing (*monodzukuri*: Japanese-style manufacturing) which is useful in the society of the future, in collaboration with physical science for theory-based prediction and analysis of the properties of materials, biology that analyzes the mechanisms of biological substances and biofunctions at the molecular level and develops materials utilizing those substances and functions, and engineering for device fabrication.

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

1. Background and Basic Policy

Only human beings are capable of creating substances that do not exist in nature. Since antiquity, techniques for this purpose have been accumulated on the basis of experience. Assuming modern science began from the end of the 18th century, those techniques evolved scientifically, and diverse material synthesis methods were devised in organic chemistry, inorganic chemistry, coordination chemistry, organometallic chemistry, polymer chemistry, and supramolecular chemistry, leading to the invention of new materials that contributed to the creation of an affluent society. Many innovative material groups have been created in recent years, including dendrimers, metallic nanoparticles and clusters, porous coordination polymers and metal-organic framework materials (PCP/MOF), supramolecules (catenane, *rotaxane, molecular cages, artificial DNA, etc.), new carbon (fullerenes, carbon nanotubes, graphene, etc.)* and 2-dimensional substances, among others. The interest of these new materials is not limited to their shape; characteristics such as dimensionality, hierarchy, homogeneity and heterogeneity, isotropy and anisotropy, symmetry and asymmetry, and complexity, can induce unique chemical, physical, biological and mechanical properties and functions. Moreover, the super-structures created by densely combining heterogenous materials express high-order functions such as coupling of signal output and chemical phenomena when an external field such as an electric field, light or magnetic field is applied. Remarkable progress is also being achieved by linkage between material/structural development and various analytical techniques, such as chemical structure analysis, crystal structure analysis, nano-array structure analysis, precise atomic-level analysis techniques, and precise predictive/analytical methods for structures, chemical properties and physical properties utilizing large-scale calculation techniques.

Against this background, the time is approaching when original research to determine what new materials and structures will express outstanding properties/functions, and conversely, what new substances and structures are suitable for intentionally expressing properties/functions, will open the way to the future of materials science. Therefore, the aim in this Research Area is to create a platform where researchers who are involved in original research challenging the future of materials science from various directions and angles can come together, and their mutual exchanges can give birth to fascinating new science.

2. Assumed Research Fields and Policy for Call/Screening of Proposals

It is assumed that this Research Area will include materials science and its various related fields. In terms of general categories, there are no particular limitations on chemistry, physics, biology, electronic engineering, material engineering or other related fields. Research proposals should

consider both synthesis of new materials/structures based on original atomic/molecular arrangement and expression of their properties and functions, but because PRESTO research is a type of individual research, it is not necessary for one researcher to cover the entire content of research. However, applicants should clearly separate the research subthemes and content which are your special strengths, and those which will require the cooperation of joint researchers in or outside of the PRESTO program. Since this research will begin in the future, it is not necessary to decide the actual researchers who will participate in such joint research. Please describe the content of the proposal so that the originality, feasibility, and scientific and social impacts of the content can also be understood by researchers in other fields. In screening proposals, we will consider the possibility of development of future research and the creation of new research fields, not limited to the PRESTO research period. This is the final (third) application for this research area. We expect proposals for original research that disparate from the research themes of the first and second term PRESTO researchers.

3. Research periods and research funds

The upper limit of the initial research budget is a total of ¥40 million (direct expenses) for one project. The research period is within three and a half years from the fiscal year in which the project was selected.

4. Management Policy

In this Research Area, we intend to create an environment in which researchers involved in a wide range of materials science fields can carry out original, attractive research while making use of their individual technological strengths and distinctive characteristics. The time until research outcomes are obtained will differ depending on the objects and contents. In PRESTO research, it is necessary to set achievement targets in the research period and accomplish those targets, but it is also important to pursue how the research will develop and what kind of new science it will lead to in the future. For this purpose, we plan to conduct substantial, free and frank exchanges of views among the Research Supervisor, Area Advisors and researchers whose proposals are selected. Moreover, the area as a whole will provide support so as to draw out the appeal of the research of each researcher to the fullest possible extent, and produce research based on new perspectives and concepts through interaction between researchers. We will also encourage scientific exchanges with external parties and cooperation with the CREST area “Precise arrangement towards the functionality of molecular systems” being implemented under the same strategic objectives. We hope that the research in this field will lead to research on a higher stage, while also having a ripple effect on various fields.