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

Precise arrangement towards the functionality of molecular systems

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Overview

The aims in this Research Area are to rationally control energy landscapes of atomic/molecular organized structures, by developing new fundamental methodologies to intentionally control the arrangement and orientation of the atoms/molecules, and to create generic technologies for realizing chemical, physical or biological functions that are unique to those organized structures.

The research fields cover a wide range of molecular-, supramolecular- and nano-materials, including organic molecules, biomolecules, polymers, metal ions, metal complexes, inorganic compounds, metallic clusters, nanocarbon and so forth. For example, (i) functional molecules and nanomaterials with their internal chemical bonding between homo-or-hetero atoms precisely controlled, and (ii) oligomeric, polymeric or supramolecular materials with the constituting molecular sequence precisely regulated via covalent or non-covalent bonding could be involved as the target molecules (or materials), and studies on their intramolecular structuring or sequence-controlled intermolecular assembly in solution, at surfaces or interfaces or in the solid-state will be involved. It will require the ability to control their hierarchical structures in arbitrary (1-, 2- and 3-) dimensions and sizes ranging from the subnano-, nano-, meso- to the macroscopic scales. This Research Area focuses on the development of methodologies or techniques for intentionally controlling — with precision on the level of organic chemistry — the sequence and orientation of the respective structural elements, nanostructures, functional units of interest in the atomic/molecularly organized systems obtained thereby. Furthermore, it also involves the studies on technologies and theoretical/computational science techniques for characterization of the electronics states and energy landscapes of the obtained superstructures at the atomic and single-molecular levels. It is essential that these approaches to control and characterize the alignment (sequence-)/orientation-/assembly-controlled structures are directed to create specific functions peculiar to these superstructures. Accordingly, all the studies need to elucidate the correlation between the controlled structures and the specific functions — such as electronic, magnetic, optical functions or chemical functions (we define these as “molecular system’s functions”) — created for the first time by intentionally controlling the atomic/molecular arrangement/orientation structures. The systematization of the acquired scientific knowledge would provide a basis for the creation and development of science for molecular systems.

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

1. Background

Self-organization and self-assembly are essential phenomena in life and also in various academic disciplines from social science to molecular-related research fields, including biology, chemistry, physics, and engineering. The researches to create integrated molecular structures by employing self-assembly of designed molecules, and utilization of their structural characteristics (i.e., shape, nano-space) have been actively promoted all over the world. To date, the JST has promoted a number of research projects related to self-assembly, including "Organization and Functions," "Structure Control and Function," "Nanosystems and Emergent Functions," "Molecular Technology," "Hyper-nano-space Design," and "Two-Dimensional Films." On the other hand, in order to utilize the self-assembly science and technology to solve important social problems, including those related to the global environment and human health/safety, it is indispensable further to develop its potential to a higher level by transcending the frameworks of the current technologies and scientific disciplines.

In this context, this Research Area aims to develop new methodologies to rationally control energy landscapes, typically that of electronic states, by controlling the alignment of functional molecules or nanomaterials in which the spatial position of constituent atoms and their chemical bonding are precisely determined. In terms of controlling the molecular alignment, both the molecular sequences in oligomer or polymer molecules and the alignment of functional molecules, nanomaterials would be controlled via covalent-or-non-covalent bonding (i.e., molecular or chemical information). The formation of their intramolecular or intermolecular superstructures would be investigated in solution, at surfaces or interfaces, and also in the condensed state. New methodologies will be developed to spatially control molecular arrangement, alignment, and orientation of functional molecules in the assemblies with atomic/molecular precision.

It is now more important than ever to develop scientifically valuable functions which are unique to the controlled atomic/molecular arrangements — such as sequence, spatial arrangement, orientation, assembly — and their structural hierarchy (we shall call such sophisticated functions peculiar to the well-controlled structures as molecular systems function). It is considered essential to elucidate the correlation between these atomic/molecular arrangements, hierarchical superstructures, and their-derived novel functions.

By developing such molecular systems functions and their causal relationships to the controlled superstructures, we also aim to create a new basic principle in the Molecular Systems Science. In this Research Area, from the fundamental perspective of the JST Strategic Basic Research Program, we invite challenging proposals that address brilliant "scientific questions", that show creativity and clarity in the purpose of research, and original research projects with scientific significance by international standards. The proposed researches are expected to produce scientific as well as technological outcomes, which will be highly evaluated by the international scientific community and to make an important contribution to future innovation in science and technology. We thus expect ambitious proposals that attempt to create basic principles in molecular systems science; methodologies, and techniques to create controlled atomic/molecular systems' structures and their unique functions. It would be essential to design the sequence-or-alignment-controlled molecular systems by starting from the particular image of "ultimate molecular system functions" that would solve the critical issues confronting humankind.

2. Principle of invitation project and selection

(1) The assumed objects of this Research Area cover a wide range of scientific disciplines related to molecular materials and nanomaterials, including organic molecules, biomolecules, oligomers, polymers, metal ions, metal complexes, inorganic compounds, and inorganic clusters, and nanomaterials. Candidate materials are not limited to hard crystalline structures but may also include flexible soft materials. The self-assembly of organic molecules is a field with a long history, but we welcome ambitious proposals related to the design of unique molecular structures based on the development of new flexible arrangement and orientation technologies, and the creation of molecular system functions that make the most of these characteristics.

(2) In developing molecular systems whose atomic/molecular arrangements and orientations are intentionally controlled, both covalent and non-covalent bondings are employed as appropriate. The definition of self-assembly in this Research Area encompasses the formation of higher (or super-) structures from intramolecular processes (such as folding) to bottom-up intermolecular assembly processes, under a condition of thermodynamic equilibrium or dynamic self-assembly under non-equilibrium conditions. Top-down methods such as photolithography, microcontact printing, nanolithography, inkjet printing, and their integrated approaches are available, and the solid phase synthesis of sequence-controlled polymers, formation of atomically or molecularly layered structures by chemical vapor deposition (CVD), molecular beam epitaxy, and molecular assembling techniques such as Langmuir-Blodgett (LB) films and the layer-by-layer (LbL) method have been established. However, in this Research Area, we expect original concepts that overcome the limitations of conventional methodologies and high-impact proposals for new multi-molecular or nanomaterials production that trigger the development of new technologies. They may also include technologies, for example, to produce precisely alignment-controlled film structures which are uniform at the cm^2 area scale or larger. Moreover, in order to lead to future technological innovation, it is desirable that the concepts and methodologies developed in this Research Area are generally applicable, and not restricted to the use of specific materials and devices.

(3) Remarkable progress has been achieved in measurement technologies in recent years, and sub-Å spatial resolution, attosecond temporal resolution, and μ eV energy resolution have been realized. The research in this Research Area would reap the benefit of these recent advances and the studies for developing precise, i.e., atomic/molecular-level structural analysis technologies and theoretical/computational science techniques for clarifying the arrangement/orientation-controlled structures, and their (non-self-evident) hierarchical structures would be involved.
(4) In fields such as inorganic materials, organic materials, polymers and their composites, there have been examples to utilize artificial intelligence to derive materials with desirable physical properties. The use of data-driven material development approaches in this Research Area, however, may not necessarily be easy because the arrangement/orientation-controlled molecular systems would include a variety of hierarchical structures. Meanwhile, it would be essential to develop AI-supported systems that correlate physical properties/functions and molecularly organized structures in question. Based on integrated approaches that intend a tie-up with data science, ambitious proposals to develop precise arrangement and orientation of molecules towards the innovation of functionality of molecular systems are also welcome.
(5) As functions of molecular systems developed in this Research Area, physical properties such as electronic conductivity, magnetism, optical or spectroscopic properties, thermal properties, etc. and chemical properties such as catalytic functions, molecular recognition, selective separation, and so forth are conceivable. However, as the functions of arrangement/orientation-controlled molecular systems are not limited to these examples, and we have the utmost respect for scientific values. We hope to receive proposals based on flexible thinking beyond the existing frameworks.

We underline that the purpose of this Research Area is not only the development of new methodologies or technologies for intentionally controlling the atomic/molecular-level arrangement, orientation, and organization of molecules or nanomaterials. The elucidation of the correlation between the obtained superstructures and their physical properties/functions is of high importance. We expect the scientific and technological outcomes in this Research Area would contribute to the innovation of science and technology that solve problems in a diverse range of disciplines, including the information-communication technology, energy, environment, medical and nanobiotechnology, and lead to the creation of new social and economic values.

3. Research Implementation System

Since CREST is team research, applicants should form the best research team, transcending the boundaries of academy, industry, and government to realize challenging research concepts, which are drafted by the Research Directors themselves, at an internationally outstanding level. Since team organization is indispensable for concept realization, please bear in mind the need for a sufficient collaborative system that is capable of making a substantial contribution to achieving the purposes of the research. In case collaboration with other research fields, etc. is recognized as useful, the Research Supervisor may request changes in the research plan, for example, implementation of joint research, a review of the team organization, etc.

4. Research periods and research funds

The upper limit of the initial research budget is a total of ¥300 million (direct expenses) for one project. The research period is within five and a half years from the fiscal year in which the project was selected.

5. Principle of research-area management

This CREST program is administered as the “Atomic/Molecular Systems Science” network laboratory. We attempt to form networks for information exchange, and collaboration between fellow researchers in different teams (including individual researchers in the PRESTO Research Area under the same strategic objectives), and researchers in and outside the Research Area, in industries. At the initial period of the research, we conduct site visits to each research project, which are also conducted to inspect the research environment. Research progress reporting meetings will be held in the Research Area once or twice each year. An interim evaluation of individual projects will be conducted approximately 3 years after the start of the research, and a final evaluation will be conducted at the end of the project. We also plan to hold public symposiums and workshops to publicize the results in this Research Area. We hope that the research in this area will open a new area on the cutting age of Science for Molecular Systems and having a ripple effect on various fields.