

Research Outline of Research Areas

Supra-ceramics: Molecule-driven frontier of inorganic materials

<http://supraceramics.jp>

Number of Research Area	: 22A205	Term of Project	: FY2022-2026
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Research Institution	: Tokyo Institute of Technology, School of Science		

1. Details of Research Area

In this research area, we define "supra-ceramics" as a group of materials in which molecular units (molecular ions, complexes, clusters, etc.) are incorporated into inorganic materials, and create new materials with innovative properties and functions through cross-disciplinary research that brings together researchers from different fields. The objective is to revolutionize the academic system of materials science, focusing on inorganic materials. In this research area, the target supra-ceramics are classified into the following two types according to the way in which molecular units are incorporated, and the creation of new materials of both types will be pursued.

Endospheric supra-ceramics: New materials that contain molecular ionic species within the lattice of inorganic crystals. Based on the strong electronic interactions within the narrow space of the crystal, new properties and functions that cannot be created by conventional molecular ion-containing materials (MOFs, etc.) are expected to be created.

Exospheric supra-ceramics: New materials that have outstanding properties and functions by placing functional molecules at specific locations on the surface of inorganic solids. Unlike conventional organic-inorganic hybrids, perturbations from crystal surfaces or interfaces are maximally utilized to create new structures and electronic states that inorganic solids or molecules alone do not possess, leading to modulation of physical properties and functions.

2. Call for Proposals and Expectations for Publicly Offered Research, etc.

In this research area, we will construct a materials design science of supra-ceramics based on close collaboration among "synthesis," "analysis and theory," and "physical properties and functions". Research Teams A01 and A02 are defined as Group A, and Research Team A03, which consists of publicly offered researches, is established in Group A. Similarly, Groups B and C are defined, and Research Teams B03 and C03 are established, respectively. We wish to expand the entire research area by including important research topics that are not included in the current research plan as publicly offered research, thereby providing a driving force for research in the area. We expect applications from various materials-related fields, such as solid-state chemistry, coordination chemistry, crystallography, supramolecular chemistry, catalysis, and condensed matter physics. We consider the possibilities of the following subjects in each research category, for example, but also welcome original one that is not covered by these categories.

Group A: Research on the synthesis of materials using electric fields, high pressure, etc., synthesis of materials under special atmospheres, development of processes to precisely control the chemical composition and arrangement (regular or irregular arrangement) of molecular ions and organic ligands, and establishment of guidelines for controlling dimension and morphology including nano- and macrostructure.

Group B: Structural dynamics of supra-ceramics, development of electronic structure measurement devices and analytical methods for light elements, analytical methods using first-principles calculations, etc., of data from analytical electron microscopes and various spectroscopic methods, chemical bonding of supra-ceramics, understanding and prediction of physical properties Theoretical calculation techniques for understanding and predicting chemical bonding and physical properties of supra-ceramics, prediction of materials and composition using materials informatics, etc.

Group C: Experimental/theoretical studies on the creation of properties and functions of supra-ceramics. Bulk properties of materials, interfacial properties including thin films, electronic devices, catalysts, biomaterials, etc.

3. Research Group, Upper Limit of Annual Budget and Number of research projects scheduled to be selected

Research Team Number	Research Group	Upper Limit of Annual Budget (Million yen)	Number of research projects scheduled to be selected
A03	Development of new synthesis method and dimensional/morphological control of supra-ceramics	Experiment, 2.5	7
B03	Design and advanced structural analysis of supra-ceramics	Experiment, 2.5	4
C03	Development of new properties and functions of supra-ceramics	Experiment, 2.5	7
A03	Development of new synthesis method and dimensional/morphological control of supra-ceramics	Theory, 1.5	4
B03	Design and advanced structural analysis of supra-ceramics		
C03	Development of new properties and functions of supra-ceramics		