【Grant-in-Aid for Transformative Research Areas（A）】

Supra-ceramics: Molecule-driven frontier of inorganic materials（Supra-ceramics）

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Research Area Information	Number of Research Area : 22A205　Project Period (FY) : 2022-2026 Keywords : Molecular ions, Metal complex, Materials Informatics

Purpose and Background of the Research

●Outline of the Research

Inorganic materials (ceramics) are an indispensable part of our social life, and the discovery of innovative inorganic materials has contributed greatly to the development of human society. Until now, research on inorganic materials has revolved around the science of cations (represented by metal oxides) and anions.

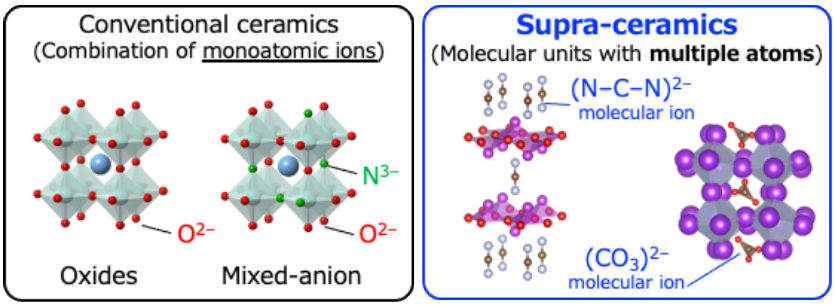

Figure 1. Conventional ceramics and supra-ceramics

On the other hand, discoveries and technological innovations in the past decade are transforming the existing values of inorganic materials, such as "hard", "brittle" and "homogeneous". For example, the possibility of acquiring new functional properties that cannot be realized with conventional inorganic ceramic materials has become apparent.

In this research area, we define "**supra-ceramics**" as a group of materials incorporating molecular units (molecular ions, complexes, clusters, etc.), which are covalently linked by multiple atoms, as a completely different direction from conventional inorganic ceramics research centered on monoatomic ions. New materials with innovative properties and functions will be created through cross-disciplinary research that brings together researchers from different fields. The aim is to revolutionize the academic system of materials science, focusing on inorganic materials.

However, research related to supra-ceramics has been sporadic, and there are few methods for synthesizing and analyzing materials, as well as scientific principles for creating desired physical properties and functions.

In this research area, we will classify our target supra-ceramics into the following two types based on the differences in the way molecular units are incorporated, and aim to create new materials of both types.

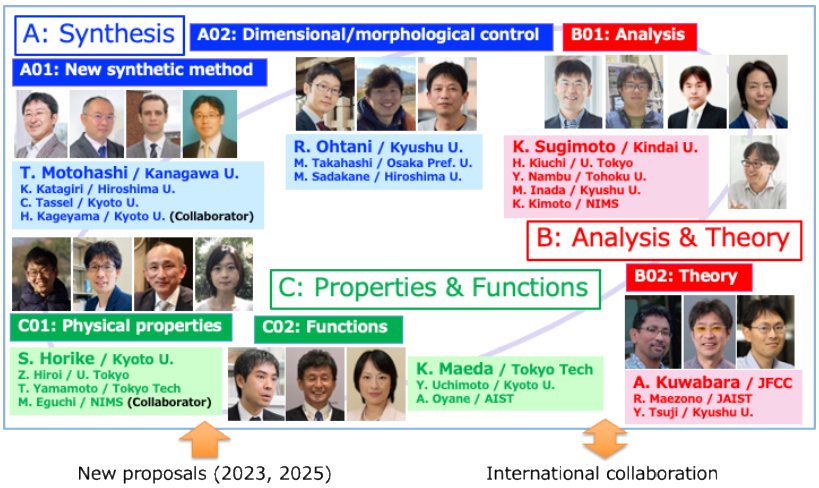

Figure 2. Research structure of the "supra-ceramics" area

●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.

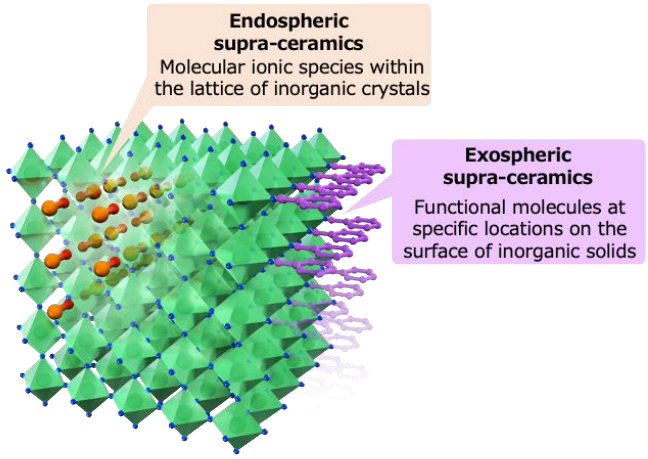

Figure 3. Endo and exospheric supra-ceramics

Expected Research Achievements

Molecular units contained in the supra-ceramics have anisotropic properties, which give rise to new degrees of freedom in terms of orientation, arrangement, and dynamic properties. As a result, various physical properties and functions can be expected to be created.

In fact, we are now discovering that innovative properties and functions can be created in inorganic materials by using the concept of manipulating molecules within inorganic materials.

For example, we are beginning to see new developments in inorganic materials chemistry that could contribute to solving social problems, such as the huge modulation of electronic properties based on the different orientation of molecular anions, ultra-high capacity of secondary batteries using molecular anion formation, and high-performance CO_2 conversion catalysts.

In this study, through research on inorganic materials including molecules, we will explore new properties and functions based on the new degree of freedom provided by molecular units, and systematically clarify the correlation between static and dynamic structures, properties, and functions of materials and substances. Through this research, we will create a new trend and lead the world by providing a new axis for the design of inorganic materials.

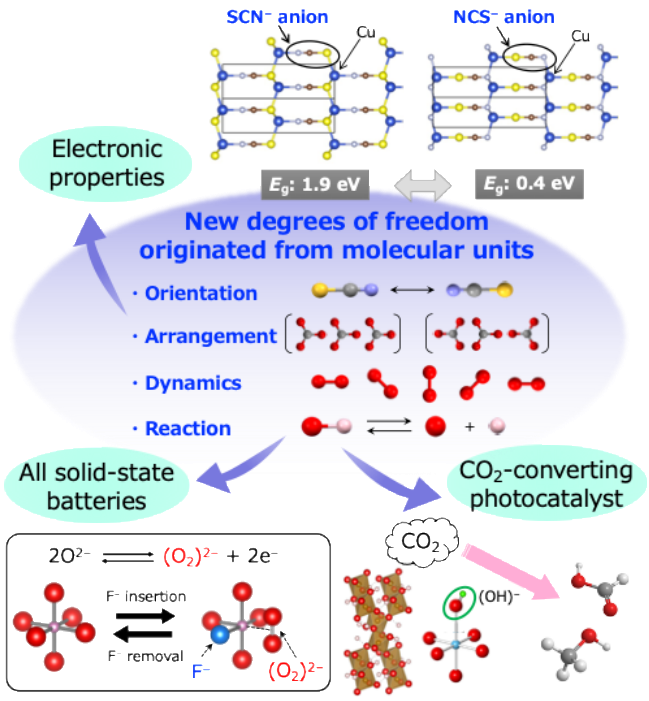

Figure 4. Creation of physical properties and functions based on new degrees of freedom of molecular units

Homepage Address, etc.	https://supraceramics.jp (Website) https://twitter.com/supraceramics (Twitter)