Title of Project : Synthesis of Mixed Anion Compounds toward Novel Functionalities

Hiroshi Kageyama
(Kyoto University, Graduate School of Engineering, Professor)

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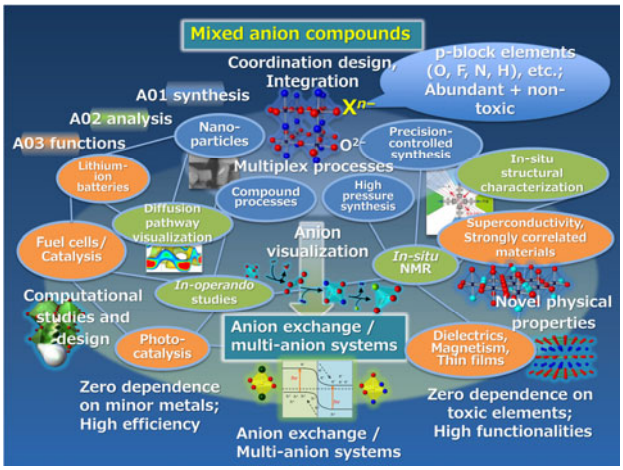
【Purpose of the Research Project】

Given the scarcity of resources for our nation, keeping a technological advantage is vital for preserving our industry's competitiveness as a whole. We believe the development of new materials is necessary for this. Recently, mixed anion compounds consisting of multiple anions within a single compound have gathered attention. The use of multiple anions enables unusual coordination modes and crystal structures, giving them a huge potential for new properties when compared to existing oxides or nitrides. While mixed anion compounds will occupy a central stage in materials development, the field is still quite new. In this project we will establish the scientific foundations of mixed anion chemistry, establish Japan's pre-eminent position in the field, and contribute to industry by providing new mixed anion materials.

【Content of the Research Project】

The scientific community in materials science is divided into many narrow disciplines. This project will unite the community and field using mixed anion systems as a rallying point. We envision a multidisciplinary team working together to develop new mixed anion compounds and explore their functions. Our team will be divided into subgroups addressing the synthesis, analysis, and functional properties of mixed anion compounds, based on these key components of the materials discovery cycle. These subgroups will work together to solve problems difficult to address with conventional non-mixed anion systems. Our multidisciplinary approach will also be invaluable in training new scientists for the next generation.

The synthesis subgroup (A01) will focus on the discovery of new mixed anion compounds based on various synthesis techniques. The group's efforts will involve complex reactions, establishing the principles controlling crystal structure, and use computational techniques for material design. The analysis group (A02) will use various diffraction and spectroscopy techniques to solve various characterization issues inherent to mixed anion systems. Combining these results with insight obtained from *ab initio* calculations will enhance our understanding of the materials' physical properties. The functions subgroup (A03) will channel these materials to provide solutions for various energy-related applications. The subgroup will make various connections between function and crystal/electronic structure, providing feedback to the further synthesis of new mixed anion compounds.



【Expected Research Achievements and Scientific Significance】

Mixed anion materials differ greatly from conventional materials, making radically new functions and applications possible. Additionally mixed anion systems focus on the effects of elements such as hydrogen, chlorine, phosphorus, carbon, etc. (in anionic form). As these elements are quite ubiquitous, our approach to materials development is relatively unimpeded by conventional problems of resource scarcity and distribution.

Until now, individuals separated by various fields and applications have led materials development. In this project, young scientists will be trained without such conventional barriers between fields. While training the next generation of scientists, we will contribute to raising the overall level of our nation's academic and technological prowess.

【Key Words】

Mixed anion compounds, ubiquitous elements, crystal chemistry, crystal engineering, analytical techniques, synchrotron radiation, theoretical calculations, electronic structure, local structure, chemical bonding, fuel cells, catalysis, rechargeable batteries, photocatalysis, photoelectrochemistry, dielectrics, fluorescent materials, magnetic materials, thermoelectrics, superconductors.

【Term of Project】 FY2016-2020

【Budget Allocation】 1,022,800 Thousand Yen

【Homepage Address and Other Contact Information】

http://mixed-anion.jp
The secretariat: k.hayashi@cstf.kyushu-u.ac.jp