



**Title of Project : Exploration of nanostructure-property relationships for materials innovation**

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**【Purpose of the Research Project】**

Nanostructures, or unique atomic configurations and electronic structures localized at surfaces, interfaces, and point defects, often play a critical role in determining materials properties. There have been significant recent advances in experimental and computational techniques to characterize individual atoms in nanostructures and to gain quantitative information. This Project aims to further accelerate exploration of frontiers in nanomaterials science, and to strongly promote integration of information to utilize accumulated knowledge regarding nanostructures for design and innovation of actual materials. The collaboration of researchers from diverse disciplines, such as materials science, applied physics, solid state chemistry, and catalytic chemistry, would create a new trend in materials science.

**【Content of the Research Project】**

This project is based on the following two research strategies:

- (1) Investigate unexplored frontiers in nanomaterials science at the state-of-the-art level. Nano-scale built-in experiments, nano-scale measurements, and accurate first-principles calculations are used intimately together to systematically collect previously unknown nanostructural information.
- (2) The newly obtained nanostructural information is used to guide design and innovation of actual materials through integration of information by combining theoretical and experimental results. The effectiveness of the present approach is verified and would be established as a new research area.

The individual research topics and planned research are outlined as follows:

A01: Frontier explorations in nanomaterials science

A02: Functional design and search through nanostructural information synthesis

A03: Innovation of new materials through nanostructure design

The organizational framework is designed to encourage collaboration between experimentalists and theorists, and the research team leaders take responsibility for collaborative research involving experimental and theoretical approaches.

This research project will evolve nanomaterials science, establish methods of its application, and create common concepts and infrastructure for researchers to collaborate over the boundaries of specific research fields. Young researchers who will inherit this foundation will be fostered, and measures for sharing scientific foundations with researchers domestically and internationally will be taken, for example through conferences.

**【Expected Research Achievements and Scientific Significance】**

Modern society demands new concepts and advances in innovative materials development various fields including energy problems, securing safety and security, environmental conservation, and information technology. Establishment of creating new materials and functionalities based on nanostructural information, which is the goal of this project, can provide many seeds in materials science for nanotechnology, and should result in significant advances.

**【Key Words】**

Nanostructural information: quantitative insight into relationship between the nanostructure and functionalities of materials

**【Term of Project】** FY2013-2017

**【Budget Allocation】** 1,028,300 Thousand Yen

**【Homepage Address and Other Contact Information】**

<http://nanoinfo.mtl.kyoto-u.ac.jp>