【Grant-in-Aid for Scientific Research (S)】

Construction of physical property correlation based on entropy and creation of new thermal control materials

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Project Information	Project Number : 23H05457 Keywords : Entropy, Caloric effect, Transition-metal compounds, Structure-property relationship	Project Period (FY) : 2023-2027

Purpose and Background of the Research

●Outline of the Research

As we face various problems in the environment of our society, there is a strong need to develop new materials to solve these problems. One of the major challenges in the energy- and environment-related fields is "thermal control". In modern society, it is reported that 25~30% of the electricity produced in the world is used for cooling purposes such as air conditioning and refrigeration. Furthermore, in the future society, it is essential to develop cooling technology for hydrogen liquefaction and storage. This research project thus aims to develop new thermal control materials that will create new fundamental science and industrial technology fields in the future.

In the project, “Material synthesis”, “Materials evaluation”, and “Theoretical calculation” research teams are organized. The material synthesis team focuses on new materials synthesis and aims to find novel functional properties. Stable structure search by machine learning will also be used. The materials evaluation team carries out atomic-level structure characterization using synchrotron X-ray, neutron, and electron quantum beams complimentary. Electronic structures of the novel materials will also be analyzed by a spectroscopic analysis technique. The theoretical calculation team conducts first-principles electronic structure calculation. Strong and complementary collaboration of the research teams with unique and cutting-edge methods will develop new interdisciplinary materials science research.

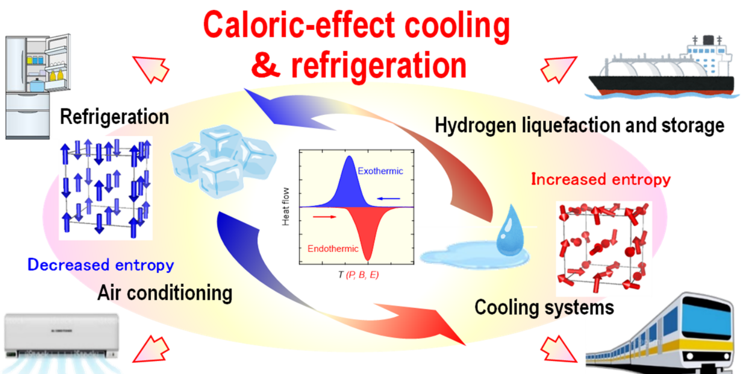

Figure 1. Project research overview

●Advantages of Solid-State Caloric-Effect Materials

The caloric effect in a solid can control heat through its entropy change caused by the application of external fields such as pressure, magnetic fields, and electrical voltages. The caloric effect can provide highly efficient refrigeration compared to conventional gas refrigeration systems and can eliminate the need for hydrofluorocarbon refrigerants. Next-generation environmentally-friendly cooling technologies can be achieved.

● Research Approach

In this study, we focus on phase transitions in transition-metal compounds with strong correlations in charge, spin, and lattice degrees of freedom. In a strongly correlated charge-spin-lattice system, the entropy change can be enhanced. In addition, thermal properties of the charge-spin-lattice correlated system can be controlled by the entropy change in multiple mays by various external fields such as electric and magnetic fields and pressure. We will construct new principles to realize such a new type of thermal control based on the entropy changes in the strongly correlated charge-spin-lattice system.

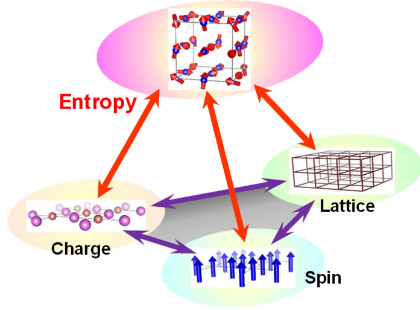

Figure 2. Physical property correlation based on entropy

Expected Research Achievements

● Methods of the Research and Organization

We will search for new transition-metal compounds that exhibit giant entropy changes by phase transitions. Specific synthesis methods like high-pressure synthesis, epitaxial thin film growth, and topotactic material transformation will be used. Computational structure search using machine learning will also be incorporated. We will also attempt to search for new materials by predicting not only crystal structures but also physical properties of the compounds and provide the information in the actual material synthesis.

For the identification of newly synthesized materials, we use high-resolution synchrotron X-ray and neutron diffraction and atomic-image analysis by electron microscopy. Thermal properties including the caloric-effect properties under various applied fields are evaluated in addition to electronic and magnetic properties. Electronic structures are discussed both from X-ray- and electron-spectroscopy analysis and first-principles theoretical calculations. The microscopic structural and electronic information will help us to understand the nature of the characteristic phase transition behaviors that induce huge entropy changes.

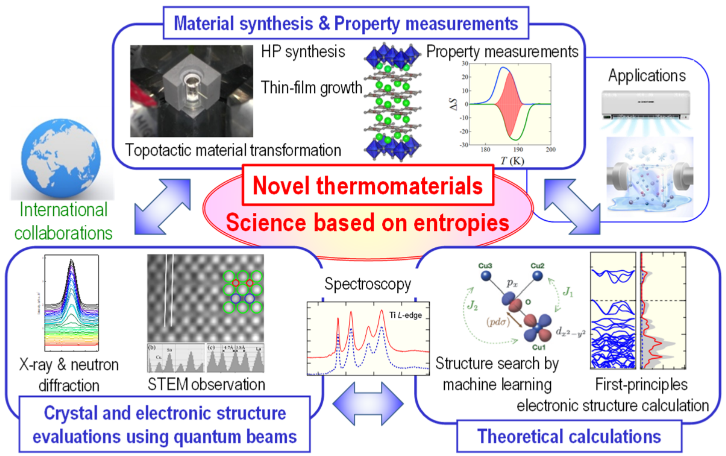

Figure 3. Methods of the research and organization

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