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

Comprehensive exploration of metastable strongly correlated materials as post-spintronics

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Purpose and Background of the Research

●Outline of the Research

Metastable magnetic materials exhibit unique magnetism and magneto-transport phenomena due to strong orbital hybridization, and are expected to become new spintronics materials. However, the high-pressure synthesis of these materials is inefficient, and the use of computational and informatics has been limited. In this research, we will conduct high-pressure synthesis based on structure prediction and prediction of magnetic and cross-correlation responses using first-principles calculations that effectively incorporate the applicant's knowledge, aiming to efficiently develop metastable strongly correlated materials with innovative spintronics functions that make use of the peculiarities of spin and electronic structures.

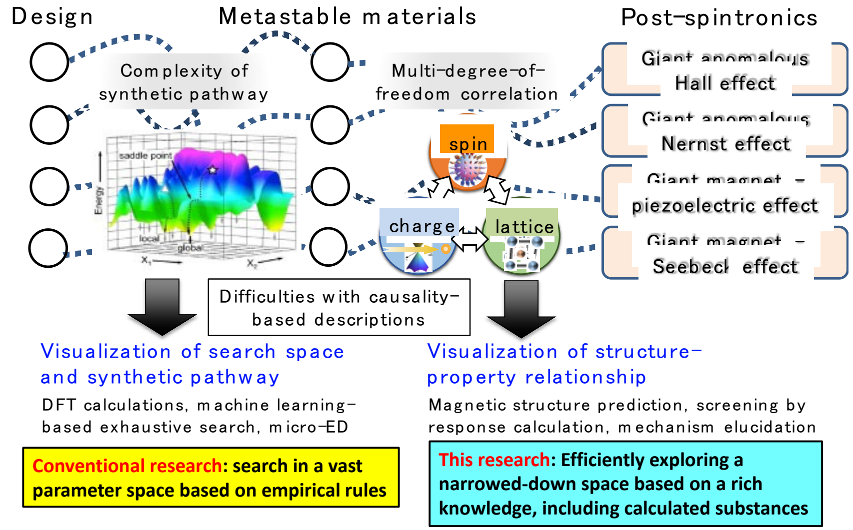

Figure 1. Schematic diagram of the materials design and exploration in this research.

●Problems to be solved and the goals of this research

While the search space for metastable materials is vast, the number of known materials synthesized at high pressures is small, making it difficult to extract descriptors based on databases. For this reason, to make use of informatics in high-pressure synthesis, it is essential to narrow down the search space through modelling based on human knowledge, and collaboration between computational scientists and experimentalists is desirable. The goal of this research project is to “fully exploit the potential of metastable strongly correlated materials as spintronics”, and to achieve this, we will (1) utilize computational and informatics to search for stable structures over a wide range and design materials based on predictions of novel functions, and (2) promote the visualization of synthesis routes under extreme conditions.

Expected Research Achievements

●Exhaustive search for metastable strongly correlated oxides

Based on the evaluation of enthalpy under high pressure using first-principles calculations, we perform high-pressure synthesis of oxides that are expected to have unusual magnetism, such as topological helimagnets. We focus on oxides that contain unusual valence ions such as Fe^{4+}, Co^{4+}, $Pt^{3+/5+}$, and $Au^{2+/3+}$, and develop spintronics functions that arise from valence instability and strong spin-orbit interactions. By evaluating the enthalpy of intermediate phases in addition to the target one, it will be possible to visualize the complex synthesis pathway. In addition, phases with oxygen deficiency order and cation order are compatible with modelling and structure searches using Bayesian estimation. Furthermore, using these structure searches as a reference, we will develop novel metastable strongly correlated oxides through multi-step topochemical synthesis combining high-pressure synthesis and soft chemical synthesis, and evaluate their magnetic and electronic transport properties. We will also perform machine learning on the database, and aim to visualize empirical rules related to high-pressure synthesis of metastable phases and construct new descriptors.

● Search for giant responses derived from unique spin and electronic structures

In this theme, we will promote the development of new materials based on the perspective of post-spin-electronics functionality. As specific systems, in addition to the oxides mentioned above, we will focus on Zintl compounds that contain magnetic cations with strong spin-orbit interactions. For these, we visualize structure-property relationship through magnetic structure prediction based on cluster multipole theory and exhaustive response calculations, and based on this, we will select promising metastable phases and perform high-pressure synthesis, and then study external field response, including electrical resistance, Hall resistance, Seebeck effect, Nernst effect, and lattice strain. We will narrow down the list of candidate materials by calculating the responses of promising systems with such characteristics and structural stability. Through this research, we aim to observe the world's highest level of anomalous Hall and Nernst effects, as well as magnetothermal and piezoelectric effects, and to establish the basic principles for the design and development of metastable spintronics.

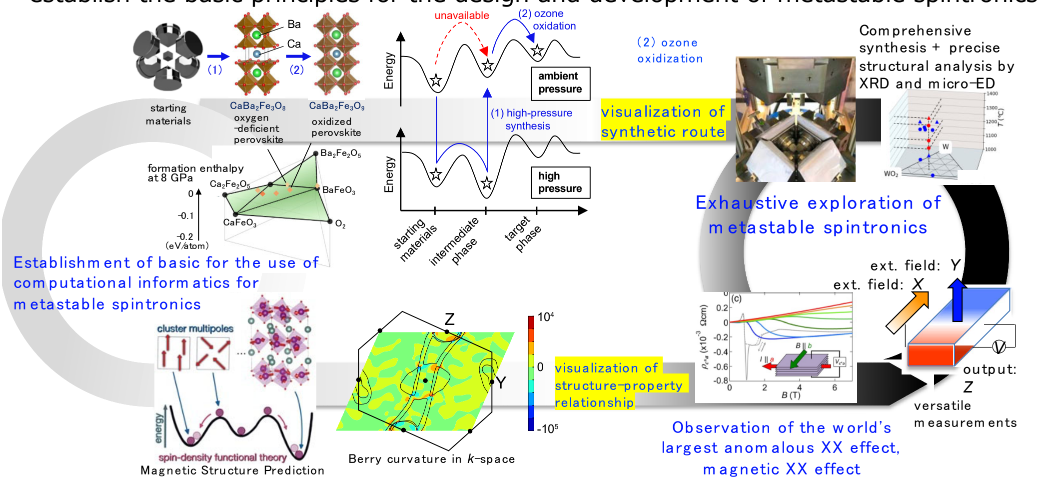

Figure 2. Methods and anticipated results.

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