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

# Exploring quantum emergence through correlation design science


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| Project Information | Project Number : 25A201 | Project Period (FY) : 2025-2029 |
| | Keywords : correlation effects, quantum emergent phenomena, materials design, new material development, precise measurement | |


## Purpose and Background of the Research

**●Outline of the Research**

Recently, there has been a notable increase in successful research on quantum materials. These successes are frequently rooted in new theoretical ideas, concepts or computational findings, which directly pave the way for the synthesis of new materials or the discovery of new phenomena. This trend is especially significant in the exploration of quantum emergent phenomena, such as high-temperature superconductivity.

Quantum emergent phenomena stem from interactions between various degrees of freedom, often resulting in properties and functionalities that go beyond naive expectations. The vast potential of these complex many-body effects cannot be fully explored through serendipity alone.

The objective of our project is to develop a comprehensive scientific approach "correlation design science" that integrates phenomenological modeling, first-principles calculations, material synthesis, and precise measurements, with the goal of spearheading new breakthroughs in condensed matter physics.

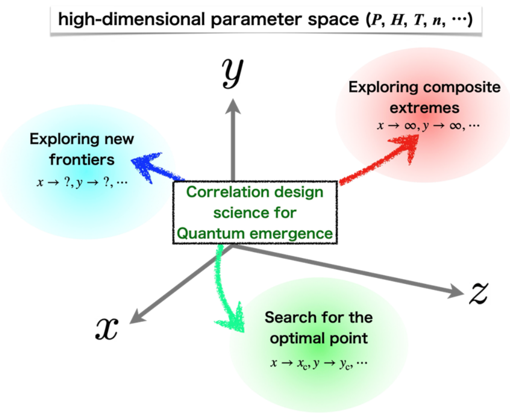


Figure 1. Illustration of materials design and exploration based on correlation design science.

**●Research background**

The role of theoretical research in condensed matter physics is rapidly evolving, driven by advances in analytical and computational techniques. These improvements have unlocked new capabilities to accurately and non-empirically calculate previously intractable phenomena. In parallel, experimental advancements have not only expanded the variety of materials that can be synthesized but also enhanced measurement accuracy and broadened experimental possibilities. Moreover, the explosive growth of artificial intelligence (AI) is significantly influencing this field. These technological advances are expected to revolutionize not just computational and data sciences but also materials science. As we edge closer to enabling AI to provide comprehensive insights into materials like room temperature superconductors, the collaboration between theoretical and experimental research becomes increasingly vital.

**●Research Objective**

We aim to realize quantum materials that can be observed across a wide parameter space, potentially impact various application areas, and serve as a platform for developing new concepts in condensed matter physics. The targeted quantum materials include:

1. Materials that maintain their properties under extreme conditions such as high temperatures, strong magnetic fields.
2. Materials that exhibit gigantic and ultrafast responses.
3. Materials that may serve as the birthplace for discovering new laws, principles, and phenomena.

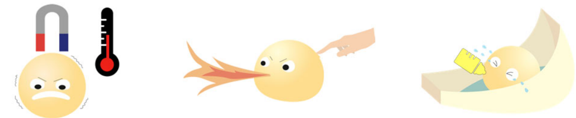

Figure 2. Illustrative diagram of the quantum materials targeted in the research project

## Expected Research Achievements

**●Research framework and goals**

This project consists of six teams, and the objectives of each team are as follows.

Team A01 will conduct research on magnetic materials, focusing on the exploration of new quantum phases in frustrated magnets. Their work will include studying electron correlations and spin moiré engineering in topological magnetic structures, as well as investigating new systems such as altermagnets and multipolar ordered systems.

Team A02 will conduct research on novel quantum metals, focusing on the exploration of new quantum phases in materials such as kagome superconductors, multilayer graphene, and cuprates, nickelates, and iron-based high-temperature superconductors. Specifically, they will focus on odd-parity orders, strong correlation-driven topological phase transitions, electron pair density waves, quasicrystal superconductivity.

Team A03 will establish control and probing methods for exotic superconductors and explore new functionalities, particularly targeting spin-triplet superconductors, parity-lacking superconductors, and two-dimensional heterostructures.

Team B01 will design and explore novel topological materials and states by leveraging correlations in materials. Specifically, they will explore magnetic Weyl semimetals and propose and design spin devices, establish new methods for identifying symmetries in unconventional superconductors and elucidate new functionalities.

Team B02 will explore new non-equilibrium quantum phases that are not seen in equilibrium states, especially aiming for theoretical proposals and experimental observations of new electronic states on ultrafast timescales of picoseconds or less.

Team B03 will develop methodologies and construct databases fundamental to theory-driven materials development. They will also develop efficient strongly-correlated first-principles calculation methods.

**●International collaboration, fostering young researchers**

We actively engage with international projects that align with our academic vision and objectives. These partnerships are crucial components of our long-term strategic plan, aimed at fostering the next generation and enhancing participation in the global exchange of young researchers.

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