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

Computational materials science based on quantum-classical hybrid algorithms

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Research Area Information	Number of Research Area : 23B205 Project Period (FY) : 2023-2025 Keywords : First-principles calculations, quantum embedding, variational wavefunction theories, quantum circuits	

Purpose and Background of the Research

●Outline of the Research

In recent years, quantum computers, which could exponentially accelerate computations using quantum mechanical superposition, have been rapidly developed, with potential applications in quantum many-body calculations. If it becomes possible to quantitatively predict physical properties that arise from the strong quantum entanglement of many electrons, it could be a key to solving unsolved fundamental problems in materials physics and chemistry, as well as energy and environmental issues facing humanity. However, the quantum computers that can be realized in the near future have severe resource limitations, and existing quantum algorithms alone cannot realize quantitative property prediction. In this research area, we will construct a new first-principles computational theory that integrates information compression methods in materials physics, chemistry, and quantum information to maximize the capabilities of both quantum and classical computers, and form an integrated core community.

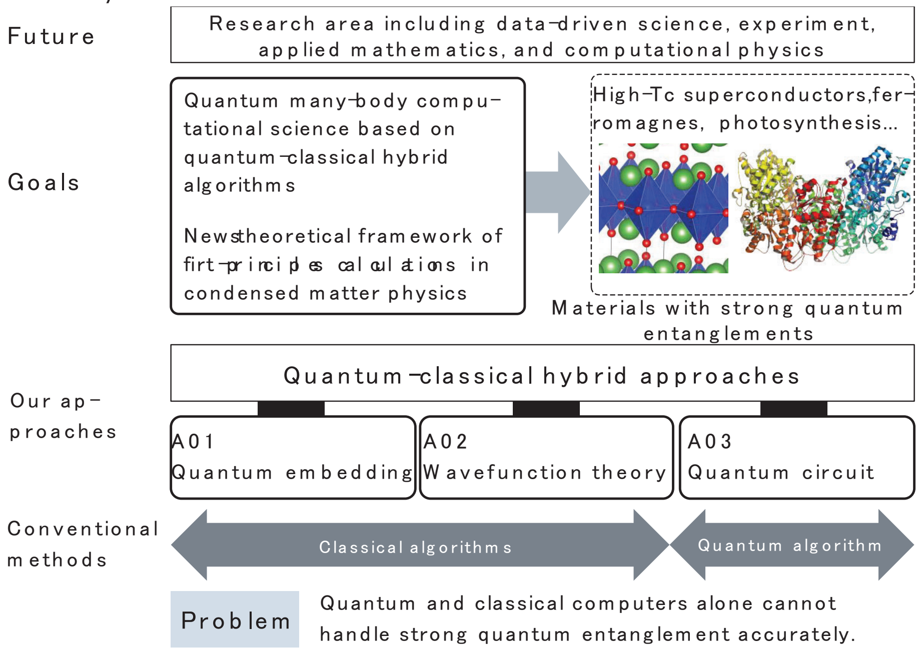

Figure 1. Overview

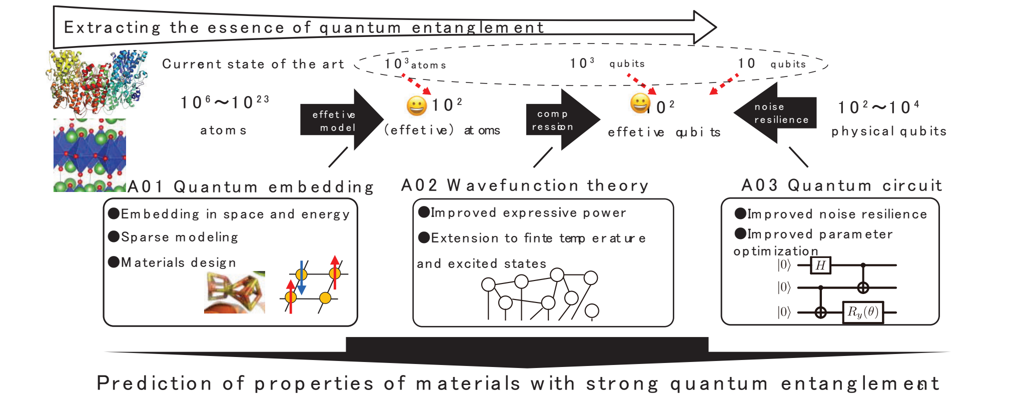

Figure 2. New theoretical framework

Expected Research Achievements

●Expected Research Achievements

By extracting the essence of quantum entanglement and constructing a multi-stage scheme to compress degrees of freedom (information), we will establish a first-principles calculation method that can solve matter groups with strong quantum entanglement with the assumed performance of NISQ (10,000 qubits). To this end, we will explore quantum embedding theory to extract essential degrees of freedom from materials（A01), compressed representations of quantum entanglement (A02), and implementation methods for quantum circuits (A03).

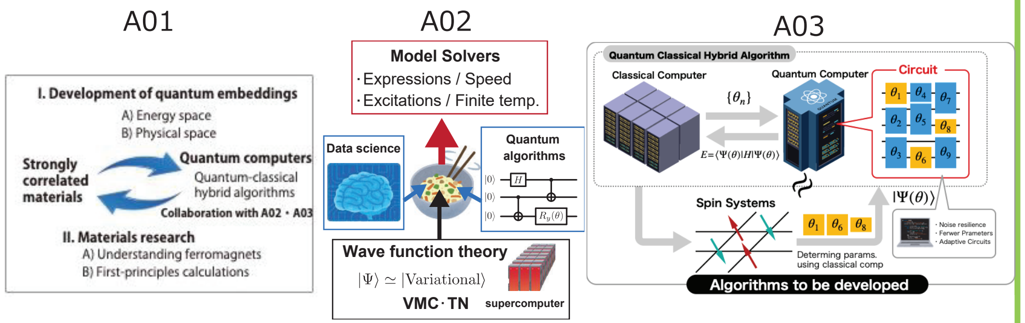

Figure 3. Research plans and expected achievements

●Outreach activities

1. Open-source software
・MateriAppsLIVE!
・Hands-on workshop

2. Online two-way communication
・Twitter
・Online seminars

3. Cooperation with industry
Cooperation with start-up companies, chemical manufacturers, etc.

Figure 4. Outreach activities

Homepage Address, etc.	https://qc-hybrid.github.io