Quemix and Mitsui Kinzoku Develop New Technology for Materials Calculation on Quantum Computers

Accelerating the Practical Application of Materials Simulation

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TerraSky Co., Ltd.

Quemix Inc. (“Quemix”; Head Office: Nihonbashi, Chuo-ku, Tokyo; CEO: Yu-ichiro Matsushita), a group company of TerraSky Co., Ltd. (Head Office: Chuo-ku, Tokyo; Representative Director, President & CEO: Hideya Sato), engaged in the research and development of quantum computing algorithms and software, and Mitsui Kinzoku Company, Limited (“Mitsui Kinzoku”; President & Representative Director: Seiji Ikenobu), are pleased to announce that they have jointly developed a new technology that significantly improves the efficiency of materials development using quantum computers.

In materials development, discovering high-performance new materials requires extensive trial and error, resulting in significant time and cost challenges. To address these issues, the use of computer simulations for more efficient materials development has been advancing in recent years. However, there remains a strong need to achieve both higher analytical accuracy and shorter computation times simultaneously. Quantum computing is attracting attention as a promising solution to these challenges.

In this joint research, the companies focused on the Dynamical Mean-Field Theory (DMFT) method, which is capable of highly accurate calculations but has traditionally suffered from long computation times. To enable efficient execution of DMFT on quantum computers, the researchers developed a new computational workflow and improved the performance of Quantum Phase Estimation (QPE), a key component in the computational process. As a result, they achieved both high-speed and high-accuracy calculations, paving the way for the early practical application of DMFT calculations using quantum computers.

The newly developed technology, named “QAVG (QPE Averaged over Variable Grids),” is an enhanced version of Quantum Phase Estimation (QPE), a core technology for materials calculations on quantum computers. Conventional QPE methods face the challenge that increasing energy resolution also increases the number of gate operations and computational costs. QAVG makes it possible to

improve both the accuracy and speed of DMFT calculations on quantum computers while suppressing the increase in computational cost.

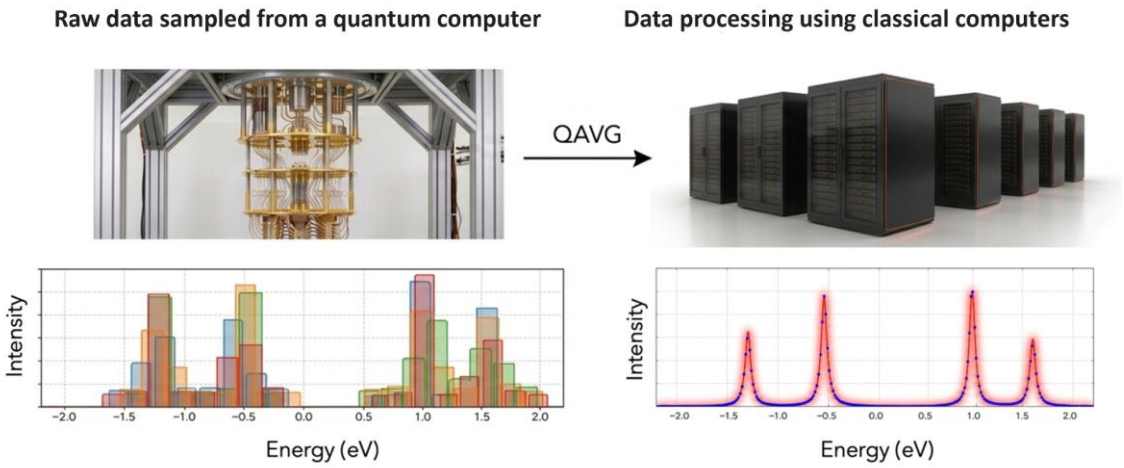


Figure: Conceptual Illustration of QAVG

Lower left: Four types of data obtained by executing QPE on a quantum computer (distinguished by four different colors).
Lower right: Continuous spectrum obtained by applying QAVG to the four datasets acquired from the quantum computer (blue dots indicate the actual QAVG results, while the red line represents the exact solution).

In this joint research, the two companies conducted simulations assuming catalytic materials on Quantinuum's quantum computing hardware and confirmed that QAVG, a key component of the DMFT computational workflow, is effective even in real hardware environments. Furthermore, QAVG enabled the current quantum hardware to achieve a level of computational accuracy that would normally be expected to be realized approximately two years later through hardware evolution alone.
These results suggest the possibility of accelerating the timeline for applying DMFT calculations using quantum computers to practical materials simulations. In addition, since QPE is a widely used technique in the field of materials calculations, the newly developed QAVG technology is expected to have applications and broader impacts not only for DMFT calculations but also across the entire field of computational materials science.
Both companies will continue to promote the development of algorithms for the practical application of quantum chemical calculations and contribute to solving social challenges through advances in materials development.
The results of this research are also scheduled to be presented by researchers from Quemix and Mitsui Kinzoku at the international conference "Q2B 2026 Tokyo," to be held in Tokyo in June 2026.

Q2B 2026 Tokyo Official Website: https://q2b.qcware.com/conference/2026-tokyo

For the press release issued by Quemix regarding this matter, please visit the following link:
https://www.quemix.com/en/post/en-20260601-mitsuikinzoku

About Quemix Inc.
Quemix Inc., a consolidated subsidiary of TerraSky Co., Ltd. (Headquarters: Chuo-ku, Tokyo; CEO: Hideya Sato), conducts research and development in quantum computing, quantum sensing, and computational materials science.
Under its vision of "realizing the future humanity has dreamed of through quantum technology," Quemix supports breakthrough innovations for companies leading the next generation of quantum technologies.
Since its establishment in 2019, the company has focused on research and development of algorithms for fault-tolerant quantum computers (FTQC), including the development and patenting of the "Probabilistic Imaginary-Time Evolution (PITE®)" quantum chemistry algorithm, which has been mathematically proven to achieve quantum acceleration.
As a leading company in FTQC algorithm research in Japan, Quemix is actively advancing research and development aimed at the practical application of quantum computing in materials computation and simulation by 2030.

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