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Quemix and Honda R&D Develop New Technology for Exponential Acceleration of Density Functional Theory Calculations on Quantum Computers

~ Advancing Quantum Computing Technology for Density Functional Theory, a Core Technology of Materials DX~

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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 Honda R&D Co., Ltd. (“Honda R&D”; Head Office: Wako City, Saitama Prefecture; President and Representative Director: Toshihiro Akiwa), the research and development subsidiary of Honda Motor Co., Ltd., have successfully developed the world’s first quantum algorithm capable of exponentially accelerating calculations based on Density Functional Theory (DFT), a core technology in Materials DX, as a result of their joint research. Today, DFT calculations serve as one of the foundational technologies in computational materials science, and accelerating DFT calculations is regarded as an extremely important core technology with broad impact across virtually all fields of materials development. Through the world’s first successful development of a quantum algorithm for accelerating DFT calculations, this joint research has opened the possibility of performing DFT calculations on extremely large-scale systems that would have been impossible to realize using conventional computers. Going forward, practical application of this algorithm is expected to accelerate the development of new materials, an area on which Honda R&D is placing significant focus.

Background: DFT as the Core of Materials DX and Expectations for Quantum Computing

In recent years, the field of materials development has faced an urgent need to transition from conventional experiment-driven approaches based on “experience and intuition” to “Materials Digital Transformation (Materials DX),” which leverages computational science. At the core of Materials DX lies Density Functional Theory (DFT), an electronic structure calculation method. Because DFT enables prediction of material properties at the atomic level, it has become an indispensable tool in

modern materials design.
At the same time, quantum computers are attracting attention as next-generation computational platforms. Research efforts around the world are accelerating toward the realization of both high-speed and highly accurate simulations that would be difficult to achieve using conventional classical computers.

Previous Challenges: Overemphasis on Accuracy Improvements and the Absence of Practical Acceleration Algorithms

To date, most research on quantum-computing-based materials simulations has focused primarily on improving calculation accuracy. This is because quantum computers are particularly well suited for rigorously handling electron-electron interactions (electron correlation effects).

[Targets for High-Accuracy Calculations]
- Strongly correlated materials, where electron-electron interactions are extremely significant
- Excited-state analyses, such as optical and photochemical reactions

[Challenge]
However, many materials of high industrial relevance — including those used in drug discovery, semiconductors, and battery materials — are classified as weakly correlated materials. For these systems, conventional DFT calculations are generally sufficient in terms of accuracy, and what is more strongly required is not further accuracy improvement, but rather faster computation and the ability to handle larger-scale systems.
Furthermore, despite DFT being a central technology for Materials DX, no effective quantum algorithm had previously existed for accelerating DFT calculations. The primary reason was the extreme technical difficulty of incorporating the nonlinear computational processes specific to DFT into the fundamentally linear operational framework of quantum computers.
More specifically, the Gram–Schmidt orthogonalization process used in DFT calculations involves nonlinear operations, creating a major obstacle for implementation within quantum circuits. In addition, evaluating total energy requires expressions defined as nonlinear functionals of electron density distributions. Consequently, conventional approaches required sequential readout (sampling) of electron density distributions. The enormous computational cost associated with this readout process represented another major bottleneck preventing practical implementation.

This Achievement: Development of the World's First DFT Acceleration Algorithm

Quemix and Honda R&D have successfully developed the world's first quantum algorithm capable of exponentially accelerating DFT calculations using quantum computers.

This algorithm introduces a new quantum-computing approach that avoids the use of the Gram–Schmidt orthogonalization process. In addition, the researchers established a method for directly calculating the total energy of DFT systems from the sampling results of Quantum Phase Estimation (QPE) circuits without requiring explicit readout of electron density distributions. As a result, the companies successfully constructed, for the first time in the world, a high-speed DFT calculation scheme that eliminates the need for electron-density readout.

Results of the Demonstration Experiments

The developed algorithm was executed on an emulator, and the following results were confirmed:

- Exponential acceleration:
  As the computational scale increased, the calculation time was shown to decrease exponentially compared with conventional algorithms.
- Accuracy comparable to conventional methods:
  The algorithm successfully achieved highly accurate results comparable to those of conventional DFT calculations in determining interatomic distances and structural constants (crystal structure parameters).
- Advanced physical-property prediction:
  The researchers demonstrated that the algorithm can calculate electronic band structures, which determine the electrical properties of materials.

Future Outlook: Roadmap Toward Industrial Applications

This achievement significantly expands the potential applications of quantum computers from limited classes of special materials, such as strongly correlated materials, to broader and more practical materials-development fields including semiconductors and battery materials. Going forward, the companies will advance implementation of this algorithm on actual quantum hardware while promoting joint research with partner companies. Through these efforts, they aim to contribute to realizing "true Materials DX" capable of dramatically shortening the development cycles of next-generation devices and new pharmaceuticals.

The results of this joint research are scheduled to be presented by researchers from Quemix and Honda R&D at “Q2B 2026 Tokyo,” an international conference on quantum technologies to be held at the Grand Hyatt Tokyo on June 4–5, 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-20260603-hondard

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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