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To Whom It May Concern

Quemix Inc.
Asahi Kasei Corporation
The University of Tokyo
National Institutes for Quantum Science and Technology

Prediction of Quantum Bit Candidate Structures in Aluminum Nitride through Classical-Quantum Hybrid Computing

-Material Exploration with FTQC Algorithm on an Actual Quantum Computer-

Key Points of the Announcement:

・In recent years, research and development of (gate-based) quantum computers*1 has shifted to the era of developing "Fault Tolerant Quantum Computer (FTQC*2)" that can detect and correct computational errors during calculation. To maximize the performance of FTQC, it is essential to develop and demonstrate quantum algorithms*3 specialized for FTQC. Aluminum nitride is an ultra-wide bandgap semiconductor material currently used in UV-LEDs and the subject of high expectations as a next-generation semiconductor. Due to its characteristics, it has also been considered as a potential base material for quantum bit (qubit) materials.

・Presently, a research group from Quemix Inc. (hereinafter Quemix), Asahi Kasei Corporation (hereinafter Asahi Kasei), the University of Tokyo, and the National Institutes for Quantum Science and Technology (hereinafter QST) successfully demonstrated the potential for new applications of aluminum nitride by performing quantum chemical calculations*4 using hybrid computing that links a Quantinuum quantum computer and the supercomputer at the Institute for Solid State Physics, the University of Tokyo. In particular, the execution of an FTQC algorithm for ground state calculation on logical qubits using quantum error detection (QED) codes on an actual quantum computer is a world-first endeavor (as of the end of February 2025 based on a survey of published papers performed by Quemix). Defects*5 in the aluminum nitride crystal, which was the target of the calculation, presented challenges in calculation accuracy with conventional quantum chemical calculation methods, but in this case quantum-supercomputer hybrid computing enabled high-precision calculation of physical property values. As a result, it was revealed that aluminum nitride has high potential as a base material for qubit materials.

・In the future, with the full-scale practical application of FTQC algorithms, further development and acceleration of the quantum chemical calculation field and the materials informatics*6 field are expected. In addition, the development of new applications of aluminum nitride as a base material for qubit materials is expected to expand, and attention to high-quality aluminum nitride single crystal substrates and advanced thin film crystal growth technology is expected to increase.

Research Overview

Hirofumi Nishi (General Manager, Research and Development Department, Quemix), Taichi Kosugi (Senior Researcher, same), Yuki Takei (Group Leader, Platform Laboratory for Science & Technology, Corporate Research & Development, Asahi Kasei), Shunsuke Mieda(Principal Researcher, same), Yutaka Natsume (Senior General Manager, Informatics Initiative, Digital Value Co-creation, Asahi Kasei), Takeshi Aoyagi (Senior Fellow, same), Yu-ichiro Matsushita (Project Chief, Quantum Materials Theory Project, Quantum Functional System Research Center, QST, and Project Associate Professor, School of Science, The University of Tokyo) and others performed quantum chemical calculations using hybrid computing consisting of a Quantinuum quantum computer and the supercomputer at the Institute for Solid State Physics, the University of Tokyo, and revealed the possibility that composite defects in aluminum nitride function as new qubits. In addition, they performed quantum chemical calculations for the first time in the world (as of the end of February 2025 based on a survey of published papers performed by Quemix) using an FTQC algorithm on logical qubits using QED codes on a quantum computer, demonstrating that quantum-supercomputer hybrid computing is a powerful tool in the quantum chemical calculation field and the materials informatics field.

It is known that composite defects*7 present in semiconductor materials exhibit new functions that are not present in the base material. Composite defects can be said to be the ultimate ultra-fine nanotechnology. Qubits, which are indispensable for quantum technology, are an example of new functional devices that have been attracting attention in recent years. Qubits are important components that make up various quantum devices*8, and are expected to be used in quantum computers, quantum sensors, quantum engines, quantum batteries, and more (Figure 1). Since qubits are to be incorporated into various quantum devices in future society, material design suitable for each application is required. Therefore, diversity is also required for qubit materials, and the search for new qubit materials is an indispensable research area for the further development of quantum technology. Among these, wide bandgap semiconductors*9

such as aluminum nitride are known to have great potential as qubit base materials for producing a variety of qubit materials due to their large band gap. In recent years, attempts to accelerate new material exploration through computer-based approaches using information science and simulations called materials informatics have been made all over the world, involving industry, academia, and government (Figure 2). This joint research is also part of an attempt to utilize computer simulations for new qubit material exploration.

Figure 1: Spin defects and quantum technologies utilizing them.

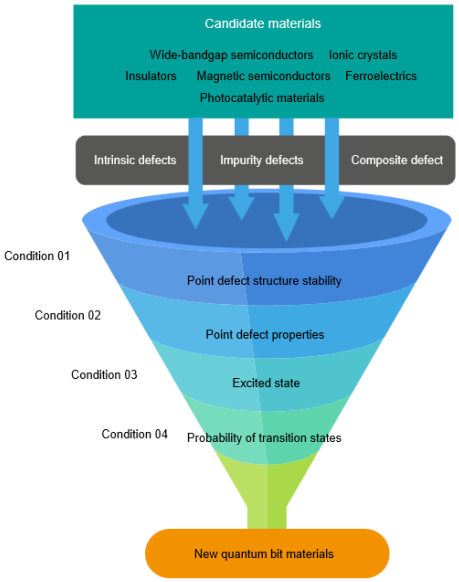

Figure 2: Conceptual flowchart of new spin defect material exploration using simulations.

In order to examine the characteristics of qubits quantitatively and in detail, it is necessary to precisely understand the behavior of electron spin (minute magnetism caused by the rotation of electrons) in both the ground state (the most energetically stable state) and the excited state (the state in which the electron energy is high enough to affect the properties of the substance at room temperature). Therefore, it was necessary to perform quantum chemical calculations with higher accuracy than the conventional method using density functional theory*10. However, when trying to perform quantum chemical calculations with higher accuracy than the conventional density functional theory, it is known that the calculation time increases exponentially as the scale of the calculation (specifically, the number of atoms to be simulated) increases. Therefore, the development of approaches to calculation for executing high-precision calculations at higher speed has become an important issue.

In recent years, the development of quantum computers has been remarkable, and in particular, the improvement of hardware performance and the innovation of error correction technology have been rapidly progressing worldwide. Research on quantum computers so far has mainly focused on quantum computers called NISQ (Noisy Intermediate-Scale Quantum) devices, in which errors occur during calculation, and the main subject of research for the past 10 years since 2014 has been how to develop effective calculation algorithms (NISQ algorithms) and applications with NISQ devices. However, FTQC and its pre-stage Early-FTQC, which were initially thought to be in the distant future, are having roadmaps to accelerate their realization announced in succession, and research and development of quantum computers is entering the next phase. Research and development of quantum algorithms (FTQC algorithms) that maximize the performance of FTQC and their verification are becoming important. In particular, quantum chemical calculation is the field in which hardware manufacturers believe that the business use of quantum computers will start the earliest. This is because the material design at the nano-level of atoms and molecules, which are the targets of quantum chemical calculations, is originally a world dominated by quantum mechanics, and it is considered that a quantum computer is the optimal computer for describing the quantum world. Currently, the development and actualization of practical application examples of FTQC algorithms to quantum chemical calculations is an important issue.

In this joint research, quantum chemical calculations were performed using hybrid computing that links a Quantinuum quantum computer and the supercomputer at the Institute for Solid State Physics, the University of Tokyo. Since current quantum computers have a limited number of qubits, there are limits to solving realistic problems. Therefore, the supercomputer "ohtaka" at the Institute for Solid State Physics, the University of Tokyo, was used to perform rough calculations using density functional

theory for the calculation target including 300 atoms. Then, by using a calculation method called the downfolding method, the scale of the problem was reduced without reducing the calculation accuracy, and the essentially difficult problem area that requires high-precision calculation was extracted (Figure 3). Specifically, only the electronic state near the composite defect was extracted while taking in the contribution from the aluminum nitride base crystal surrounding the composite defect. Next, high-precision calculations were performed by executing the FTQC algorithm for the extracted problem using the actual Quantinuum ion trap quantum computer "H1-1". However, since current quantum computers do not yet have error correction technology implemented, they are susceptible to quantum noise, and errors occur in the calculation results. In this research, by using a (QED) code called the Iceberg code, the influence of quantum noise (calculation error) was reduced, and the execution of a high-precision FTQC algorithm was made possible. The Iceberg code is a code suitable for current quantum computers because it requires only 4 auxiliary qubits for encoding and syndrome measurement (Figure 4). In this way, in this research, it became possible to detect calculation errors during quantum calculation by using a QED code. If an error during calculation was detected by the QED code, the calculation result was discarded. By using a QED code in this way, it became possible to analyze only the calculation results in which no error occurred during calculation, and it was possible to execute the FTQC algorithm on the current actual machine. The probabilistic imaginary time evolution (PITE) method, which has been jointly developed by Quemix, the University of Tokyo, and QST, was used as an FTQC algorithm for accurately calculating the quantum state of composite defects. The PITE method, a quantum algorithm that has been designed for the FTQC era, is mathematically proven to accelerate quantum chemical calculations. It should be noted that this is the world's first report of the execution of calculations combining QED codes and an FTQC algorithm for ground state calculation on an actual quantum computer. As a result of actually performing the calculations, it was possible to effectively reduce errors by QED and obtain both the ground state and the excited state of the composite defect with high accuracy (Figure 5). In fact, it was demonstrated that 98% of the accuracy of an ideal FTQC machine can be realized even with current quantum computer hardware. This extremely high accuracy indicates that current quantum computer hardware is approaching a degree of completeness that allows practical use. In addition, QST, which has detailed analysis technology for qubit states, performed analysis of the calculation results. As a result, it was shown that $Zr_{Al}V_N$, $Ti_{Al}V_N$ and $Hf_{Al}V_N$ composite defects have high potential as qubits. Specifically, all of them have a spin triplet state (a state in which two electron spins are aligned in the same direction in the vicinity of the composite defect), which is the same electronic state as the diamond NV center, which is a promising qubit material, as the ground state, and they all have a spin singlet state (a state in which

all electron spins in the vicinity of the composite defect are directed in opposite directions to each other and cancel out the magnetism of the spins) as the excited state. In addition, it was found that the wavelength of light required to excite in the spin triplet state is approximately 400 nm, which is the highest known energy wavelength band of excitation light. On the other hand, it was found that the excitation state in the spin singlet state is 2500 nm, which is low energy. The result of this research thus revealed unique quantum physical property values that differ greatly in the excitation state depending on the spin state. While diversity of qubit materials is required, unique qubit states not seen in other materials could be found in aluminum nitride crystals. Although calculations can be performed with current supercomputers when the calculation target is of limited scale, as with this research, the superiority of quantum computers will become clear as the problem scale increases in the future. This research represents an important step in quantum chemical calculations using quantum computers, and is not only a milestone towards the practical application of FTQC algorithms, but is also expected to contribute to the development of future qubit materials.

The results of this research were published online in Physical Review Applied on March 10, 2025 (U.S. local time).

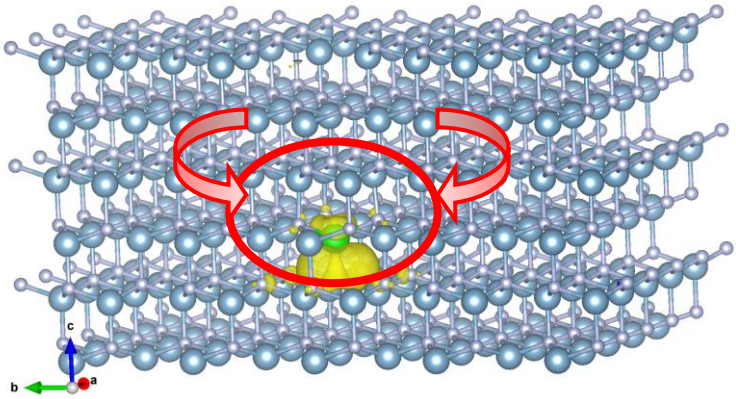

Figure 3: Calculation system of atomic structure used in this study (300 atoms). The large blue spheres represent aluminum atoms, and the small white spheres represent nitrogen atoms. The yellow-green spheres represent hafnium atoms in the aluminum nitride crystal. The yellow surface represents the localized spin density derived from the composite defect, which is strongly localized in the hafnium atom and the vacancy structure at the adjacent site. The red arrows indicate the process of extracting the problem of describing the electronic state near the composite defect, incorporating the contribution from the electronic state of the aluminum nitride crystal surrounding the composite defect.

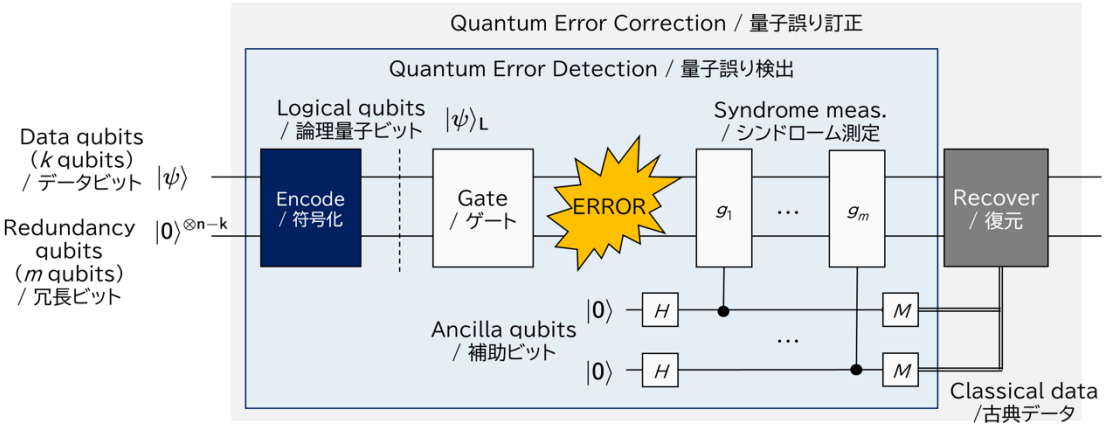

Figure 4: Conceptual diagram of quantum error detection and quantum error correction technology. In current NISQ devices, errors (shown in yellow in the figure) may occur during calculations. If an error occurs during calculation, it can be detected by syndrome measurement performed during calculation (quantum error detection). Quantum error correction is to perform restoration gate operations based on the information on the presence or absence of detected errors. In this study, only quantum error detection is performed due to the depth of the quantum circuit.

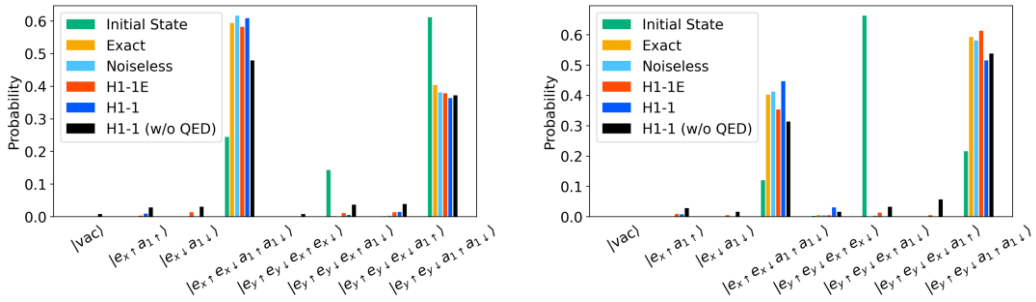

Figure 5: Execution results on an actual quantum computer. Results for the ground state (left figure) and results for the excited state (right figure). In each figure, the initial state is shown in green, the exact imaginary time evolution method in yellow, the ideal quantum computer without noise in light blue, the simulation results incorporating the noise model in red, the results on the actual quantum computer using the quantum error detection code in blue, and the results on the actual quantum computer without using the quantum error detection code in black.

Explanation of Terms/Notes

*1. Gate-based quantum computer: A computer that operates based on quantum mechanics, which enables general-purpose calculations by applying gate operations to the quantum states of qubits (a time series of gate operations is called a quantum circuit).
*2. Fault Tolerant Quantum Computer (FTQC): A gate-based quantum computer that incorporates a quantum error correction mechanism. Since errors can be corrected even if they occur during calculations, highly reliable quantum calculations can be realized.
*3. Quantum algorithm: An algorithm that is executed on a quantum computer. In classical computers, various calculations are executed using four arithmetic operations as basic operations, so all desired calculations are rewritten and executed with four arithmetic operations. On the other hand, in quantum computers, since unitary operations are basic operations, it is necessary to rewrite all desired calculations with unitary operations and execute them. Therefore, it should be noted that algorithms that run on current computers do not necessarily run on quantum computers as they are.
*4. Quantum chemical calculation: A calculation that attempts to reproduce and predict the properties of a substance in a virtual space by constructing a substance in a virtual space of a computer and simulating the behavior of electrons and atomic nuclei by quantum mechanical calculations.
*5. Defect: A disorder that appears in the arrangement of a crystal structure. For example, there are "vacancy" defects which are the absence of an atom in the crystal structure, and "substitution" defects in which elements other than those in the crystal replace atoms within the crystal.
*6. Materials informatics: A method to improve the efficiency of material development by utilizing information science and AI (artificial intelligence). It aims to accelerate the discovery and development of new materials by analyzing vast amounts of experimental data and simulation data and predicting the composition of substances that can realize desired material properties.
*7. Composite defect: A defect structure in which more than one type of defect appear together as a pairs. For example, there is a "vacancy-substitution" pair defect in which a "vacancy" defect and a "substitution" defect are paired.
*8. Quantum device: A general term for devices that operate based on the principles of quantum mechanics. It utilizes phenomena unique to quantum, in contrast to devices that can be understood by classical mechanics, such as conventional electronic devices.
*9. Wide bandgap semiconductor: A semiconductor material with a larger bandgap

than conventional silicon semiconductors. It has high heat resistance, pressure resistance, and high-frequency characteristics, and is expected to be applied in various fields such as power devices and sensors in high-temperature environments.

*10. Density functional theory: One of the theories for handling many-body problems in quantum mechanics. It calculates the energy of a system using electron density and predicts the properties of a substance. It is used in a wide range of fields such as material development and chemical research.