Fujifilm, Keio University and blueqat Develop Workflow for Quantum Chemical Calculations of Large Molecules on Fault-Tolerant Quantum Computers

Joint research paper published in the international journal *Physical Chemistry Chemical Physics*

FUJIFILM Corporation (headquartered in Minato, Tokyo, President and CEO, Representative Director: Teiichi Goto, hereafter, Fujifilm), Keio University (headquartered in Minato, Tokyo; President: Kohei Itoh), and blueqat Corporation (headquartered in Shibuya, Tokyo; CEO: Yuichiro Minato; hereinafter blueqat) have announced the development of a groundbreaking workflow for Fault-Tolerant Quantum Computing (FTQC) aimed at conducting quantum chemical calculations of large molecular weight molecules. This innovative workflow's validity was demonstrated using three types of molecules, including benzene and its substituents. These research findings were published online in the international journal *Physical Chemistry Chemical Physics* on December 3, 2024 (JST).

FTQC incorporates a mechanism for correcting errors[1] that occur in the calculation process. As it is believed that FTQC can perform highly accurate calculations in a considerably shorter time than conventional computers, making it suitable for tasks such as predicting the physical properties of molecules when developing materials. Due to these capabilities, FTQC is a highly anticipated technology with many practical applications. Specifically, the application of quantum chemical calculations[2], a computational method for clarifying important properties of molecules, is attracting attention because it is expected to enable extremely fast and accurate simulations of the electronic structure and reactivity of molecules and solid-state materials. However, the practical application of quantum chemical calculations will require not only the development of technology to correct errors generated by qubits during calculations, but also the development of a workflow to efficiently execute large-scale calculations with a small number of qubits, as well as the development of a method to calculate the chemical properties of molecules with large molecular weights.

Fujifilm, Keio University, and blueqat have jointly developed a workflow that can be widely applicable to the quantum chemical calculations of large molecules with FTQC. This workflow was implemented on a quantum simulator with state-of-the-art GPUs developed by Fujifilm and blueqat, featuring algorithms developed and implemented by Fujifilm and Keio University. The newly developed quantum circuit[3], which converts electronic states that significantly affect the physical properties of molecules into a format that can be selected and calculated and the algorithm using iterative quantum phase estimation[4], enable quantum chemical calculations of molecules with large molecular weights with little calculation and a small number of qubits and quantum gates. This innovative workflow is expected to significantly

reduce the time required for developing materials compared to current methods using conventional computers.

This research was supported by JPMJPF2221, the program on open innovation platform for industry-academia co-creation.

Journal Information

Journal: *Physical Chemistry Chemical Physics*

Title of paper: Workflow for practical quantum chemical calculations with a quantum phase estimation algorithm: electronic ground and π-π* excited states of benzene and its derivatives

Author: Yusuke Ino, Misaki Yonekawa, Hideto Yuzawa, Yuichiro Minato, and Kenji Sugisaki

Link: https://pubs.rsc.org/doi/D4CP03454F

Inquiries about the research should be directed to

Kenji Sugisaki, Project Associate Professor, Graduate School of Science and Technology, Keio University

Email: ksugisaki@keio.jp

blueqat Corporation

Email: info@blueqat.com

ICT Strategy Division, FUJIFILM Holdings Corporation

Email: fh-dx_program_office@fujifilm.com

Keio University Office of Communications and Public Relations

Email: m-pr@adst.keio.ac.jp

Reference

Research Result

This research study [A] showed the development of a quantum chemical calculation workflow based on a fault-tolerant quantum algorithm applicable to various molecules, and [B] demonstrated this workflow on a quantum simulator.

[A] Development of a quantum chemical calculation workflow using error-resistant quantum algorithms applicable to a variety of molecules

The following workflow was developed for this study

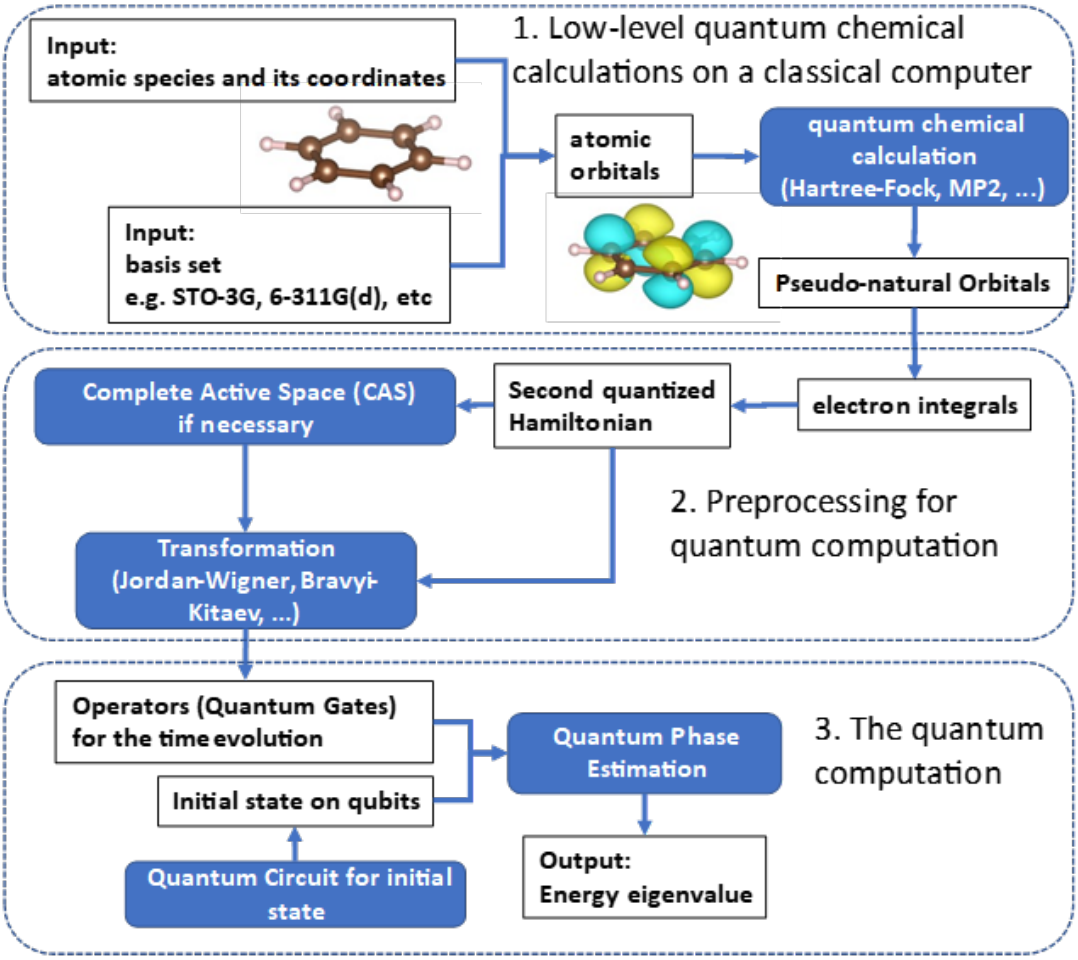

Figure 1: Workflow of quantum chemical calculations on a quantum computer proposed in this research.

This workflow consists of three parts. In “low-level quantum chemical calculations on a classical computer,” the type and coordinates of the atoms constituting the molecule to be calculated are given as input, and quantum chemical calculations are performed at a level that can be easily performed on a classical computer. Based on the results of 1., a quantum circuit is constructed in 2. “Preprocessing for quantum computation“, where the problem size can be reduced by selecting the active space that is expected to play an important role in the

electronic state in the natural orbital basis. In addition, the number of ancilla qubits and quantum gates required for the calculation is reduced by using the iterative quantum phase estimation method, which allows the calculation to be performed with fewer qubits.

[B] Demonstration of the same workflow on a quantum simulator

The research group demonstrated this workflow on three types of molecules with large molecular weights, including benzene and its substituents, which are also widely used in practical applications. The calculations were performed using a quantum simulator implemented on Fujifilm's proprietary GPU computing environment[5].

		Molecule		
		Benzene	Chlorobenzene	Nitrobenzene
Excitation energy [eV]	Experimental	4.9	4.72	4.38
	with CAS-CI	6.091	5.998	5.951
	with IQPE	6.092	6.008	5.925

The numbers are accurate!

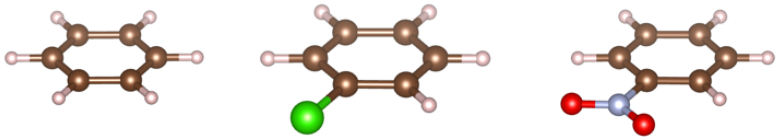

Figure 2: Molecules used in this study to validate the workflow and their calculation results. The results agree with the corresponding most accurate quantum chemical calculation results (CAS-CI) in the range of chemical accuracy.

The results obtained by the quantum algorithm (“with IQPE” in Figure 2) are in agreement with existing calculations (“with CAS-CI”) and successfully capture the trend of the corresponding experimental results (“Experimental”).

Glossary

1. Quantum bits, the basic unit of computation in a quantum computer, are affected by various influences from the outside world and errors (quantum errors) occur. Only after correcting these errors can the targeted quantum computational operations be performed. Currently, about 1,000 qubits are required to realize a single logical qubit, but in recent years, a series of groundbreaking achievements have been reported in this field (*Quantum Insider*, “Year in Review: The Big Stories That Rocked Quantum Research and Quantum Business in 2023,” 12/29/2023). It is expected that error correction will be achieved with fewer qubits in the future.

2. Quantum chemical calculations are methods to calculate important properties of molecules, such as excitation energy, by obtaining the electronic state through approximate solution of the Schrödinger equation (a fundamental equation that maps the type and coordinates of atoms constituting a molecule to the state of electrons in the molecule). From the obtained electronic states, physical properties of molecules (wavelength of absorption, elastic modulus, polarization ratio, dielectric constant, etc.) can be obtained.

3. In general, as the number of electrons constituting a molecule increases, the computational resources required increases exponentially. In this study, the researchers confirmed that by focusing on the complete active space among molecular orbitals, they could reduce the total number of calculations required while preserving the properties of the molecule.

4. Iterative quantum phase estimation is a quantum algorithm that uses a quantum computer to compute eigenvalues of unitary operators, such as the time evolution operator that describes how a wave function changes with time, making it exponentially faster than a classical computer. They have been applied to a wide variety of problems, including quantum algorithms for solving linear equations as well as quantum chemical calculations. In this study, the researchers employed iterative quantum phase estimation. While this algorithm can suppress the amount of computational resource required, the drawback is that it is difficult to estimate errors. In this study, based on previous research findings, the researchers constructed a computational flow that is both simple to implement and used to identify errors.

5. Fujifilm was one of the first companies to build a computing environment including GPGPU, with technological innovations including the introduction of NVIDIA DGX-2™ (the world's most advanced GPU server at the time).