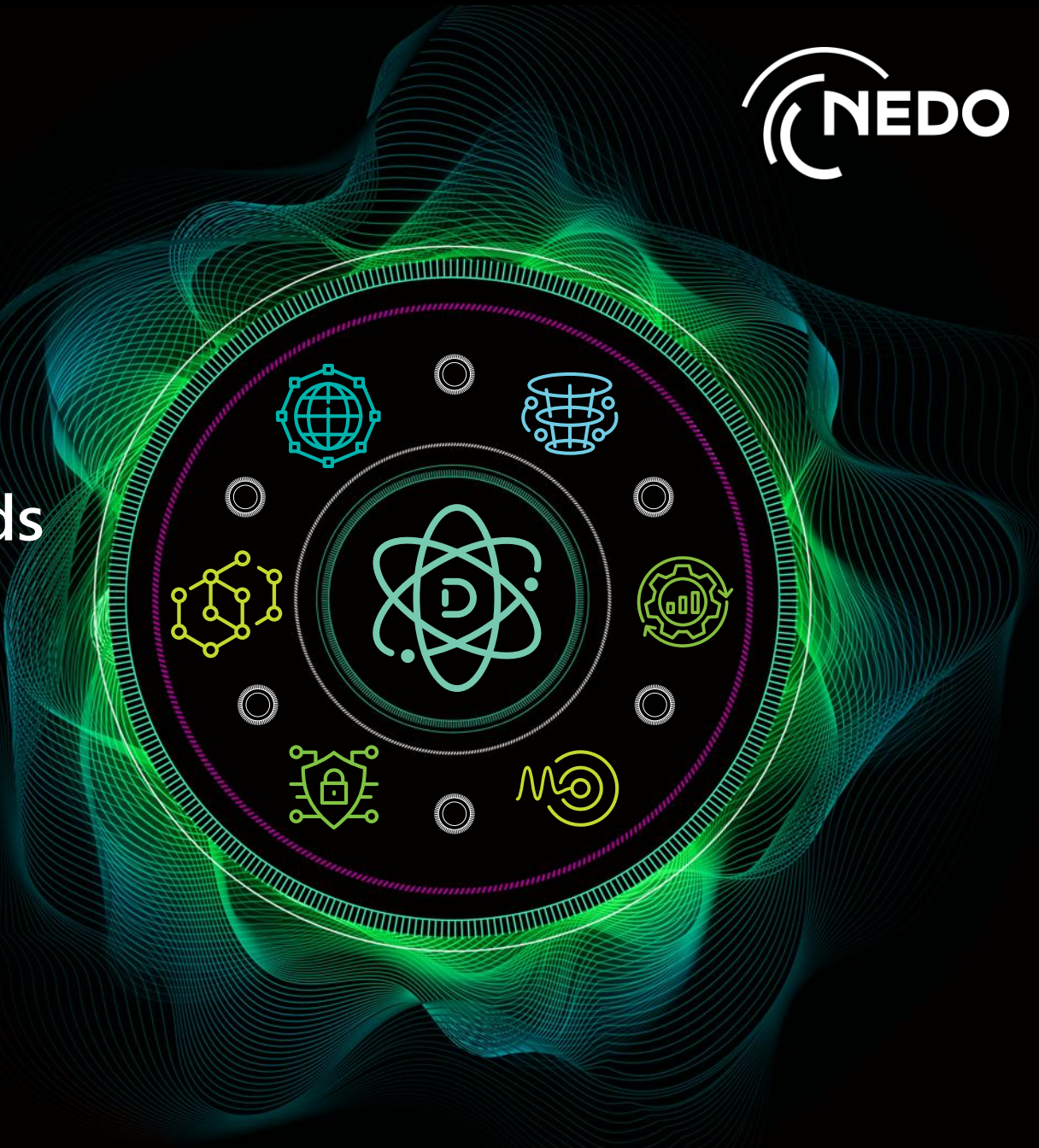
Quantum Computing Use Cases

High-precision energy calculation for large-scale molecules and solids

Mitsubishi Chemical, Keio University, and IBM



New Energy and Industrial Technology Development Organization (NEDO)

Mitsubishi Chemical, Keio University, and IBM: High-precision energy calculation for large-scale molecules and solids [2024/06] 1/2

Validation

Industry	Process Manufacturing
Process	research and development
Method	Simulation
Category	Gate*

Background

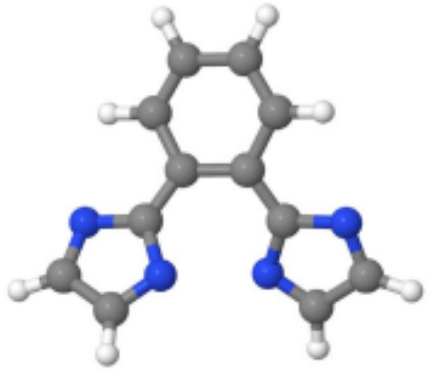
- Physical properties of molecules and solids can be determined by calculating the states of electrons contained in substances.
- However, since the calculation of the electronic state **increases exponentially with the number of electrons,** the current method is **approximated**
- **DFT (density functional), which approximates electron correlation,** is widely used to calculate the ground state of electrons, the lowest energy state, but **it is difficult to obtain sufficient accuracy for materials with complex electronic structures with strong Coulomb repulsion.**

Issues and motivation to be solved

- Quantum computers are expected to **improve the accuracy of electron ground state calculations in materials with complex electronic structures.**
- While current quantum computers are limited in the number of qubits and gates, Mitsubishi Chemical, Keio University and IBM worked together to **develop a calculation method for a large-scale, high-precision calculation that exceeds the performance of a single quantum computer**

Expected business benefits

- Combining the two developed calculation methods **HTN + QMC** and **pseudo-Hadamard test**, we calculated the photochromic model molecules monoallyldiimidazole, *1 and *** 1**. As a result, we were able to **calculate the ground state with high accuracy**
  - ✓ Concretely, it was calculated with an accuracy of 0.042±2.0 milli-Hartree *2, **higher than the accuracy for understanding general chemical phenomena (1.6 milli-Hartree)**



Structure of Monoallyldiimidazole Calculated in the Present Study
Gray represents carbon, white represents hydrogen, and blue represents nitrogen.

Reference: Keio Gijuku "Quantum Computer Technique for Large-Scale High-Precision Energy Calculations for Molecules and Solids Published in Nature Research" (https://www.keio.ac.jp/ja/press-releases/files/2024/6/10/240610-1.pdf)
*Gate（gate-based）: A computing approach in which operations are applied sequentially to qubits to perform calculations. Similar in concept to logic circuits in classical computers, it can address a wide range of problems.

*1: A compound consisting of one allyl group and two imidazoles. Imidazoles are used in a variety of applications, from pharmaceuticals to commodities.
*2: Atomic units used in quantum chemistry to deal with atomic and electron scales

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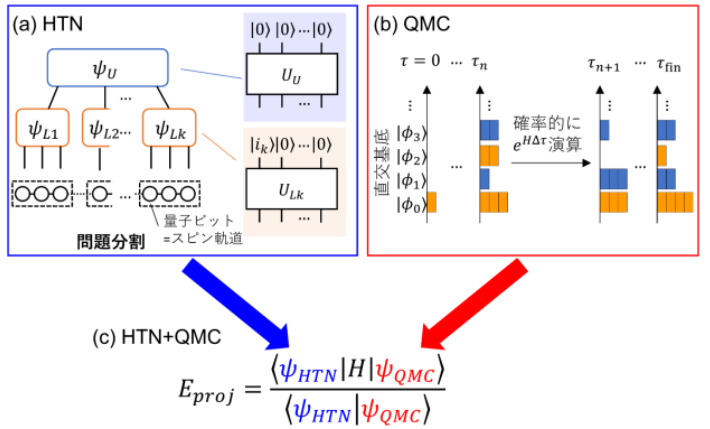
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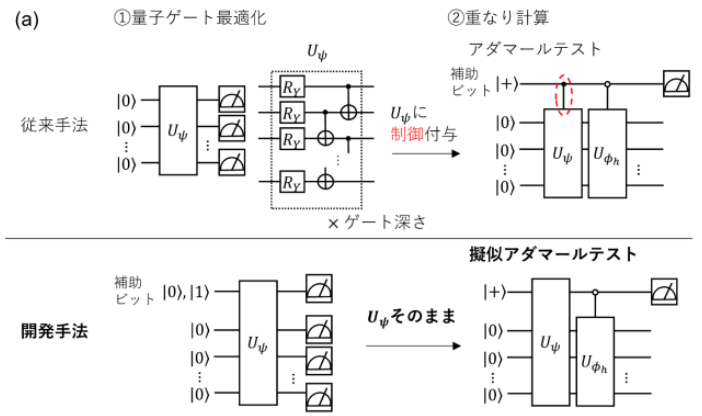
Problem setting as a quantum computer

- **Two calculation methods were** developed **to obtain the energy of large-scale molecules and solids with high accuracy.**
  - ✓ **HTN + QMC** is developed by combining the hybrid tensor network (HTN), which divides a quantum state larger than the size of a quantum computer into smaller tensors (blocks) using a quantum computer and a classical computer to connect the tensors, and the quantum Monte Carlo (QMC), a high-precision energy calculation method.
  - ✓ **Pseudo Hadamard Test** to Calculate Overlap Between Quantum States Effectively on a Quantum Circuit
- Using this calculation method, **photochromic model molecule,** * and **energy calculation of** were performed.
- The machine used was **IBM's gated commercial quantum computer, IBM Quantum System One.**

*: the property of the material to change color as the intensity of light changes;



HTN+QMC approach



simulated Hadamard test

Reference: Keio Gijuku "Quantum Computer Technique for Large-Scale High-Precision Energy Calculations for Molecules and Solids Published in Nature Research" (https://www.keio.ac.jp/ja/press-releases/files/2024/6/10/240610-1.pdf)

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More use cases are available on our website. We invite you to explore them.
https://www.quantum-computing-use-cases.nedo.go.jp/english/

More Use Cases

New Energy and Industrial Technology Development Organization (NEDO)
AI and Robotics Department (e-mail: quantum_ai@ml.nedo.go.jp)

This collection of use cases was obtained as a result of the work commissioned by the New Energy and Industrial Technology Development Organization (NEDO) "Cyber-Physical Development Business of Quantum/Classical Hybrid Technology/Study of Use Case of Quantum Technology" and the “Post-5G Information and Communications System Infrastructure Reinforcement R & D Project (Quantum Industrialization)/Comprehensive Study for Promoting the Industrialization of Quantum Computers”.