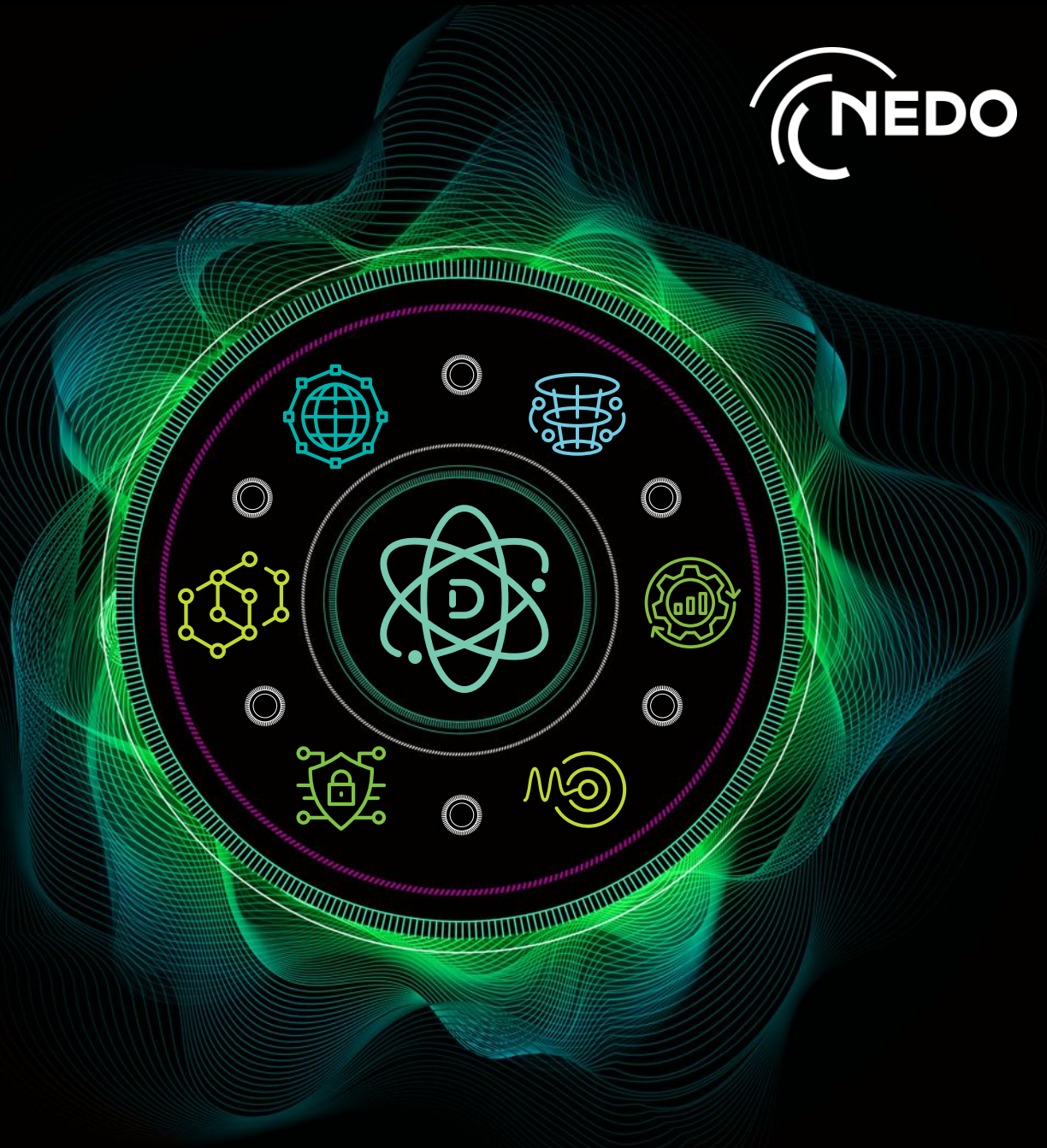
Quantum Computing Use Cases

Accelerated platform for material design and reaction analysis

Mitsui



New Energy and Industrial Technology Development Organization (NEDO)

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Concept

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

Background

- **In the fields of drug discovery, materials, and chemistry, the link between computation and experiment, which requires molecular-level precision, has become important. On the other hand, the maturity of quantum computation technology, the shortage of human resources, and the introduction cost have become bottlenecks, and many companies remain at the evaluation and examination stage.**
- Materials development requires complex computational processes that link quantum mechanical microphenomena with macroscopic product performance, and requires an environment in which leading-edge computational chemistry, quantum computation, and AI are integrated.
- Mitsui integrates the strengths of Qsimulate's classical computing software and Quantinuum's quantum computing software, and starts providing "QIDO," a quantum-classical hybrid platform that can be easily used in the cloud.

Issues and motivation to be solved

- **By improving the precision of molecular design, we will promote the introduction of quantum computers in the fields of drug discovery, materials, and chemistry, which are expected to bring innovation to drug discovery and material development.**
- Enhance molecular simulations by seamlessly connecting highly practical classical and advanced quantum computations

Problem setting as a quantum computer

- High-precision chemical reaction analysis is performed with QSimulate's classical calculation software "QSP Reaction" and applied to Quantinuum's quantum calculation software "InQuanto" to make quantum calculation more efficient

Reference: Mitsui & Co., Ltd.: "Launch of "QIDO," a quantum/classical hybrid platform aimed at accelerating drug discovery and material development" (https://www.mitsui.com/jp/ja/topics/2025/1251846_14877.html)
*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.

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Expected business benefits

- By utilizing the cloud environment, QIDO will be able to provide an environment that enables rapid and flexible experimental analysis of various research themes, and will promote the spread of quantum chemical technology, which previously required specialized knowledge, to more research sites.
- The user interface and automated analysis allow researchers to select the most appropriate method and conduct research efficiently.
  - Companies and research institutions can efficiently implement quantum technologies and contribute to accelerating their adoption
- **Use cases such as drug discovery, catalyst and enzyme design, sustainable materials, and energy technology are envisaged, including the search for chemical reaction pathways and excited state calculations. In the future, we plan to expand the functions specialized in each field sequentially with a view to application to battery technology and biotechnology.**



Conceptual image of QIDO

Reference: Mitsui & Co., Ltd.: "Launch of "QIDO," a quantum/classical hybrid platform aimed at accelerating drug discovery and material development" (https://www.mitsui.com/jp/ja/topics/2025/1251846_14877.html)
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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".