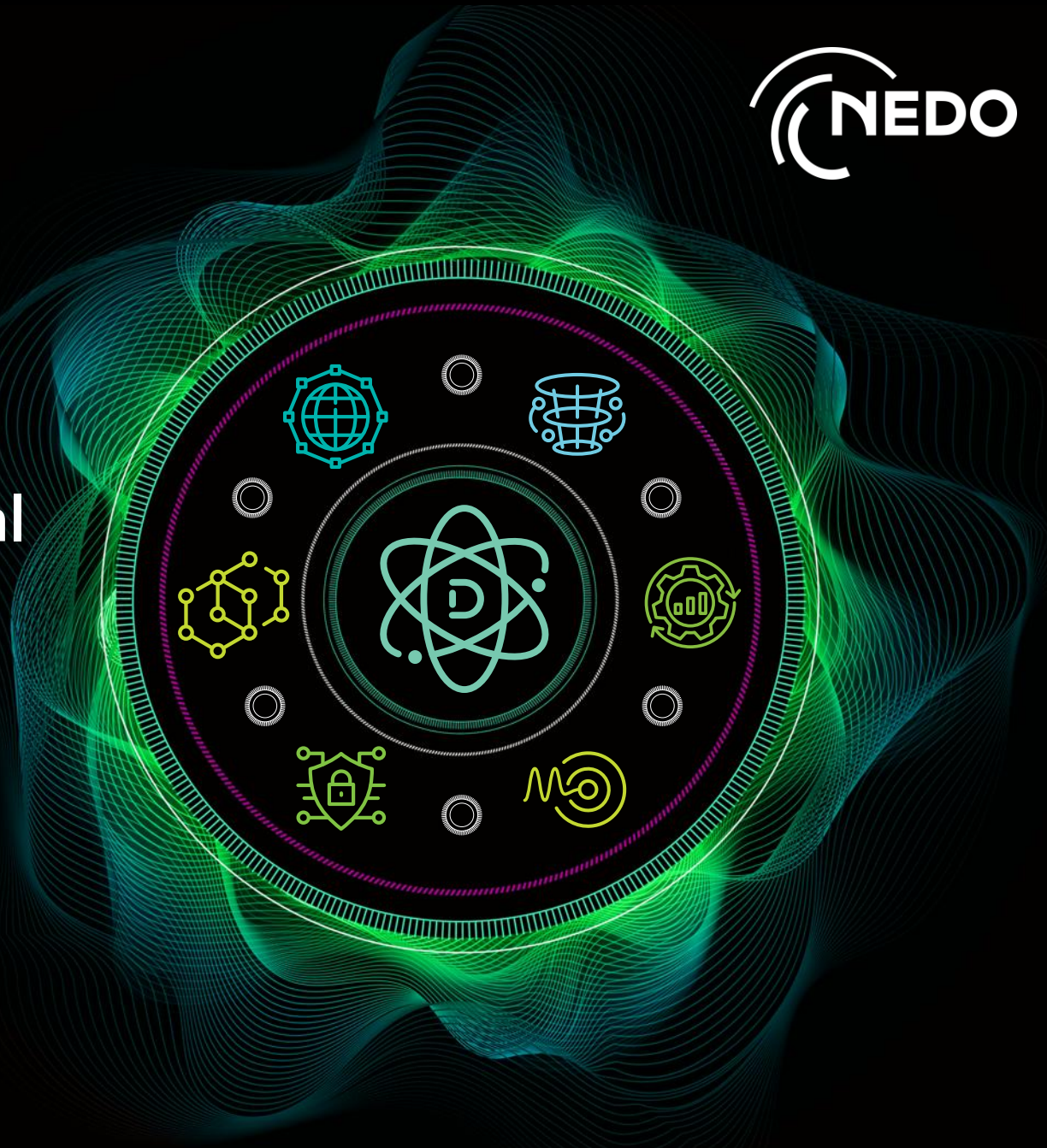
Quantum Computing Use Cases

Prediction of material properties and simulation of various chemical reactions

TOPPAN, The University of Osaka



New Energy and Industrial Technology Development Organization (NEDO)

TOPPAN The University of Osaka: Prediction of material properties and simulation of various chemical reactions [2023/04] 1/2

Concept

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

Background

- Quantum computers are expected to be a revolutionary technology that will revolutionize various industries.
  - ✓ In particular, **in the field of chemistry, the creation of innovative new materials is expected.**
- Materials development so far **requires a lot of time** because researchers design molecular structures that are expected to have desired physical properties based on past data and experience, and search for promising compounds by repeating synthesis and measurement of physical properties.
- In recent years, efforts have been made to **accelerate research and development by utilizing new methods such as materials informatics (MI).**
  - ✓ Computational chemistry to elucidate mechanisms of functional expression
  - ✓ Efficient screening of vast amounts of material data using AI and other technologies

Issues and motivation to be solved

- By using quantum computers for computational chemistry, there is a growing expectation that **there is a possibility of high-speed, high-precision calculations of complex molecules that cannot be calculated with classical computers.**
- Molecular structures and properties calculated by quantum computers are expected to become important learning data for MI, and to greatly expand the search area for screening.
- Toppan Printing and the The University of Osaka Research Center for Quantum Information and Quantum Life (QIQB) have started **joint research to develop and demonstrate quantum chemical calculation algorithms.**

Expected business benefits

- Through this joint research, we aim to **reform and speed up the process of material development and evaluation, and create innovative new materials and functional materials.**

Reference: TOPPAN Holdings Co., Ltd. "Toppan Printing and The University of Osaka Quantum Information and Quantum Life Research Center start joint research on materials development and evaluation methods using quantum computers." (https://www.holdings.toppan.com/ja/news/2023/04/newsrelease230411_1.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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Problem setting as a quantum computer

- Development of a quantum chemical calculation algorithm **to calculate physical properties of new materials and perform analytical simulations of chemical reactions on a quantum computer**
  - ✓ Prediction of physical properties of materials developed and manufactured in Toppan's business area, such as semiconductors and display-related components, architectural materials, and packages
  - ✓ Operations such as analytical simulations of various chemical reactions
- These will **verify whether it is possible to calculate molecules that could not be calculated with classical computers.**
- use the **gate method** to perform quantum chemical calculations

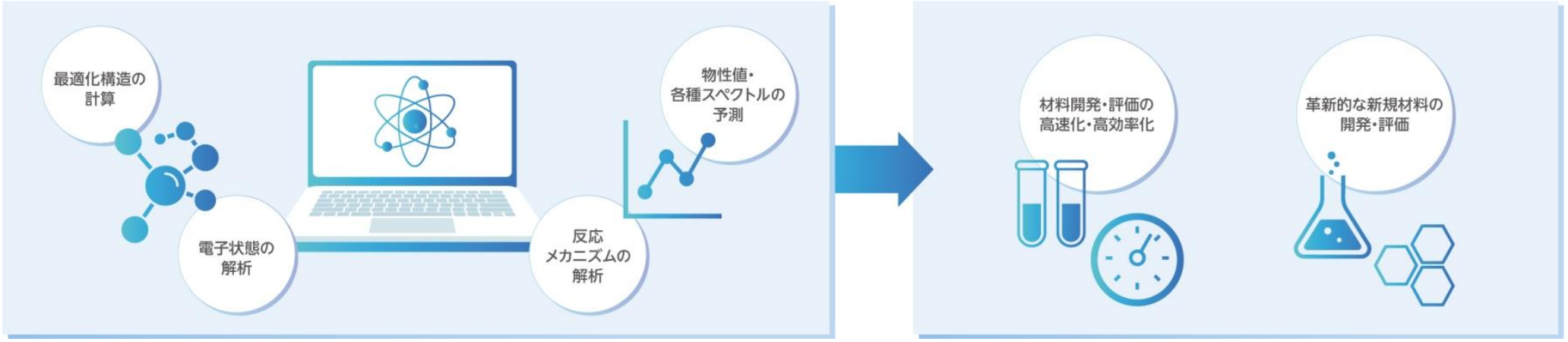


Image of quantum computer utilization

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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".